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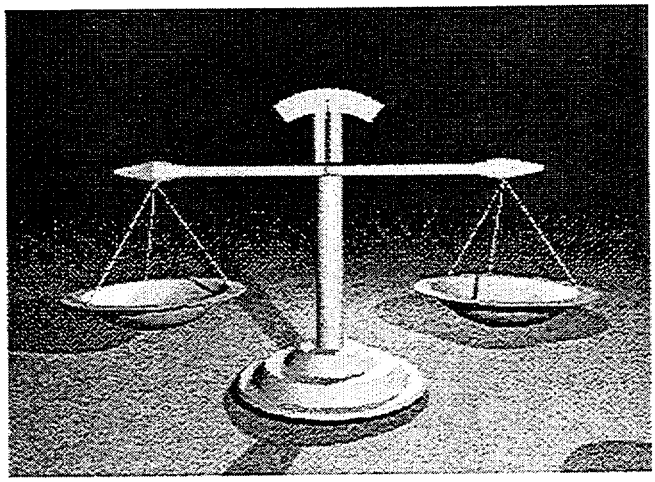
Vol. 3

SCALE

Version 4.4

A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation



Miscellaneous

Oak Ridge National Laboratory

Prepared for
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Vol. 3

SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation

Miscellaneous
M1 – M17

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ABSTRACT

SCALE, a modular code system for Standardized Computer Analyses Licensing Evaluation, has been developed by Oak Ridge National Laboratory at the request of the U.S. Nuclear Regulatory Commission. The SCALE system utilizes well-established computer codes and methods within standard analysis sequences that (1) allow an input format designed for the occasional user and/or novice, (2) automate the data processing and coupling between modules, and (3) provide accurate and reliable results. System development has been directed at problem-dependent cross-section processing and analysis of criticality safety, shielding, heat transfer, and depletion/decay problems. Since the initial release of SCALE in 1980, the code system has been heavily used for evaluation of nuclear fuel facility and package designs. This revision documents Version 4.4 of the system.

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***Cancelled. Included in Section C4.

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*Obsolete with SCALE-4.0 release.
**Not included in SCALE-4.4 release.
***Cancelled. Included in Section C4.

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*Obsolete with SCALE-4.0 release.
**Not included in SCALE-4.4 release.
***Cancelled. Included in Section C4.

PREFACE

Introduction

This Manual represents Revision 6 of the user documentation for the modular code system referred to as SCALE. The previous revision documented version 4.3 of SCALE, released in October 1995. This revision documents version 4.4a of SCALE. Prior to the release of version 4.4a, SCALE 4.4 was released in September 1998. Many minor corrections and enhancements have been made since that time and are being included in SCALE 4.4a. The corrections and enhancements in versions 4.4a and 4.4 are documented separately below. All modifications in version 4.4 are included in version 4.4a.

Background

The history of the SCALE code system dates back to 1969 when the current Computational Physics and Engineering Division at Oak Ridge National Laboratory (ORNL) began providing the transportation package certification staff at the U.S. Atomic Energy Commission with computational support in the use of the new KENO code for performing criticality safety assessments with the statistical Monte Carlo method. From 1969 to 1976 the certification staff relied on the ORNL staff to assist them in the correct use of codes and data for criticality, shielding, and heat transfer analyses of transportation packages. However, the certification staff learned that, with only occasional use of the codes, it was difficult to become proficient in performing the calculations often needed for an independent safety review. Thus, shortly after the move of the certification staff to the U.S. Nuclear Regulatory Commission (NRC), the NRC staff proposed the development of an easy-to-use analysis system that provided the technical capabilities of the individual modules with which they were familiar. With this proposal, the concept of the Standardized Computer Analyses for Licensing Evaluation (SCALE) code system was born.

The NRC staff provided ORNL with some general development criteria for SCALE: (1) focus on applications related to nuclear fuel facilities and package designs, (2) use well-established computer codes and data libraries, (3) design an input format for the occasional or novice user, (4) prepare "standard" analysis sequences (control modules) that will automate the use of multiple codes (functional modules) and data to perform a system analysis, and (5) provide complete documentation and public availability. With these criteria the ORNL staff laid out the framework for the SCALE system and began development efforts. The initial version (Version 0) of the SCALE Manual was published in July 1980. Then, as now, the Manual is divided into three volumes — Volume 1 for the control module documentation (Sections C4, C6, D1, S1- S5, and H1), Volume 2 for the functional module documentation (Sections F1- F17), and Volume 3 for the documentation of data libraries, and subroutine libraries, and miscellaneous utilities (Sections M1- M17).

System Overview

The original concept of SCALE was to provide "standardized" sequences where the user had very few analysis options in addition to the geometry model and materials. Input for the control modules has been designed to be free-form with extensive use of keywords and engineering-type input requirements. The more flexible functional modules have a more difficult input logic and require the user to interface the data sets necessary to run the modules in a stand-alone fashion. As the system has grown in popularity over the years and additional options have been requested, the control modules have been improved to allow sophisticated users additional access to the numerous capabilities within the functional modules. However, the most

important feature of the SCALE system remains the capability to simplify the user knowledge and effort required to prepare material mixtures and to perform adequate problem-dependent cross-section processing.

The modules available in Version 0 of SCALE were for criticality safety analysis sequences (CSAS) that provided automated material and cross-section processing prior to a one-dimensional (1-D) or multidimensional criticality analysis. Since that time the capabilities of the system have been significantly expanded to provide additional CSAS capabilities, new shielding analysis sequences (SAS) that also include depletion/decay capabilities for spent fuel characterization, and a heat transfer analysis sequence (HTAS). At the center of the CSAS and SAS sequences is the library of subroutines referred to as the Material Information Processor or MIPLIB (see Section M7). The purpose of MIPLIB is to allow users to specify problem materials using easily remembered and easily recognizable keywords that are associated with mixtures, elements, and nuclides provided in the Standard Composition Library (see Section M8). MIPLIB also uses other keywords and simple geometry input specifications to prepare input for the modules that perform the problem-dependent cross-section processing: BONAMI, NITAWL-II, and XSDRNPM. A keyword supplied by the user selects the cross-section library from a standard set provided in SCALE (see Section M4) or designates the reference to a user-supplied library. Several utility modules from AMPX[1] have been included to provide users with the capability to edit the cross-section data and reformat user-supplied libraries for use in SCALE.

Over the history of the project several modules have been removed from the system because they are no longer supported by the development staff at ORNL. Tables 1 and 2 provide a summary of the major applications of each of the control modules and functional modules currently in the SCALE code system. The control modules were designed to provide the system analysis capability originally requested by the NRC staff. The CSAS module (sometimes denoted as the CSAS4 module and documented in Section C4) is the primary control module designed for the calculation of the neutron multiplication factor of a system. Eight sequences enable general analysis of a 1-D system model or a multidimensional system model, capabilities to search on geometry spacing, and problem-dependent cross-section processing for use in executing stand-alone functional modules. CSAS6 is a newer criticality control module to provide automated problem-dependent cross-section processing and criticality calculations via the KENO-VI functional module. The SAS1 and SAS3 modules (see Sections S1 and S3, respectively) provide general 1-D deterministic and 3-D Monte Carlo analysis capabilities. The SAS2 module (see Section S2) was originally developed to perform a depletion/decay calculation to obtain spent fuel radiation source terms that were subsequently input automatically to a 1-D, radial shielding analysis in a cylindrical geometry. Over time the depletion/decay portion of the SAS2 module has been significantly enhanced and interfacing to the other shielding modules has been provided. An alternative sequence for depletion/decay calculations is ORIGEN-ARP (Section D1), which interpolates pre-generated ORIGEN-S cross-section libraries versus enrichment, burnup, and moderator density. The SAS4 module (see Section S4) enables automated particle biasing for a Monte Carlo analysis of a transportation package-type geometry. The HTAS1 module (see Section H1) is the only heat transfer control module and uses the various capabilities of the HEATING code to perform different sequences of steady-state and transient analysis that enable the normal and accident conditions of a transportation package to be evaluated. Like SAS4, the HTAS1 module is limited to a package-type geometry. The capability to perform a point-kernel shielding analysis within the SCALE system has been developed in the QADS control module.

A 238-energy-group neutron cross-section library based on ENDF/B-V[2] is the latest cross-section library in SCALE. All the nuclides that are available in ENDF/B-V are in the library. A 44-group library has been collapsed from this 238-group library and validated against numerous critical measurements.[3] These libraries are available in this version of SCALE.

Technical Assistance and Updates

To obtain technical assistance regarding the installation and use of SCALE, download software updates, or report problems, you may contact us through the following channels:

- E-mail questions to **scalehelp@ornl.gov**
- The SCALE Users Electronic Notebook on the Web:
  http://www-rsicc.ornl.gov/ENOTE/enotscal.html
- SCALE Web Site (including Download, Training, Benchmarks, and Newsletter pages):
  http://www.cped.ornl.gov/cad_nea/text/scale-home.html
- SCALE Newsletter:
  http://www.cped.ornl.gov/cad_nea/text/scale_news.html
- FAX to SCALE Help, 815-327-6460 or 865-576-3513

Significant Updates in SCALE 4.4a

A significant number of updates have been made to SCALE since the initial release of SCALE 4.4 in September 1998. Most of these updates were minor corrections or enhancements. Because some of these updates could be important to SCALE users, this interim release of SCALE 4.4a is being made available.

SAS4 and PICTURE were enhanced to allow the generation of two-dimensional (2-D) plots when the "PARM=CHECK" option is used. This option is similar to the plotting option in the CSAS criticality sequences. Another innovation was the addition of an option that allows users to specify an X-Y, X-Z, or Y-Z plot and have the code automatically calculate the cosines used for the plot.

A discrepancy in scoring boundary crossings of surface detectors was corrected in MORSE. Contributions to user-specified surface detectors in MORSE in SCALE 4.4 could have been underestimated because of a failure to determine which surface detector to score. This failure was due to the comparison of a single precision variable to a double precision variable. Most affected cases would have a zero result for the surface detector, indicating that no particles have crossed the surface detector boundary. Detector location coordinates of four digits or less would not be expected to experience this problem.

A coding error introduced in QAD-CGGP in SCALE 4.4 has been identified and corrected. Because of inconsistent array dimensions, if more than a very limited number of bodies are input in one zone, the additional zone data are lost or stored incorrectly. This situation typically causes the code to fail. Though extremely unlikely, it might be possible for a case like this to run if the incorrectly stored geometry happened to be valid. SCALE 4.4 users should check under the "input zone data" header in the QAD-CGGP output to verify that the zone data agree with their input.

SAS2 was corrected to fix an error introduced in SCALE 4.4 that caused the PARM=OLDSAS2 option to fail. Another discrepancy introduced in SCALE 4.4 caused spent fuel isotopic data written to file FT72F001 to be incorrect in certain cases. This error, which has been corrected, occurred in cases where burnable poison rods or other inserts are removed from or inserted into the fuel assembly between fuel cycles. SAS2 can now correctly handle multiple fuel zones in the path B model. A minor discrepancy was corrected where invalid characters were being written to title records in the ORIGEN-S binary library. Some text editors could not read the SAS2 output file when invalid characters were present.

A large number of enhancements were made to XSDRNPM. The Fortran source for XSDRNPM was converted to Fortran 90 free format. The input/output units were all moved to the 0$ array. The energy of the

average lethargy causing fission was added to the balance tables. The output files from the balance tables and the activities were modified and converted to ASCII files. A new ASCII file was created that contains the input and derived data from a problem. The coarse mesh generation algorithm used in rebalancing the inner iterations was modified to correct a problem that prevented convergence for a very small class of problems. The code was modified to recycle if the final iteration performed after convergence failed the convergence test. For group banding cases, convergence is now reset after initial convergence to an order of magnitude less than overall convergence to prevent looping through iterations and never converging. The default value for flux convergence tolerance, PTC, was reduced from 10^{-4} to 10^{-5}. The calculation of activities by interval, an option that was available many years ago, was reintroduced in the code.

The XSDRNPM mesh generation algorithm in MIPLIB was modified to address two problems: (a) insufficient number of mesh intervals for thick reflectors of low absorbing material and (b) too many mesh intervals for highly absorbing regions. New input options to override the automatic mesh generation were added. Although this enhancement was designed primarily for CSAS1X, it potentially affects all control modules except SAS2H that use XSDRNPM.

KENO-VI was modified to detect intersecting HOLEs in the global unit. A problem will now terminate if intersecting HOLEs are detected in the global unit. Intersecting HOLEs are illegal in KENO-VI geometry but were not detected in the global unit in SCALE 4.4. Intersecting HOLEs in units other than the global unit are detected during tracking of particles through the intersecting regions. Several corrections were made to KENO-VI to prevent a particle from becoming lost and causing the code to enter an infinite loop.

MORSE was updated to correct a problem in determining the correct day of the week for dates after December 31, 1999.

Many other minor changes included in SCALE 4.4a are listed under "SCALE 4.4a Minor Modifications."

SCALE 4.4a Minor Modifications

In addition to the major enhancements noted above, SCALE 4.4a contains many minor modifications, including corrections to errors in SCALE 4.4 and changes to improve portability to different computing platforms. Note that some of these modifications may be duplicate listings of items mentioned in the previous section.

PICTURE **MRR98-056**

Updated to handle the call by SAS4 when the "PARM=CHECK" option (added to the SAS4 control module in MRR98-057) is used. Also, added an option that allows users to specify an X-Y, X-Z, or Y-Z plot and have the code automatically calculate the cosines used for the plot.

SAS4 **MRR98-057**

Added a "PARM=CHECK" option that calls PICTURE from within the SAS4 to plot geometry but not run MORSE. SAS4 prepares or reads MARS geometry input data, reads PICTURE input, and calls PICTURE. Several other changes were made to error messages and formats.

SAS2 **MRR98-058**

Updated to correct an error introduced in SCALE 4.4 that caused the PARM=OLDSAS2 option to fail. Also corrected another problem introduced in SCALE 4.4 that caused spent fuel isotopic data written to file FT72F001 to be incorrect in certain cases where burnable poison rods or other inserts are removed from or inserted into the fuel assembly between fuel cycles.

MORSE **MRR98-059**

Corrected a discrepancy in scoring boundary crossings of surface detectors. A roundoff error caused by comparison of a double precision variable to a single precision constant resulted in boundary crossings not being scored. The epsilon value for the comparison was also increased from 0.0005 to 0.001.

SAS4 **MRR98-060**

Updated to correct the dimensions on two arrays. Also changed a test comparing 2 floating point variable names equivalenced to integer variables to use function ISET. (This test has previously caused floating point underflows on some platforms.)

QADS **MRR98-061**

Added a test on the MIPLIB error flag that terminates execution of the problem if an error occurred.

KENO-VI **MRR98-062**

Updated to allow a particle to cross from one hole directly into an adjacent hole even if the crossing is outside the allowed tolerances. This prevents some cases from entering an infinite loop.

SAS2 **MRR98-063**

Corrected minor discrepancy that resulted in invalid characters being written to title records in ORIGEN-S binary library. Some text editors could not read SAS2 output file when invalid characters were present.

MIPLIB **MRR98-064**

Updated to allow control modules to specify a sensitivity library from NITAWL and to allow number density input for an element that has multiple isotopes.

XSDRNPM **MRR98-065**

The Fortran source for XSDRNPM was converted to Fortran 90 free format. The input-output units were all moved to the 0$ array. The energy of the average lethargy causing fission was added to the balance tables. The output files from the balance tables and the activities were modified and converted to ASCII files. A new file was created which contains the input and derived data from a problem. The flux file was changed to double precision. The code was modified to not run with fluxes out of core unless explicitly requested in the input. The coarse mesh generation algorithm used in rebalancing the inner iterations was modified to correct a problem that prevented convergence a very small class of problems.

C5TOC6/K5TOK6 **MRR98-066/MRR98-067**

The input file generated for CSAS6/KENO VI incorrectly labeled regions generated to surround HOLEs if there were more than one region in a unit that contained HOLEs. Because of a change in KENO-VI, these regions should no longer need to be generated. Subroutine PUNCH_GEOM was modified to not generate these regions.

QAD-CGGP **MRR98-068**

Updated to correct an error introduced in SCALE 4.4. The dimension on one variable in the geometry was not updated when the input format was changed to match that of MARS input. This caused some jobs to fail. Also, updated to correct misspelled name of unit used for error output.

ARPLIB **MRR99-001**

Updated to accept either lower or upper case input.

PRISM **MRR99-002**
Updated to accept either lower or upper case input.

XSECLIST **MRR99-003**
Updated to accept either lower or upper case input.

SAS2 **MRR99-004**
Updated for compatibility with the newest revisions to XSDRNPM (MRR98-065). The routines that wrote the XSDRNPM input files needed to be changed to account for the changes to XSDRNPM input. Subroutine COPYNX had to be changed to add the 0$ array to the XSDRNPM input file, and to move setting the logical unit number of the flux output file from the 2$ array to the 0$ array.

UNIXLIB **MRR99-006**
Changes to update XSDRNPM required a double precision ERF function. This function is part of the Fortran intrinsic library for the DEC Alpha's and the IBM RS/6000, but is not part of that library for the HP or the SUN workstations. This modification provided an update for the necessary routines to compute the double precision ERF when it is not part of the intrinsic library.

BONAMI **MRR99-007**
Updated to correct a problem that caused cases to fail when zero number density input is used.

SAS4 **MRR99-008**
Updated to change the convergence criteria because the criteria in XSDRNPM were changed. Also added an input variable NDAB to allow the user to specify the number of direct access blocks allocated.

XSDOSE **MRR99-009**
Added option to turn off angular flux print and made the default to be no angular flux print.

MODIFY **MRR99-010**
Updated subroutine LODATA for compatibility with changes in MRR98-064(MIPLIB).

XSDRNPM **MRR99-011**
(1) The code was modified to re-cycle if the final iteration performed after convergence failed the convergence test. For group banding cases, convergence is now reset after initial convergence to an order of magnitude less than overall convergence to prevent looping through iterations and never converting. (2) The default value for flux convergence tolerance, PTC, was reduced from 10^{-4} to 10^{-5}. (3) Errors were corrected in the calculation of activities by interval. This previously undocumented option is now documented in the XSDRNPM input description.

KENO-VI **MRR99-012**
Modified KENO-VI to detect intersecting HOLEs in the global unit. A problem will now terminate if intersecting HOLEs are detected in the global unit. Intersecting HOLEs are illegal in KENO-VI geometry but were not detected in the global unit in SCALE 4.4. Intersecting HOLEs in units other than the global unit are detected during tracking of particles through the intersecting regions.

ORIGEN **MRR99-014**
A new subroutine was added to provide the user the option of more significant digits in the output tables. Unit 71 was set as the default file number for the binary file containing concentrations and spectral data.

MIPLIB **MRR99-015**

The XSDRNPM mesh generation algorithm was modified to address two problems: (a) insufficient number of mesh intervals for thick reflectors of low absorbing material and (b) too many mesh intervals for highly absorbing regions. New input options to override the automatic mesh generation were added too. Consistent with MRR99-011, the default value of PTC was reduced from 10^{-4} to 10^{-5}. Although this enhancement was designed primarily for CSAS1X, it potentially affects all control modules that use XSDRNPM.

KENO-VI **MRR99-016**

The code was corrected to define LCHK as a logical variable in subroutine POSIT. In addition, an IMPLICIT NONE statement has been added to the beginning of the subroutine. All variables have been explicitly typed as appropriate.

MODIFY **MRR99-017**

Program MODIFY was changed for consistency with the change in the direct access file made in MRR99-015(MIPLIB).

KMART **MRR99-018**

An error that resulted in calculated volumes of zero for hemicylinders and arrays (if an array number was skipped) was corrected.

CSAS6 **MRR99-019**

The argument list for the call to subroutine PRTPLT was modified for consistency with changes made to KENO-VI in MRR99-012.

SAS2 **MRR99-020**

Calls to subroutine EPSIG were changed for consistency with MIPLIB modifications in MRR99-015.

MORSE **MRR99-021**

The code was updated to correct a problem in determining the day of the week for dates after December 31, 1999.

KENO-VI **MRR99-022**

The code was updated to fix a roundoff problem that sometimes caused particles to get into an infinite loop when they transferred from one array location to another but in the process missed the unit boundary.

SUBLIB **MRR99-023**

Subroutine YREAD turns off the normal invalid character check done by the free form reading routines, but does not make any checks of its own for invalid characters. This can lead to erroneous results in some cases where a user mistypes a character when entering the array data to KENO. Checks were added to the array reading routine to give warning messages if illegal characters are read. Corrections were also made so YREAD would store correctly a double precision array.

KENO-VI **MRR99-024**

The code was updated to fix a problem where the unit boundary shares surfaces with other geometry regions and the unit is in an array. This problem could result in an infinite loop because the code fails to detect a particle crossing the boundary.

SAS2 **MRR99-025**

The following modifications were made: (1) The calculation of the light element concentrations in ORIGEN-S was corrected when multiple fuel zones (MX=500) are used in the PATH B model. The code previously assumed only one fuel zone was present, and did not sum the zone volumes when multiple zones were present, resulting in erroneous light element concentrations in the ORIGEN-S depletion calculations. (2) The depletion of light element nuclides with mixture numbers 50 through 59 is now permitted. (3) The use of 1$ data for MXT (input level 3) when reading a second working library in NITAWL is now permitted.

HEATING **MRR99-027**

The code was updated, including Fortran 90 dynamic memory allocation, to improve portability on both workstation and PC platforms.

UNIXLIB **MRR99-028**

Subroutine JSTIME was modified to return time to the precision supplied by the system.

SAS4 Sample Problems **DRR99-001**

Updated SAS4 sample problems 1, 3, and 5 to remove references to variables FR1, FR2, FR3, and FR4, which became obsolete in SCALE 4.4.

XSDOSE Sample Problem **DRR99-002**

The XSDOSE section of the SCALE Manual documents the output of the sample problem and includes the printing of the fluxes. The input was modified to turn on the new angular flux print option in XSDOSE (see MRR99-009).

KENO V.a Sample Problems **DRR99-003**

Input data for sample problems 17 and 18 were changed. The number of neutrons started in sample problem 18 was changed to agree with the number per generation. Problem 17 was changed to specify the NBK parameter because the default was not large enough.

238- and 44-Group ENDF/B-V Libraries **DRRs 99-004 and 99-005**

Changes were made because problems were discovered with ^{238}Np, ^{250}Cf, ^{253}Cf, ^{249}Bk, ^{242}Am, and ^{233}Pa. The corrections for ^{250}Cf, ^{233}Pa, and ^{249}Bk were very minor and should have no important effects. However, significant errors were identified for ^{238}Np, ^{253}Cf, and ^{242}Am. In addition, these three nuclides do not have fission cross sections specified in the fast region in ENDF/B-V. This omission is obviously wrong, and because it could lead to very non-conservative answers for k_{eff}, these three nuclides were removed from the library.

Major Enhancements in SCALE 4.4

Many enhancements and corrections were made to SCALE in the three years between the release of SCALE-4.3 and 4.4. SCALE 4.4 is compatible with the year 2000 (see "SCALE 4.4 is Year 2000 Compliant"). User-specified surface detectors have been added to SAS4/MORSE to improve its computational flexibility and efficiency (see "Improvements to SAS4 and MORSE"). The KENO-VI input requirements for HOLEs have been simplified and made more consistent with KENO V.a (see "KENO-VI HOLE Input is Simplified"). Additionally, some significant improvements to the speed and stability of KENO-VI have been made (see "KENO-VI Stability and Speed Improvements"). A large number of changes have been made to the SAS2H depletion module (see "SAS2H Corrections and Enhancements").

Several enhancements have been made to the PC version of SCALE 4.4. A significant effort has been made to minimize the programming differences between the PC and Unix workstation versions. Both versions

will contain the same modules. The heat transfer modules HTAS1, HEATING, and the HEATING auxiliary codes are now available in the PC version for the first time. The PC version can recognize MS-DOS, Windows 95, Windows 98, and Windows NT operating systems and run under any of these systems from a single user command. CSAS can now be run directly from the CSASIN input processor.

ORIGEN-ARP, which was first released in the PC version of SCALE-4.3, has been enhanced and now runs under the SCALE driver, so it can run easily on workstations as well as PCs. ORIGEN-ARP has been improved significantly. ARP now interpolates on moderator density as well as burnup and enrichment for BWR fuel types. Several auxiliary codes have been added that enable users to generate their own ORIGEN-ARP cross-section libraries via SAS2H.

The default number of histories in KENO V.a and KENO-VI have been increased to 200,000 to produce more statistically accurate results. Color plots are now the defaults in both these codes.

PICTURE has been upgraded to generate two-dimensional (2-D) color plots of MORSE/MARS and QADS/QAD-CGGP geometry models like the color plots generated by KENO V.a and KENO-VI in SCALE-4.3. A new utility, LEGEND, has been created that adds a color/material legend and title to the color plots generated by KENO and PICTURE.

KMART is a new module to allow post-processing of a KENO V.a restart file, along with a working format cross-section library, to generate activities and/or broad-group fluxes and to compute the fission production activity if the components are available in the working cross-section library for the requested nuclide.

The group banding procedure in XSDRNPM was modified to significantly improve convergence for many large problems. Two examples of improvement include a fixed-source calculation with an 85% reduction in run-time and a k_{eff} calculation with a 50% reduction in run-time.

A correction was made to MIPLIB to allow the use of moderator in the gap region of a lattice cell calculation. Prior to this correction, if the same mixture number was specified in the moderator and the gap regions, the moderator density was incorrectly increased by a factor of two in the Dancoff factor calculation. In CSAS or CSAS6, this error results in a non-conservative calculated k_{eff} value that is approximately 0.5 to 1% low.

Other additions to SCALE 4.4 include the capability to perform a one-dimensional criticality search in CSAS1X (see "Criticality Search in CSAS1X"); the new KENO biasing weights library for 16-, 27-, 44-, 218-, and 238-group problems (see "New KENO Weights Library and Modules to Generate Weights"); the C5TOC6 and K5TOK6 conversion utilities for KENO-VI, and the Q0RDPN binary to ASCII conversion utility for functional module FIDO input files (see "New SCALE Utility Programs"); and the new zirconium hydride cross section data in the 238- and 44-group ENDF/B-V libraries (see "Zirconium Hydride Cross Sections").

The SCALE manual is distributed in electronic format on CD with the software. The manual is formatted in PDF files that can be read, searched, and printed using Adobe Acrobat Reader with Search. Users who desire a hard copy of the manual may obtain one from RSICC for an additional charge to cover reproduction costs.

Many other minor changes included in SCALE 4.4 are listed under "SCALE 4.4 Minor Modifications."

SCALE 4.4 is Year 2000 Compliant

Current and earlier versions of SCALE should calculate results correctly beyond the year 2000. However, when the year 2000 occurs, the output from some codes in these earlier versions will incorrectly display the year as 1900 instead of 2000. All known instances of this problem have been corrected in SCALE 4.4.

Improvements to SAS4 and MORSE

SAS4 and MORSE have been enhanced to allow users to specify multiple non-overlapping surface detectors on each surface (previously defaulted to 4 locations). These surface detectors can be divided into "sub-detectors" that enable the user to obtain detailed dose rate profiles. The flexibility in the use of these surface detectors makes them suitable for the substitution of point detectors, which are much less computationally efficient. Another enhancement to SAS4 was the addition of two options to pass data to PICTURE for plotting. One option generates geometry data only for the purpose of running PICTURE to view 2-D slices of the geometry. The other option provides "PARM=CHECK" option that calls PICTURE from within the SAS4 to plot geometry but not run MORSE. SAS4 prepares or reads MARS geometry input data, reads PICTURE input, and calls PICTURE.

Improvements to MORSE include orderly termination of a problem when errors in tracking to detector exceed a limit, an option to print/not print flux output after each batch, user capability to specify the number of direct-access blocks allocated on scratch units, compatibility with the year 2000, and reduction of the amount of error output in some cases.

KENO-VI HOLE Input Is Simplified

HOLE input in KENO-VI has been simplified. These changes are significant improvements requested by many users. The HOLE boundary no longer needs to be specified in the unit containing the HOLE. The HOLE boundary is automatically added by the program based on the unit specified in the HOLE record and its ORIGIN and ROTATE data. HOLEs cannot intersect. An example of the original and the new methods for adding HOLEs to a unit is given below. The input data no longer required are highlighted in the old input.

```
********** Old KENO-VI input *************
unit 1
hexprism  10  1.0  10.0 -10.0
media  1  10
boundary  10
unit 2
cuboid    10  6p20.0
hexprism  20  1.0  10.0  -10.0  origin x=5.0 y=3.0  rotate a2=90
media 2  10  -20
hole  1  20 origin x=5.0 y=3.0 rotate a2=90
boundary  10
******** New KENO-VI input ***************
unit 1
hexprism  10  1.0  10.0 -10.0
media  1  10
boundary  10
unit 2
cuboid    10  6p20.0
media  2  10
hole   1  origin x=5.0 y=3.0 rotate a2=90
boundary  10
```

Note that in addition to the lack of a geometry record which defines the HOLE boundary, the HOLE record no longer has a vector definition array. The new version of KENO-VI should be able to read most old input files correctly, but they will take longer to run.

KENO-VI Stability and Speed Improvements

Improvements have been made to KENO-VI since the last Web update to increase the stability and the speed of KENO-VI. To improve the code's stability, logic has been added to KENO-VI to check if a particle is still in the boundary region of a unit when it is no longer in any region. If this occurs, an error message is printed and the program terminates. This situation is often caused by an undefined volume in a unit and could previously lead to the program entering an infinite loop.

To improve the execution speed of KENO-VI, the following modification has been made: When a particle is in an array, the particle is tracked both in the unit where it is currently within the array and in the unit containing the array. It needs to be tracked in the unit containing the array so it knows when it crosses out of the array. Previously, the crossing distance to every surface in that unit was calculated. The code has been changed to calculate only the crossing distance to the surfaces related to the array boundary. This change will significantly reduce the running time of problems where particles spend most of the time in an array or where the array is in a complex unit containing many additional regions unrelated to the array boundary. Running times have been reduced by as much as 15% for arrays contained in complex units.

SAS2H Corrections and Enhancements

A large number of corrections and enhancements have been completed in SAS2H for the release of SCALE 4.4. They are listed below.

- Two errors were corrected for cases where there were more than three zones prior to the mixture 500 zone in the Path B model: (1) The atomic densities were not updated with depleted values in the cross-section processing/spectrum calculations when fuel was input to more than one zone (including the cell-weighted mixture 500 zone). (2) Nuclides that only appear in the moderator were depleted. An example of a model that would be affected is a BWR Path B model with Gd-poisoned fuel pin, gap, clad, moderator, and mixture 500. Usually these discrepancies cause only slight errors in the neutronics part of such BWR cases, but could significantly impact the results for some unique fuel models.

- Input checks and error messages were improved.

- A programming error that caused problems with "MXREPEATS=0" cases to fail on PCs was corrected. These cases are typically used to remove or insert burnable poison rods from one cycle to the next in a depletion.

- A modification was made to correctly calculate the fuel bundle area printed in the shipping cask geometry for the triangular-pitch lattice type of fuel.

- The FUELBNDL input parameter was changed from integer to floating point to allow fractions of fuel assemblies.

- The temperatures of the zones (except the gap) in the Path A model may now be changed for each cycle, similar to the BFRAC and H2OFRAC variables.

- The limit on the total number of libraries (NCYC*NLIB/CYC) was increased to 9,999. However, because the number of unique output file names in SCALE is currently limited to 10,000 and there are typically 11 output files per pass in SAS2H, the practical limit for users is approximately 900 total libraries.

- A significant change was implemented to enable fixed sources (volumetric source or angular flux at a boundary) to be used with INPUTLEVEL=3 cases. This change gives users the capability to model cases such as the irradiation of target materials without explicitly including the irradiation facility in the SAS2H model. Previously the driver geometry and its specific power were required as input to govern the depletion calculation. This fixed-source option is specified in the INPUTLEVEL=3 data as either a volumetric or boundary source. SAS2H then determines the flux based on this fixed source and passes it to ORIGEN-S for use in a flux-driven depletion calculation.

- SAS2H was modified to allow two zones in the Path A model to contain the same nuclide, one at a density of 10^{-20} and the other at a density of greater than 10^{-10}.

- The fixed dimension of 1000 for the Path B mixing table arrays was removed where possible and increased otherwise. The size needed for these arrays can be as large as five times the Path A mixing table size (currently a maximum of about 300 in the 44-group library) plus the number of nuclides outside the zone of mixture 500. The dimension of the arrays that remain fixed was increased to 5000. The remaining arrays were variably dimensioned to the maximum of 2000 or the sum of the Path B mixing table size plus 100 (to allow increases of at least 100 nuclides for INPUTLEVEL=3).

Criticality Search in CSAS1X

MIPLIB has been updated to add input options to MORE DATA that allow specifying an XSDRN adjoint solution, a zone width search, a unit number for the balance table file, and suppressing the cross section weighting. The addition of the zone width search option now gives CSAS1X the capability to perform one-dimensional criticality searches on the size of a geometry zone in XSDRNPM.

New KENO Weights Library and Modules to Generate Weights

Because there was a need to be able to automatically generate a set of weights for use in KENO for arbitrary group structure and material, a new control module GWAS and a new functional module GENWGTS have been added. GWAS sets up an adjoint XSDRNPM case and generates weights automatically from the fluxes. GENWGTS is called by GWAS to read the adjoint fluxes, automatically generate the KENO weighting functions from them, and write an output file for use by program WGT. The biasing weights library for KENO V.a and KENO-VI was updated using the new modules GWAS and GENWGTS. The library contains weights for paraffin, water, concrete, and graphite in 16, 27, 44, 218, and 238 energy groups. The new library was created because there were no biasing data for use with the new ENDF/B-V 44- and 238-group libraries that were released in SCALE-4.3. The old library only contained data for 16, 27, and 123 groups. Note that the 123-group library was removed in SCALE-4.3. Results using this new weights library with the 16- and 27-group cross-section libraries will be different but should agree within statistical uncertainty.

New SCALE Utility Programs

Several new utility programs have been developed for SCALE. A new utility LEGEND has been created that adds a title and legend to the color GIF files generated by KENO V.a or KENO-VI. LEGEND was released last summer with the updated version of KENO-VI (see the June 1996 issue of the Newsletter). The versions of KENO V.a and PICTURE in the next release of SCALE will use LEGEND as well.

K5TOK6 and C5TOC6 are new utilities that convert KENO V.a and CSAS input files to KENO-VI and CSAS6 input files by translating the KENO V.a geometry input to KENO-VI format. Since the converted input files are based on the KENO V.a geometry input, they are generally not the most effective in terms of the

KENO-VI geometry features. They do provide the user with a working KENO-VI input file that can be modified for improvements.

Another new utility is Q0RDPN. It converts a binary input file generated by a CSAS or SAS control sequence for one of the functional modules that use FIDO input such as BONAMI, NITAWL-II, ICE, and XSDRNPM, to an ASCII input file. The user can easily edit the ASCII input file to run a modified version of a problem. This capability allows the user to specify input parameters that are not available in the standard control sequences.

Zirconium Hydride Cross Sections

The ENDF/B-V cross-section libraries in SCALE 4.4 have been updated with thermal scattering data for zirconium hydride. New standard compositions have been added to the Standard Composition Library to allow access to these new cross sections. The new standard compositions are the following:

ZRH2 - density 5.61 g/cc, 1 zirconium to 2 hydrogen atoms
ZR5H8 - density 5.61 g/cc, 5 zirconium to 8 hydrogen atoms
H-ZRH2 - density 1.0 g/cc, the hydrogen in zirconium hydride
ZR-ZRH2 - density 1.0 g/cc, the zirconium in zirconium hydride

SCALE 4.4 Minor Modifications

In addition to the major enhancements noted above, SCALE 4.4 contains many minor modifications, including corrections to errors in SCALE-4.3 and changes to improve portability to different computing platforms. Note that some of these modifications may be duplicate listings of items mentioned in the previous sections.

18-Group Gamma Library: (1) Processed through CORECTOL to mark it as NITAWL-II compatible. Could not be processed by NITAWL-II prior to this correction. (2) Updated to replace the Henderson and Claiborne-Trubey dose factors because the data overestimated the doses by about 25%. The replacement data were taken from the 22n-18g group coupled library.

27-Group Burnup Library: Updated data on rhodium-103 so that Bondarenko factors are generated in the unresolved resonance range. A test case based on 4.5 wt % UO_2 burned to 54,585 MWD/MTU, cooled for 5 years, was run. The calculated k_{eff} increased by 0.06% with the new Rh-103 cross sections.

44-Group ENDF/B-V Library: The 44-group neutron cross-section library was recollapsed from the 238-group library using the corrected version of MALOCS. The impact of the MALOCS corrections should be negligible. See MALOCS corrections below for more information.

238-Group and 44-Group ENDF/B-V Libraries: (1) Corrected negative scattering and total cross sections for minor actinides, fission products, and beryllium metal. Also corrected thermal Bondarenko factors for potassium. Only significant impact should be on cases where potassium is important in the thermal range. (2) Updated to remove resonance parameters from specially weighted stainless steel nuclides because they were being doubly applied. Also, zirconium and hydrogen cross sections for zirconium hydride were added to both libraries.

AJAX: Corrected a portability problem in subroutine ANN caused by the array D being typed real by default, and then printing variables from it using an integer format.

ARP: Updated for optional interpolation on moderator density and made more general to handle user-created basic cross-section libraries. ARP now runs under SCALE driver on PCs and workstations.

ARPLIB: This is a new utility program that creates binary ORIGEN libraries for ARP. It extracts libraries at the desired burnups from large multi-burnup library files generated by SAS2H.

AWL: Added AWL to SCALE to convert AMPX working format libraries between ASCII and binary formats. It is required for the SCALE Criticality V&V package.

BONAMI: (1) Updated to improve error handling procedure and messages. (2) Corrected a problem that caused cases to fail when zero number density input was used.

C5TOC6/K5TOK6: The input file generated for CSAS6/KENO VI incorrectly labeled regions generated to surround HOLEs if there were more than one region in a unit that contained HOLEs. Because of a change in KENO-VI, these regions should no longer need to be generated. Subroutine PUNCH_GEOM was modified to no longer generate these regions.

COUPLE: Updated for year 2000 compatibility, PC version compatibility, uppercase or lowercase input files, and for printing the banner page only when COUPLE is first called.

COUPLE Sample Problem: Updated to change the inner radii in the 3$$ array to zero for consistency with the NITAWL-II input requirements.

CSAS/KENO V.a /KENO-VI/SAS2H Sample Problems: Updated to use the 44-group library.

CSAS and MODIFY: CSAS was updated to add additional required data to the direct access file written for a search problem. MODIFY was updated to read this file. A check for valid parameter constraints and the printing of an error message if they are invalid were also added.

H7MAP: For 1-D problems, if the number of nodes is large enough that the output exceeds one page in length, only part of the output is displayed. The output from the first page is repeated, and the rest of the output is never printed. Correcting this problem involved simply moving one statement from within a DO loop to a point before the DO loop.

H7TECPLOT and H7MONITOR: Outdated comment lines in the BLOCK DATA subroutine that are used to activate or deactivate computer-system-dependent blocks of code resulted in memory not being allocated for variably-dimensioned arrays. An additional correction was made in H7TECPLOT, where the x and y axes were reversed when a translation was done from spherical to Cartesian coordinates.

HEATING Sample Problems: The input file for the second HEATING sample problem was modified to first compile and run a simple Fortran program to convert an ASCII node connector file to binary format for use by HEATING. This modification improves installation portability on different Unix workstation platforms.

KENO V.a: (1) Updated subroutine RDPLOT to correct the format used to print the error message for incomplete input data. (2) Corrected variable type in format statements for debug prints. This discrepancy causes problems on some systems, including PCs when debug print is turned on (DBG=YES). (3) Changed default plot type to color. (4) Updated to correct an error in the k_{eff} calculation that caused a doubling of k_{eff}

when using an ICE mixed AMPX format working library. This error was introduced in SCALE-4.3. (5) Updated to allow printing the frequency distributions for 1-group problems. (6) Updated to match KENO-VI with respect to matrix calculations. The calculation of lifetime was corrected because it was not based on a fair game. These changes can cause the lifetime to be substantially different. The error in the lifetime calculation has probably been in KENO V.a since its initial release in SCALE-3.

KENO-VI: (1) Updated to correctly number error messages, replace the word PICTURE with the word PLOT throughout the program, and print plot symbol data only for character plots. (2) Updated subroutine TRACK to correctly sum fluxes. The fluxes didn't sum properly for units that were crossed by an array boundary. (3) Enhanced to allow HOLEs to be used without explicitly defining a geometry region where the HOLE was to be inserted. The code automatically adds to the unit containing the HOLE the equations that define the boundary of the unit contained within the HOLE, properly rotated and translated as specified on the HOLE record. (4) Fixed problem writing restart file on Sun workstation. (5) Modified the subroutine GEOMIN to correct an infinite loop problem. A pointer to the array that contained the unit boundary x, y, and z position was improperly specified. The pointer LBOXGM has been respecified. (6) Corrected a problem where a particle's inability to cross an array boundary due to round-off problems caused an infinite loop. (7) The code was updated to correct a problem that could cause cases containing arrays with complex boundaries to incorrectly calculate k_{eff}. (8) Corrected a discrepancy that caused the code to go into an infinite loop when boundaries consisted of a body with multiple sets of paired planes. (9) Corrected an error that prevented a restart problem from producing a readable file if it stored data in the generation before the code entered the infinite loop. (10) Corrected a problem involving nested arrays and hexprisms that sometimes caused the code to go into an infinite loop if a collision occurred very near a boundary. (11) Corrected a problem that occurred when a particle crossed a boundary and immediately had a collision that reversed its direction without traveling any distance. The particle sometimes got lost and entered an infinite loop. (12) Modified subroutine TRACK to correct a problem that occurred when an array shared a boundary with a hole that contained the array. If the distance to cross out of the array is less than EPS, the particle now exits the array instead of crossing from one unit to another within the array. (13) Corrected an error in placement of starting points for start type 6. (14) Corrected an error in the flux calculation for regions containing holes or arrays. (15) Corrected a roundoff problem with arrays offset a long distance from the origin. This problem could sometimes cause an infinite loop. (16) Corrected a variable that was misnamed and, as a result, was used without being initialized. (17) Set a lower limit for the calculated crossing tolerance to prevent the code from entering an infinite loop. Also made minor changes to the particle-tracking output when parameter TRK=YES. (18) Updated to allow starting points in a volume larger than the global unit. (19) Updated to terminate a problem if a particle in subroutine TRACK gets lost. Also, updated to allow problems that contain array data but do not reference the arrays in the GEOMETRY data block to run. (20) Updated to change the logic in calculating the array boundary crossing distance (decreases running time for some problems) and to change the default plot type to color. (21) Updated to correct a problem with non-cuboidal albedo boundaries and to add additional space for matrix data. The standard deviations for average k-effective by generation skipped are now accumulated in batches. Because of these changes, any matrix information and the table of average k-effective by generation skipped in the sample problem output will be different. (22) Corrected tracking to allow simultaneous crossing of multiple shared boundaries and to correctly sum fluxes after a collision. Also corrected error related to calculating the x-offset of an array. Changed input logic for ORIGIN and ROTATE data to sum values for an auxiliary keyword for a given geometry record rather than use the last value. This last change was made for compatibility with C5TOC6. (23) Updated to allow a particle to cross from one hole directly into an adjacent hole even if the crossing is outside the allowed tolerances. This prevents some cases from entering an infinite loop. (24) Modified to detect intersecting HOLEs in the global unit. A problem will now terminate if intersecting HOLEs are detected in the global unit. Intersecting HOLEs are illegal in KENO-VI geometry but were not detected in the global unit. Intersecting HOLEs in units other than the global unit are detected during tracking of particles through the intersecting regions.

KENO-VI Sample Problems: Sample problem 22 has been altered in the KENO-VI input file. The geometry data were changed to take advantage of the simplified method of adding HOLEs.

KMART: This new module was added to allow post processing of a KENO V.a restart file, along with a working format cross-section library, to generate activities and/or broad group fluxes and compute the fission production activity if the components are available in the working cross-section library for the requested nuclide. A resonance self-shielded value is used for the fission cross section.

MALOCS: (1) An error was corrected in weighting a coupled master library using a neutron spectrum from a neutron library combined with an explicitly specified gamma-ray spectrum. Also introduced several options for truncating upscattering terms. Changes were made to properly weight the delayed and prompt values of ν. (2) A discrepancy was corrected that caused the storage of invalid data in the temperature array. In the 44-group library this caused the data for the third temperature to be overwritten and to be used for a temperature that is effectively zero degrees Kelvin.

MARSLIB: (1) Updated to change the value of epsilon used to check for round-off errors in the geometry and, thereby, reduce the number of such errors. This modification eliminated the errors previously experienced with several of the SCALE Shielding V&V problems. (2) Variables IR in subroutine AZIP and IRET in subroutine UNIS are now initialized to 0 before they are used as arguments to function IREAD. In AZIP and in UNIS a 'CALL EXIT' was changed to a 'STOP'. In subroutine ALBERT, the nH was removed from two formats and replaced with quotes.

MIPLIB: (1) Updated to allow moderator mixture in a lattice cell to be used in the gap and to add the ability to specify the inner radius to the resonance data. (2) Updated to allow a control program to suppress certain output by setting flags. Added input options to MORE DATA to allow specifying an XSDRNPM adjoint solution, a criticality search in XSDRNPM using the zone width search option, a unit number for the balance table file, and suppressing the cross section weighting. (3) Corrected an error allowing the input of a number density for a compound or alloy. This error was introduced in SCALE-4.3. (4) Updated to allow number density input for an element that has multiple isotopes.

MIPLIB, SUBLIB, UNIXLIB, COMPOZ, MODIFY: Updated to use new direct access routines for character data and replaced references to specific intrinsic FORTRAN functions with their generic names for Fortran 90 compatibility. Also corrected an error in the Dancoff factor calculation that occurs for cylinders in a MULTIREGION problem. This error results in an error in the calculated k_{eff} value of approximately 0.1% for a cylinder the size of a typical fuel rod. Note that this error did not occur in the LATTICECELL geometry option.

MORSE: (1) Updated the limit on number of tracking errors, the unit number for surface detector results, and increased dimensions on surface detector arrays. (2) Updated to include changes to surface detectors for SAS4 cases, to correct a problem in DIREC for NDSG=17 case, to allow orderly termination of a problem when errors in tracking to detector exceed a limit, to add an option to print/not print flux output after each batch, to input the number of direct-access blocks allocated on scratch units, to change the way date is output (to handle the year 2000 and beyond) and to reduce the amount of error output in some cases.

MORSE Sample Problem 8: The 10** array was modified by adding a 22r0.0 at the end.

NITAWL: Corrected the potential cross section used for higher order resonances (L>0). The impact should be negligible in most cases.

ORIGEN-S: (1) Updated cross-section edit of binary libraries to add option to change cross-section values to quantities derived from total flux (as in ORIGEN2) instead of thermal flux. (2) Corrected calculation of printed average power. (3) Added error message if number of time steps is less than 4 for reactor startup case. (4) Updated to correct the loop index for re-normalizing the R8 array. (5) Updated for year 2000 compatibility and to correct calculation of He-3 and H-3 for long time steps and high flux. (6) Updated to allow saving concentrations and then continuing with a subcase using a new library. (7) Updated to allow the flux input value for the last time step to be zero.

ORIGEN-S Master Photon Library: The library was updated to correct the photon yield data for Ra-222 and Th-226, and the photon yields for gammas accompanying (α,n) and spontaneous fission reactions were updated to reflect small changes that occurred during the last decay data update.

OSBICO/OSBIRE: Updated for compatibility with lastest version of ORIGEN-S.

PERFUME: Improved the selection of new moments when a moment is found to be invalid and converted coding to a more standard Fortran 90.

PERFUME Sample Problem: The special cross-section data file required for the PERFUME sample problem has been added to SCALE, and the sample problem input data have been updated to use it. This problem has not been included in SCALE since SCALE was moved from the mainframe to the workstation several years ago.

PICTURE: (1) The module was updated to add option of generating 2-D color GIF plot files of the geometry model input for the SCALE shielding modules MORSE or QAD-CGGP. This capability already exists in the SCALE criticality modules KENO V.a and KENO-VI. (2) The module was also updated to handle the call by SAS4 when the "PARM=CHECK" option is used. (3) An option was added that allows users to specify an X-Y, X-Z, or Y-Z plot and have the code automatically calculate the cosines used for the plot.

PRISM: This is a new utility program for ARP that can read a single SAS2H or other type of input file and generate multiple copies by replacing generic symbols with specified values.

QADS/QAD-CGGP: (1) Updated to make the combinatorial geometry input data have the same format as the combinatorial portion of the MARS geometry input which is used in other SCALE modules. Old input files will no longer run. (2) Updated to add error checks for limits on number of compositions and elements and to fix the code to handle upper- or lower-case input. (3) Added a test on the MIPLIB error flag that terminates execution of the problem if an error occurred.

QADS and QAD-CGGP Sample Problems: Updated to change the geometry input format to agree with the changes made to QADS and QAD-CGGP.

RADE: Corrected an error in subroutine MCHEK that caused RADE to fail on a Sun workstation. A constant was passed as an argument to subroutine MCHEK to be used for dimensioning, but MCHEK later used the same variable for other purposes. The argument was renamed and used in the dimension statement.

SAS1: Scratch unit N16 was not opened when SCALE driver returned to SAS1 after cross-section processing and prior to XSDRNPM shielding calculation. This problem caused SAS1 to fail on the PC. The OPEN statement was moved to the beginning of main program so it would always be opened.

SAS2H: (1) Updated to fix a problem where the reload feature failed to reload correctly for the final cycle type. (2) Modified subroutine SZNSEG so that it would not cause the ORIGEN library creation to fail by not recognizing the cross-section library specified. The problem was an uninitialized variable ERSET. The change was to initialize the variable as "FALSE" before calling subroutine GETLIB. A change was also made so that the library name was passed to GETLIB instead of only the first 4 characters. (3) Updated to correct an error in the mass of the clad when the clad was input as an isotope and the mass was not input as a light element in Data Block 15. (4) A problem was corrected where the atomic densities were not updated with depleted values in the cross-section processing/spectrum calculations when fuel was input to more than one zone (including the cell-weighted mixture 500 zone) and there were more than three zones prior to the mixture 500 zone. For example, consider a BWR Path B model with Gd-poisoned fuel pin, gap, clad, moderator, and mixture 500, where there are four zones prior to the mixture 500 zone. Usually this discrepancy causes only slight errors in the neutronics part of such BWR cases, but could significantly impact the results for some unique fuel models. (5) The module was updated for compatibility with the newest revisions to XSDRNPM. The routines that wrote the XSDRNPM input files needed to be changed to account for the changes to XSDRNPM input. Subroutine COPYNX had to be changed to add the 0$ array to the XSDRNPM input file, and to move setting the logical unit number of the flux output file from the 2$ array to the 0$ array.

SAS3: (1) Variable IR in subroutine OAKTRE is now initialized to 0 before it is used as an argument to function AREAD. Subroutine RINPUP was updated to initialize the variables JMK and IML in COMMON JOMK because they are used when SAS3 calls MARSLIB routines and they were not being defined prior to the calls to JOMIN. (2) Updated to be compatible with the new MORSE input options and to implement the PARM=SIZE parameter which was not being passed to MORSE.

SAS4: (1) Subroutine MORINP was updated to add common JOMK and to initialize the variables JMK and IML in common JOMK because they are used when SAS4 calls MARSLIB routines and they were not being defined prior to the calls to JOMIN. (2) The code was modified to translate the user input to lowercase. This change was necessary to make SAS4 capable of handling input files in either upper or lowercase, as the other SCALE neutronic codes already do. (3) The code was updated to correct the dimensions on two arrays. Also changed a test comparing 2 floating point variable names equivalenced to integer variables to use function ISET. (This test has previously caused floating point underflows on some platforms.) (4) Added a "PARM=CHECK" option that calls PICTURE from within the SAS4 to plot geometry but not run MORSE. SAS4 prepares or reads MARS geometry input data, reads PICTURE input, and calls PICTURE. Several other changes were made to error messages and formats. (5) The convergence criteria was updated because the criteria in XSDRNPM were changed. (6) The input variable NDAB was added to allow the user to specify the number of direct access blocks allocated.

SAS4 Sample Problems: (1) A ninth sample problem was added to illustrate the new enhanced surface detector option. (2) SAS4 sample problems 1, 3, and 5 were updated to remove references to variables FR1, FR2, FR3, and FR4, which became obsolete in SCALE 4.4.

SCALE Driver: (1) Updated to allow processing the rest of the input data after invalid input data are detected. (2) The driver has been updated to obtain and act on error codes from the modules. The driver now prints error codes and stops further sequence execution.

Standard Composition Library: (1) The default density of B4C was corrected from 2.54 to 2.52 g/cc. This error was introduced in SCALE-4.3. For an LWR fuel problem with B_4C pins between fuel assemblies, the calculated k_{eff} value increased less than 0.2%. (2) Updated to reference the nuclides used for zirconium

hydride which have been added to ENDF/B-V libraries and to add four new standard composition names related to zirconium hydride. (3) The densities for SS304 nuclides were made identical to the standard versions of the same nuclides. (4) Updated the standard composition ZIRC2 for consistency with current technical standard and updated densities for SS304 and SS316. (5) Mass of copper was corrected (it was in atomic mass units instead of C-12 mass units). Density of C-GRAPHITE was changed from 1.0 to 2.3 g/cc. The following compositions were added: GRAPHITE, KEROSENE, KERO(H2O), NORPAR13, NORPAR(H2O), POLYVINYLCL, PVC, PVC(H2O), TBP, TBP(H2O).

SUBLIB/UNIXLIB: (1) Updated to remove year 2000 problems. These changes basically changed the year format for the QA verification table to 4 digits. Additionally, the date format was changed to use a 3-character month abbreviation so that the date would be unambiguous. A new line was added to the QA verification table printout to identify the machine on which the program was run. (2) Updated to remove an artificial limit of 8-character-length filenames for non-standard files in subroutine OPNFIL. (3) Modified subroutines LISTQA and VERGET for consistency of the length of the string containing the executable name, the creation date, and the directory path to the executable. The directory path was increased to 256 characters. (4) Updated subroutine FINDQA to place underscores in place of the blanks in the date to simplify the automatic updating of the QA verification table. (5) Replaced the CHARACTER*8 type of variable CAT with a variable length CHARACTER type in subroutine NOTE. This corrected a problem in WAX on the Sun workstation. (6) Added comments to subroutine OPENDA indicating how to replace the Fortran 90 specific INQUIRE statement with a Fortran 77 compatible statement. (7) Replaced all STOP statements with calls to EXIT with the appropriate error return code for proper detection by the driver. (8) Modified subroutine DREAD to correctly process data following the second digit of an exponent when called by the array reading subroutine YREAD. Previously, exponents of 10 or greater sometimes caused errors in the reading of FIDO-type input arrays. This discrepancy was discovered in an ORIGEN-S case. (9) Changes to update XSDRNPM required a double precision ERF function. The necessary routines were added to compute the double precision ERF when it is not part of the intrinsic library.

XSDOSE: An option was added to turn off angular flux print and no angular flux print was made the default.

XSDOSE Sample Problem: The input was modified to turn on the new angular flux print option in XSDOSE.

XSDRNPM: (1) The special activity file and balance table file were not written correctly, and the correct file structure is not what was documented. Subroutine SETUP was changed such that it would not read or write dummy records after the files were opened. These read/writes were the only way to open the files before Fortran 77, but when the code was converted to Fortran 77 and OPEN statements were added to explicitly open the files, the extra statements were not removed. (2) Updated to correct the accumulation of zone fluxes when inner-cell weighting is selected. (3) Updated to correct the value of productions/absorptions when a direct buckling search is done. (4) The code was also modified to collapse prompt υ and delayed υ using the same procedure as used to collapse the total υ. (5) Corrected calculation of broad group balance tables to be consistent with fine group tables. Broad group cross sections were not in balance when upscatters were collapsed. (6) Updated to print clearer messages when allocated memory is insufficient. Also, in these cases if an output file could not be written, any previously existing file was deleted to prevent subsequent calculations from reading it. (7) The Fortran source for XSDRNPM was converted to Fortran 90 free format. (8) The input/output units were all moved to the 0$ array. The energy of the average lethargy causing fission was added to the balance tables. (9) The output files from the balance tables and the activities were modified and converted to ASCII files. A new file was created which contains the input and derived data from a problem. The flux file was changed to double precision. (10) The code was modified to not run with fluxes out of core unless explicitly requested in the input. (11) The coarse mesh generation algorithm used in rebalancing the

inner iterations was modified to correct a problem that prevented convergence of a very small class of problems.

XSECLIST: This is a new utility program for ARP which prints lists of absorption and fission cross sections vs burnup for nuclides from ORIGEN-S multi-burnup binary libraries.

Portability

Version 4.4a of the SCALE system has been developed to ensure portability among various computing platforms. The system is maintained and enhanced at ORNL under quality assurance and configuration management plans. The system has been routinely tested on IBM and DEC workstations. In addition, a version for personal computers (PCs) is included in the package. The PC version runs on Windows 95, 98, and NT4.0 and platforms. The system also has been installed and tested by ORNL on SUN and HP workstations. Information needed to install and run SCALE on each of these systems is included in README files with the software package distributed by the code center.

Related developments

The definition of "easy-to-use" has changed considerably since the late 1970s. As funding has allowed, the ORNL development staff has sought to develop user interfaces that provide a distinct aid to novice or occasional users of the system.

The ORIGNARP input processor is a MS-DOS PC program designed to assist a user in creating an ORIGEN-S input file. It is coupled with the ARP code, which interpolates on standard LWR ORIGEN-S binary libraries, in the ORIGEN-ARP system (Section D1).

CSPAN (Criticality Safety Input Processor for Analysis) is the Windows GUI replacement for the CSASIN input processor for the CSAS criticality sequences in SCALE. CSASIN was an MS-DOS program developed in 1990–91 to assist new and occasional SCALE users. Because CSASIN is incompatible with Pentium II and later PCs, a new easier to use and more powerful Windows program has been developed. CSPAN can be used to read and modify an existing SCALE input file or to create a new input file. CSPAN can call SCALE to execute CSAS using the input file it creates. The SCALE Standard Composition library and the selected SCALE cross-section library are read by CSPAN and the user is only allowed access to those compositions available on the selected cross-section library. The program handles the entry of basic standard compositions, solutions, and arbitrary materials, unit cell data, optional parameter data, and KENO V.a input data. CSPAN can call SCALE to execute any CSAS case. CSPAN runs under Windows 95, 98, or NT. Checks for errors are included throughout the program to verify that the input is valid. The initial version distributed with SCALE 4.4a is considered a beta test version. Help files have not been developed yet, but will be made available soon.

The initial version of a Windows-based GUI for HEATING named Visual Heating is also included in the SCALE 4.4a release. Visual Heating assists the user in preparing a HEATING input file and includes a 3-D graphics display of HEATING geometry models using OpenGL. Visual HEATING can execute the HEATING case in SCALE and display the output file in a text editor. It includes an HTML Help system similar to many commercial Windows programs. The help system is accessible both from the main menu bar and by pressing the F1 key. Most of the information in the HEATING User's Manual (Sect. F10 of the SCALE Manual) is included in the help system along with explanations of Visual HEATING input screens.

Availability

The SCALE code system and the other software designated under "Related Developments" have been packaged by the Radiation Safety Information Computational Center (RSICC). The SCALE system and the related software may be obtained by contacting

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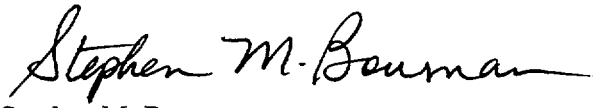
Telephone: (865) 574-6176
FAX: (865) 574-6182
E-mail: rsic@ornl.gov
Internet: http://www-rsicc.ornl.gov

Acknowledgments

The SCALE system is maintained at ORNL and enhanced to keep pace with normal technical advancements in the analysis areas of interest. Although the NRC continues its role as the controlling sponsor of the SCALE system, the U.S. Department of Energy (DOE) began assisting in the maintenance of the SCALE system in 1987. Over the years numerous individuals within these sponsoring organizations have played key roles in ensuring that the SCALE system remained a readily available, reliable system for the analysis of nuclear fuel facilities and packages. The individuals who have worked with the ORNL staff to coordinate maintenance and development activities include R. H. Odegaarden (NRC, ret.), G. H. Bidinger (NRC, ret.), C. Mauck (DOE, ret.), E. P. Easton (NRC), W. H. Lake (NRC and DOE), M. E. Wangler (DOE), and M. G. Bailey (NRC).

As demonstrated by this Manual, there are also numerous individuals from the ORNL staff who have contributed significantly to the development and enhancement of the SCALE system. Most are credited by their authorship of the sections in this Manual that correspond to their work. A few individuals have been essential to the development and maintenance of SCALE but are not credited by authorship. These individuals include: S. K. Lichtenwalter, who is responsible for implementing and controlling software system changes; C. H. Shappert, who provided the editorial review of this Manual; and L. F. Norris (ret.) and W. C. Carter, who prepared the entire manuscript. Special acknowledgement is also due to R. M. Westfall and G. E. Whitesides (ret.) who, together with R. H. Odegaarden of the NRC, developed the concept and long-range goals of the SCALE system in the late 1970s. Finally, this Project Leader will always be grateful to C. V. Parks, who served as the SCALE Project Leader for the first 15 years, and L. M. Petrie, who for 20 years has consistently provided consultation and advice on the technical direction that should be taken in development of nearly every module and cross-section library that are in the present system.



Stephen M. Bowman
SCALE Project Leader
December 1999

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Table 1 Analysis capabilities summary of the SCALE control modules

Control module	Analysis function(s)	Functional modules executed	Section reference
CSAS	1-D deterministic calculation of neutron multiplication 3-D Monte Carlo calculation of neutron multiplication Problem-dependent cross-section processing Multiplication search or spacing	BONAMI NITAWL-II XSDRNPM KENO V.a ICE	C4
CSAS6	3-D Monte Carlo calculation of neutron multiplication	BONAMI NITAWL-II XSDRNPM KENO-VI	C6
ORIGEN-ARP	Point depletion/decay of nuclear fuel and radioactive material	ARP ORIGEN-S	D1
SAS1	1-D deterministic calculation of radiation transport through shield and dose evaluation at a point Calculation of dose at detector based on leakage from critical volume	BONAMI NITAWL-II XSDRNPM XSDOSE	S1
SAS2	Point depletion/decay of nuclear fuel 1-D radial shielding analysis in cylindrical geometry	BONAMI NITAWL-II XSDRNPM COUPLE ORIGEN-S XSDOSE	S2
SAS3	Dose evaluation using MORSE Monte Carlo code	BONAMI NITAWL-II XSDRNPM MORSE-SGC	S3
SAS4	Calculation of dose outside of transportation package using MORSE code and automated biasing techniques	BONAMI NITAWL-II XSDRNPM MORSE-SGC	S4
QADS	3-D point-kernel gamma-ray shielding analysis	QAD-CGGP	S5
HTAS1	R-Z steady-state and transient analyses of a transportation package	OCULAR HEATING	H1

Table 2 Analysis capabilities summary of the SCALE functional modules

Module	Function	Section reference
BONAMI	Resonance self-shielding of cross sections with Bondarenko factors	F1
NITAWL-II	Resonance self-shielding of cross sections with resolved resonance data	F2
XSDRNPM	General 1-D, discrete-ordinates code for: • zone-weighting of cross sections • eigenvalue calculations for neutron multiplication • fixed-source calculation for shielding analysis • adjoint calculation for determining importance functions	F3
XSDOSE	Module for calculation of dose at a point based on the 1-D leakage flux from a finite shield	F4
COUPLE	Interface module for preparation of cross-section and spectral data for ORIGEN-S	F6
ORIGEN-S	General-purpose point-depletion and decay code to calculate isotopic, decay heat, radiation source terms, and curie levels	F7
ICE	Cross-section utility module for mixing cross sections	F8
MORSE-SGC	Monte Carlo code with combinatorial and array geometry features used to perform radiation shielding analysis	F9
HEATING7.2	Finite-volume, multidimensional code for conduction and radiation heat transfer	F10
KENO V.a	Monte Carlo code for calculation of neutron multiplication factors	F11
OCULAR	Calculation of radiation exchange factors	F16
KENO-VI	Monte Carlo code for calculation of neutron multiplication factors for complex geometries	F17

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SCALE SYSTEM DRIVER

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ABSTRACT

The SCALE driver was designed to allow implementation of a modular code system consisting of control modules, which determine the calculation path, and functional modules, which perform the basic calculations. The user can either select a control module and have that module determine the execution path, or the user can select functional modules directly by input.

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M1.1 DESCRIPTION

The SCALE driver was designed to allow implementation of a modular code system consisting of control modules, which determine the calculation path, and functional modules, which perform the basic calculations. The user can either select a control module and have that module determine the execution path, or the user can select functional modules directly by input.

The driver obtains the name of the module to be accessed from the module specification card, the first card in the user input data file. It then transfers data cards from the input file to unit 5 until it finds an END card (a separate card with the characters END in columns 1 through 3). The driver constructs a file of control information and accesses the module named on the first card. The control file allows the module to return control information to the driver and indicate what the next task will be. These tasks may include transferring more cards from the input file to unit 5, accessing a string of up to eight functional modules and/or terminating this module and checking the input file for another module name to be accessed. SCALE uses subroutines GETMS and RESETM to communicate data from the control file between the driver and labeled commons. This isolates the exact mechanism for communicating these data to the driver. This mechanism is one of the system-dependent parts of the SCALE system. Another system-dependent function the driver needs is the means to initiate the execution of another program.

When the driver accesses a functional module, the exit code returned by the module is checked. If the returned code is nonzero, the access string is terminated. When a string of functional module accesses is finished, the driver again accesses the control module to determine its next function.

Table M1.1 describes the four sets of data the driver passes to a control module. The data of JP and JD are message strings, IC is an integer array, and AC is a real array. JP is the string defined by the PARM= field on the module specification card.

By default, the driver reads input from SYSIN, prints a record of primary module accesses and input data to PRINT, writes the input file for the primary module to INPUT, and calls the module.

Table M1.1 Use of data in the communication block between the driver and the control module

Item	Use [a]	Control module action	Driver action
JP(1)	PARM field, string length starts on a half-word boundary followed by a character string.	Can be passed to the main program as a parameter.	(None)
JD(1)	DDNAME table, length of table starts on a half-word boundary, then 8-character names follow, binary zeros nullify.	Needed for system routine use.	(None)
IC(1)	Control module access count, termination flag.	If 1, read data from unit 5, save, set 0 for subsequent case, <0 for termination; <1 upon entry indicates an error condition.	Initialize as 0 whenever user input instructs access of a control module, add 1 prior to each access of a control module, seek new user input instructions if 0, terminate if <0.
IC(2)		Not used.	Not used.
IC(6)			
IC(7)	Task completion flag, 0 - completed successfully, ≠ 0 - failure.	If ≠ 0, execute wrap-up procedures.	Store STOP return number from code module here if it exceeds that allowed.
IC(8)	User input data transfer flag (0 - no; 1 - transfer data and access module specified by control module; 2 - transfer data and access the special processor named on the first card (A8); >2 - transfer data only).	Set to anticipate needs.	If >0, move a block to unit 5, no other tasks if >2; set to zero on successful data transfer.
IC(9)	Individual code module task completions.	Probably set 0 at the start of each separate case; nonzero upon first access indicates previous calculations have been done, perhaps under control of this or another control module.	Add 1 after each acceptable return from a code module excluding the control module.
IC(10)	Reserved for future driver control.		If 5376 ≤ IC(10) ≤ 5631, driver will print a functional module access record along with the control module access and input record.
IC(11) IC(80)	Reserved for control module use.		

Table M1.1 (continued)

Item	Use [a]	Control module action	Driver action
AC(1)	8-character control module name.	(None)	Set here.
AC(2-AC(9)	8-character code module names.	Set functional module access order here, end with a blank if <8 entries.	Initialize blank.
AC(10)	Latest input data header name.	Used here, then set blank.	Initialize blank, set here unless first record read encounters end-of-file.
AC(11)-AC(40)	Reserved for control module use.		

[a]A control module will not be summoned under the apparent error conditions of unsuccessful transfer of data to unit 5; a terminator flag in the input data is required. The driver processes the user input file seeking a subsequent request for access to a control module. The elements in the IC array are set zero and in array AC are set "BLANK" initially by the driver, and prior to a subsequent access of any control module, IC(1) - IC(8) and IC(10) are set zero and AC(1) - AC(10) set "BLANK." Upon entry to a control module, AC(1) will contain its access name, IC(1) will be 1, IC(8) is a task completion flag set for transfer of the control- module input data, IC(9) remains the code-module access count.

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SCALE SUBROUTINE LIBRARY

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ABSTRACT

A number of subroutines have been developed which are used by more than one of the SCALE program modules. The subroutines have been collected together in a library. This section contains a brief description of the function and the arguments of each subroutine.

CONTENTS

ACKNOWLEDGMENT

Many of the subroutines described here were contributed by N. M. Greene. Numerous other people have also contributed to the library.

M2.1 INTRODUCTION

The SCALE subroutine library is a collection of subroutines, each of which performs a function that may be useful to more than a single program. These subroutines have been collected into a library so that a program can easily access those it needs. In the description that follows the calling sequence, a brief description of the function, a brief description of the arguments, and the programming language used for each subroutine in the library are given. This section is written from the point of view of aiding a programmer in using these subroutines in a program. Section M3.2 gives more information on how a user inputs data to the SCALE free-form reading package. Section M10 gives similar information on using FIDO-type input.

The programming language for the subroutines refers to the distributed version of SCALE. Most of the subroutines are programmed in FORTRAN 77, with the rest being programmed in C. The C routines are used to provide functionality not available in FORTRAN 77. Section M2.2 describes the FORTRAN subroutines. Appendix M2.A contains a list of the C language routines, their FORTRAN interface, and the functionality they provide.

A number of AMPX[1] subroutines are included in the SCALE subroutine library for use with the AMPX modules included in SCALE. These subroutines are not described here, but are listed in Appendix M2.B, along with the modules that use them.

M2.2 DESCRIPTION OF FORTRAN SUBROUTINES

M2.2.1 ALOCAT

CALLING SEQUENCE:

CALL ALOCAT(PROG,LMAX,*NSRET)

FUNCTION:

ALOCAT is used to dynamically allocate an automatic array and pass it, along with its dimensions, to a subroutine supplied as an argument. The length requested is the second argument. ALOCAT passes the address of the storage and its length to a subroutine supplied by the calling program.

ARGUMENTS:

PROG is the subroutine ALOCAT is to call. The call is of the form CALL PROG(D,LEN), where D is an array of length LEN. D starts on a double-word boundary, and LEN is the number of single words in D.

LMAX is the number of words of storage to be allocated.

*NSRET is an alternative return that will be used when the system is unable to allocate the required block. ALOCAT returns to this alternative return without calling PROG.

M2.2.2 ANIS

CALLING SEQUENCE:

CALL ANIS(EG,UG,EN,UN,IDE,CX,C,MSC,MSCM,ID,IHT,IHS,ITL,MMCR,NOU,NPU,NT4, NT9,IFCT)

FUNCTION:

ANIS is used to convert an AMPX working format library to an ANISN format library (either binary or punched card).

ARGUMENTS:

EG is an array into which the gamma energy group boundaries are read.

UG is an array into which the gamma lethargy group boundaries are read.

EN is an array into which the neutron energy group bounds are read.

UN is an array into which the neutron lethargy group bounds are read.

IDE is an array of length 50 into which the nuclide identifier record from the AMPX library is read.

CX is a scratch array used to hold the cross sections from the AMPX working library.

C is an array used to construct the ANISN-formatted cross section in. Its length is ITL*(IGM + IPM), where IGM is the number of neutron groups and IPM is the number of gamma groups.

MSC is an array containing the MT numbers of the extra 1-D cross sections to be output on the ANISN library.

MSCM is the number of extra 1-D cross sections to be output on the ANISN library.

ID is the ANISN cross-section identifier. ANIS increments this by one for every set. If ID<0 when ANIS is called, it is set to 0. The first cross-section set will have an identifier of the initial ID + 1.

IHT is the position of the total cross section in the ANISN cross-section table. If IHT is 3 or greater, position IHT-1 will contain $\upsilon\sigma_f$, and position IHT-2 will contain σ_a by default. Positions 1 to MSCM will contain the cross sections specified in the MSC array.

IHS is the position of the within-group scattering cross section in the ANISN cross-section table. If the cross sections contain upscatter elements, positions for the values must be left between IHT and IHS.

ITL is the table length of the ANISN cross sections. The value should be IHS plus the number of downscatters allowed.

MMCR specifies the format of the output ANISN library. If MMCR = 1, the ANISN library will be punched card format. If MMCR = 2, the ANISN library will be unformatted binary.

NOU is the logical unit number to print messages and list cross sections on.

NPU is the logical unit number to punch the cross sections on.

NT4 is the logical unit number for the AMPX working library.

NT9 is the logical unit number for the binary ANISN library.

IFCT is a listing control flag. The ANISN cross sections are listed through order of L = IFCT. If IFCT < -1, only the P_o cross sections are output on the ANISN library.

SUBROUTINES CALLED:

CLEAR,IO,A1DX,SNST,WOT,FFPUN

M2.2.3 AREAD

CALLING SEQUENCE:

WORD = AREAD(IBR,IRET)

FUNCTION:

AREAD is a CHARACTER*4 function used to read character data in free format. AREAD returns four characters at a time. Depending on its arguments, AREAD can return the first four characters of a new record, the next four characters from the current record, or it can skip blanks and then return up to four characters. After having skipped to a nonblank character, AREAD will return up to the next four characters, but will stop and pad with blanks if it detects a blank or equal sign (or double blank or left parenthesis, depending on the argument). AREAD, on the next reference, can return the next four characters, but it remembers if a blank (or double blank) has been detected, and can return a blank word in this case. The double blank allows a string of characters with embedded single blanks to be returned as entered.

ARGUMENTS:

IBR is an option flag determining the mode of reading data.

IBR = 0 returns the next four characters in the input record.

IBR = 1 reads a new record and returns the first four characters.

IBR = 2 returns four characters starting with the first nonblank character and stopping if there are two consecutive blanks or an equal sign. Padding is with blanks if necessary.

IBR = 3 returns four characters but stops with a double (or single) blank, depending on whether the preceding call to AREAD had IBR = 2 or IBR = 4.

IBR = 4 returns four characters starting with the first nonblank character and stopping with a single blank, or an equal sign. Padding is with blanks if necessary.

IBR = 5 same as IBR = 4, but will also stop at a left parenthesis.

IBR = -1 returns the last character scanned.

IRET is a flag returned to the calling program if the scan-ahead feature has been activated (see SCANON, also see Sect. M3). If IRET = 2 when AREAD is called, it prints a message and

terminates. Otherwise, it sets IRET = 0 and continues. If the scan ahead feature is activated, and 'END' is found when scanning, IRET is set to 1. If an end of file is detected while scanning ahead, IRET is set to 2.

SUBROUTINES CALLED:

ENFILE,Y0READ

COMMONS:

UNIT,QRDBUF

M2.2.4 AZIRN

CALLING SEQUENCE:

CALL AZIRN (s,c)

FUNCTION:

AZIRN returns the sine and cosine of a uniformly distributed random azimuthal angle.

ARGUMENTS:

S is the sine of a random azimuthal angle

C is the cosine of a random azimuthal angle

SUBROUTINES CALLED:

FLTRN, SIN, COS

M2.2.5 A1DX

CALLING SEQUENCE:

CALL A1DX(CX,N,IGP,IA,C,ITL,MSC,MSCM,IHT,GR,IGM,ITRG)

FUNCTION:

A1DX finds the 1-D cross sections from an AMPX working library (see Sect. F2.4) and moves them to the correct positions in an ANISN library. It has a default set of reaction types which can be supplemented in the argument list.

ARGUMENTS:

CX is an array containing the 1-D cross sections from an AMPX working library.

N is the number of different 1-D cross sections in CX.

IGP is the number of groups + 1 in the AMPX cross sections.

IA is the offset to be added to the group number in the AMPX library to obtain the group index in the ANISN library. This offset will be zero for neutron groups, and will be the number of neutron groups for the gamma groups in a coupled library. The offset will be zero for a gamma-only library.

C is the array for the ANISN library.

ITL is the table length of the ANISN cross sections.

MSC is the array containing the identifiers of extra processes to be put in the ANISN library.

MSCM is the number of extra processes to be put into the ANISN library.

IHT is the position of the total cross section in the ANISN library. By default, $\upsilon\sigma_f$ is in position IHT-1, σ_a is in IHT-2, and the extra cross sections are lined up sequentially in positions 1 to MSCM. An "extra" cross section will override the default process if the positions overlap.

GR is a vector into which A1DX will place the difference between the cross section placed in position IHT and the total cross section. This difference is then used to correct the within-group scattering position of the transfer array.

IGM is the number of groups in the ANISN cross sections.

ITRG is a flag determining whether the cross sections are for neutrons or gammas (0 is neutrons, 1 is gammas).

M2.2.6 BDYS

CALLING SEQUENCE:

CALL BDYS(E,IGM,N6,NTYPE,IVER,NWT)

FUNCTION:

BDYS searches a group boundary library for a particular group structure, type, and version, and then reads the corresponding boundaries from the library into E. If the particular set asked for cannot be found, BDYS will generate a default set using an equal lethargy spacing. The default neutron

structure will be from 0.00001 to 1.49E+7 eV; the default gamma structure will be from 1.E+4 to 1.E+7 eV.

ARGUMENTS:

E is the array returning the group boundaries.

IGM is the number of groups.

N6 is the logical unit number for the printed output.

NTYPE is a flag determining whether a neutron or a gamma group structure is needed.
0 - neutrons
1 - gammas

IVER is the version number desired.

NWT is the logical unit number of the group boundary library.

M2.2.7 BLANK

CALLING SEQUENCE:

CALL BLANK (LC,NL)

FUNCTION:

BLANK sets a character string to blanks.

ARGUMENTS:

LC is the character string.

NL is the number of characters in the string.

M2.2.8 CLEAR

CALLING SEQUENCE:

CALL CLEAR (LD,N)

FUNCTION:

CLEAR sets an array to zero.

ARGUMENTS:

LD is the array to be zeroed.
N is the number of words to be zeroed.

M2.2.9 CLOSDA

CALLING SEQUENCE:

CALL CLOSDA (NU)

FUNCTION:

CLOSDA is used to close a random access file opened by OPENDA.

ARGUMENTS:

NU is the logical unit number of the file to be closed.

M2.2.10 CMPS

CALLING SEQUENCE:

CALL CMPS (C,L,IGM,IPM,IFTG,N,IHT,CODE)

FUNCTION:

CMPS is used to convert an expanded transfer array that allows space for all possible values to a compressed form containing magic words and with zeroes suppressed such as is used on AMPX cross-section libraries.

ARGUMENTS:

C is the array to be compressed.

L is the compressed dimension of C upon exiting CMPS.

IGM is the number of neutron groups.

IPM is the number of gamma groups.

IFTG is the first thermal group.

N is an array that points to the magic word position in the expanded array.

IHT is the number of 1-D cross-section positions in the array.

CODE is a flag determining whether a group can be completely compressed out of the array (0.0 is yes, 1.0 is no).

M2.2.11 COPY

CALLING SEQUENCE:

CALL COPY (X,N,II,IO,IGO)

FUNCTION:

COPY is used to copy a record from unit II to unit IO.

ARGUMENTS:

X is an array used in the copy.

N is the number of words to be copied.

II is the input logical unit number.

IO is the output logical unit number.

IGO is a flag keying whether the records are self-defining or not.
IGO = 1 means N must be supplied by the calling program.
IGO = 2 means N is supplied by the record to be copied.

M2.2.12 CREAD

CALLING SEQUENCE:

WORD = CREAD(IBR,IRET)

FUNCTION:

CREAD is a CHARACTER*8 function used to return eight characters according to the argument IBR. See AREAD for more details.

ARGUMENTS:

IBR is an option flag determining the mode of reading data.
IBR = 0 returns the next eight characters in the input record.

IBR = 1 reads a new record and returns the first eight characters.

IBR = 2 returns eight characters starting with the first nonblank character and stopping if there are two consecutive blanks. Padding is with blanks if necessary.

IBR = 3 returns eight characters but stops with a double (or single) blank depending on whether the preceding call to AREAD had IBR = 2 or IBR = 4.

IBR = 4 returns eight characters starting with the first nonblank character and stopping with a single blank.
NOTE: IBR = 2,3, or 4 will also stop at an '=' character.

IBR = 5 same as IBR = 4, but will also stop at a '(' character.

IBR = -1 returns the last character scanned.

IRET is a flag returned to the calling program if the scan ahead feature has been activated (see SCANON, also see Sect. M3). If IRET=2 when AREAD is called, it prints a message and terminates. Otherwise, it sets IRET=0 and continues. If the scan ahead feature is activated, and 'END' is found when scanning, IRET is set to 1. If an end of file is detected while scanning ahead, IRET is set to 2.

SUBROUTINES CALLED:

AREAD

M2.2.13 REED,RITE,RD,CREED,CRITE

CALLING SEQUENCE:

```
CALL REED (X,L,NU,NP)
CALL RITE (X,L,NU,NP)
CALL RD (LP,X,L,NP,NU)
CALL CREED (C,L,NU,NP)
CALL CRITE (C,L,NU,NP)
```

FUNCTION:

REED is used to read an array, X of length L, from the random access file pointed to by logical unit number NU, starting at block number NP. RITE is used to write X on NU at NP. RD is used to read X from NU starting with LP*th* word of block NP. CREED is used to read a character array, C of length L from NU at NP. CRITE is used to write C on NU at NP.

ARGUMENTS:

X is the array into which or from which data are read or written.

C is the character array into which or from which data are read or written.

L is the number of words to be read or written.

NU is the logical unit number of the random-access file.

NP is the block number at which data transfer is to start.

LP is the first word of block NP to be transferred to X.

M2.2.14 DATIM

CALLING SEQUENCE:

CALL DATIM (DATE,TIME)

FUNCTION:

DATIM returns the date and time of day as two eight-character strings suitable for printing.

ARGUMENTS:

DATE is an eight-character string in which the date is returned in the form mm/dd/yy, where mm is the month, dd is the day, and yy is the year.

TIME is an eight-character string in which the time of day is returned in the form hh:mm:ss, where hh is the hour, mm is the minutes, and ss is the seconds.

SUBROUTINES CALLED:

RETMTM

M2.2.15 DAZIRN

CALLING SEQUENCE:

CALL DAZIRN (DS, DC)

FUNCTION:

DAZIRN returns the double-precision sine and cosine of a uniformly distributed random azimuthal angle.

ARGUMENTS:

DS is the double-precision sine of a random azimuthal angle

DC is the double-precision cosine of a random azimuthal angle

SUBROUTINE CALLED:

FLTRN, COS, SIN

M2.2.16 DGTISO

CALLING SEQUENCE:

CALL DGTISO (DU, DV, DW)

FUNCTION:

DGTISO returns the double-precision direction cosines of an isotopically distributed random direction.

ARGUMENTS:

DU is the double-precision x-direction cosine

DV is the double-precision y-direction cosine

DW is the double-precision z-direction cosine

SUBROUTINES CALLED:

FLTRN, SQRT, SIN, COS

M2.2.17 DREAD

CALLING SEQUENCE:

WORD = DREAD(IBR,IRET)

FUNCTION:

DREAD is used to read numbers in free-form format. It returns a double-precision floating-point number. This routine is the basic number reading routine for the free-form reading package.

ARGUMENTS:

IBR can have two values.
IBR = 1 - read a new record and return the first number found.
IBR = 0 - return the next number found.

IRET = 2 will cause DREAD to terminate.

IRET ≠ 0 will cause a 0.0 to be returned. If the scan-ahead feature is activated and an 'END' is found while scanning, IRET will be set to 1. If an end of file is sensed while scanning, IRET will be set to 2.

SUBROUTINES CALLED:

ENFILE,Y0READ

COMMONS:

UNIT,QRDBUF

M2.2.18 DSET

CALLING SEQUENCE:

R = DSET (I)

FUNCTION:

DSET returns the double word at I as a double-precision floating point value.

ARGUMENTS:

I is the address of a double word containing a double-precision number.

M2.2.19 DTASET

CALLING SEQUENCE:

CALL DTASET (LOG,DSN,VOL)

FUNCTION:

DTASET returns the data set name and volume serial number pointed to by a logical unit number.

ARGUMENTS:

LOG is the FORTRAN logical unit number of the DD card.

DSN is the 44-character data set name returned.

VOL is the 8-character volume serial number returned.

SUBROUTINES CALLED:

GETFILE

M2.2.20 ECHECK

CALLING SEQUENCE:

CALL ECHECK (E,IGM,N6)

FUNCTION:

ECHECK verifies that the energy boundaries of a group structure are in descending order.

ARGUMENTS:

E is the array containing the group boundaries.

IGM is the number of energy groups.

N6 is the logical unit number on which the error messages are printed.

M2.2.21 ENERGY

CALLING SEQUENCE:

CALL ENERGY (E,IGM,N6)

FUNCTION:

ENERGY determines a set of energy-group boundaries for an IGM group neutron structure by calling subroutine BDYS. The boundaries are expected to reside on logical 47.

ARGUMENTS:

E is the array of group boundaries.

IGM is the number of energy groups.

N6 is the message unit number.

SUBROUTINES CALLED:

BDYS

M2.2.22 ENFILE

CALLING SEQUENCE:

CALL ENFILE

FUNCTION:

ENFILE is used by the free-form reading package to print an end-of-file message and stop when an end-of-file has been sensed.

COMMONS:

UNIT

M2.2.23 ERRO

CALLING SEQUENCE:

CALL ERRO (A,J)

FUNCTION:

ERRO is used to print an error message and stop.

ARGUMENTS;

A is a four-character error identifier.

J is an integer containing information relating to the error.

M2.2.24 ERRTRA

CALLING SEQUENCE:

CALL ERRTRA

FUNCTION:

ERRTRA gives a traceback of the calling chain. It is currently a dummy routine.

M2.2.25 EXPRN

CALLING SEQUENCE:

X = EXPRN ( )

FUNCTION:

EXPRN returns an exponentially distributed double-precision random number.

SUBROUTINES CALLED:

FLTRN, LOG

M2.2.26 EYENIT

CALLING SEQUENCE:

CALL EYENIT (NBLK,LBLK,NUNIT,D,LSKIP,BAL)

FUNCTION:

EYENIT is called to initialize a set of direct-access blocks. It is necessary on IBM systems, but may not be necessary on other systems. On UNIX systems, it removes any pre-existing dataset.

ARGUMENTS:

NBLK	number of blocks
LBLK	length of each block
NUNIT	FORTRAN logical unit number
D	scratch buffer array of length LBLK
LSKIP	number of blocks already existing
BAL	12-byte area where system data will be saved. *This area should be saved from the creation of the file to the destruction of the file.*

SUBROUTINES CALLED:

FILNAM

M2.2.27 E3

CALLING SEQUENCE:

Y = E3(X)

FUNCTION:

E3 returns the value of the E_3 function at the point x. $E_3(x) = \int_1^\infty \frac{e^{-xu}}{u^3}\, du$.

ARGUMENTS:

X is the point at which the value of the E_3 function is desired.

M2.2.28 FFPACK

CALLING SEQUENCE:

CALL FFPACK (ISTRNG,ICHAR,IPOS)

FUNCTION:

FFPACK is used to insert a character into a string of characters at a given position. FFPACK is used by the FIDO reading package (see Sect. M10) when transmitting character data.

ARGUMENTS:

ISTRNG is the string of 8 characters.

ICHAR is the character to be inserted.

IPOS is the position in ISTRNG at which ICHAR is to be inserted.

M2.2.29 FFPUN

CALLING SEQUENCE:

CALL FFPUN (X,N,N2)

FUNCTION:

FFPUN is used to punch a floating-point array in free-format input form. The data are punched on unit NPU, the first variable in COMMON /PUNIT/. The default unit number is 7.

ARGUMENTS:

X is the array to be punched.

N is the number of words to be punched.

N2 columns 73-76.

SUBROUTINES CALLED:

FLTFX

COMMONS:

PUNIT

M2.2.30 FFREAD

CALLING SEQUENCE:

CALL FFREAD (IN,K,V,NF,N5,N6,IPRTRG)

FUNCTION:

FFREAD is the free and fixed-field card translator for the FIDO input package. It reads a card at a time, returning the data and the number of entries read.

ARGUMENTS:

IN is the array used to hold the first subfield value of the three-subfield arrangement used by the FIDO input scheme. It generally contains the number of repeats, the array number, etc.

K is the array used to hold the second subfield in FIDO input scheme. It generally contains an operator, such as R for repeat, * for a floating-point array, etc.

V is an array used to hold the third subfield in the FIDO input scheme. It most often contains a data value.

NF is the number of entries in IN, K, and V.

N5 is the input logical unit number.

N6 is the print logical unit number.

IPRTRG is a print trigger flag signaling whether the input card images should be echoed to the print unit.

= 0 - do not echo.
>0 - do echo.

SUBROUTINES CALLED:

FFPACK

M2.2.31 FHLPR

CALLING SEQUENCE:

CALL FHLPR (CC,A,NOU)

FUNCTION:

FHLPR prints an eight-character block letter line.

ARGUMENTS:

CC is the carriage control character to be printed with the first line.

A is the eight-character string to be printed in block letters.

NOU is the logical unit number for the print.

COMMONS:

LETTER

SUBROUTINES CALLED:

YOTRNS

M2.2.32 FIDAS

CALLING SEQUENCE:

CALL FIDAS (D,LD,LPN,LOF,NER,N5,N6)

FUNCTION:

FIDAS reads a FIDO-type input data block into an arbitrary array. (See Sect. M10 for a description of FIDO-type input.)

ARGUMENTS:

D,LD are the arrays into which the floating point and the integer numbers are stored. These arrays would normally be the same.

LPN is the array containing the pointers to the beginning of each FIDO array in D and LD.

LOF is the offset to the 1$ or 1* array pointer in LPN.

NER is returned as the count of errors found in reading the current data block.

N5 is the input logical unit number.

N6 is the print logical unit number.

SUBROUTINES CALLED:

FFREAD

M2.2.33 FILNAM

CALLING SEQUENCE:

CALL FILNAM (FILE, PREFIX)

FUNCTION:

FILNAM generates a unique filename using the prefix.

ARGUMENTS:

FILE is the unique filename return upon successful completion.

PREFIX is the character string used in generating the unique filenames.

M2.2.34 FINDQA

CALLING SEQUENCE:

CALL FINDQA (PROGRAM,DATE,LIBRARY)

FUNCTION:

FINDQA returns the name of the current program, the date it was created, and the library it comes from. These data are used to print a QA table.

ARGUMENTS:

PROGRAM eight-character name of the current program

DATE eleven-character date PROGRAM was created

LIBRARY 44-character dataset name of the library containing PROGRAM

SUBROUTINES CALLED:

GETARG, GETMTM, LNBLNK, GETCWD

M2.2.35 FISCAP

CALLING SEQUENCE:

CALL FISCAP (ZA,EPF,EPC)

FUNCTION:

FISCAP is used to supply default values of energy per fission and energy per capture for a selected set of nuclides. It returns EPF and EPC unchanged if it has no data for the ZA specified. If EPF and/or EPC already have positive values, FISCAP will not change them.

ARGUMENTS:

ZA is 1000*Z+A for the nuclide for which data are to be supplied.

EPF is the energy per fission in watt-s/fission.

EPC is the energy per capture in watt-s/capture.

M2.2.36 FLTFX

CALLING SEQUENCE:

CALL FLTFX (X, IX, IEX)

FUNCTION:

FLTFX is used to convert a floating-point number to an integer and an exponent.

ARGUMENTS:

X is the floating point number to be converted.

IX is the integer derived from X.

IEX is the exponent derived from X.

M2.2.37 FLTRN

CALLING SEQUENCE:

X = FLTRN ( )

FUNCTION:

FLTRN returns a double-precision pseudo random number uniformly distributed between 0.0 and 1.0. The generator programs the algorithm described in Refs. B.1-5 for sixteen-bit computers.

M2.2.38 FLUX

CALLING SEQUENCE:

X = FLUX (E,EMAX,T,C2,EF,THETA,C1,IOPT)

FUNCTION:

FLUX supplies a flux value at E based on the other arguments. If IOPT = 1, the value is interpolated from a fast reactor spectrum. Otherwise, the spectrum is a combination of a fission spectrum to 1/E to Maxwellian at thermal.

ARGUMENTS:

E is the energy in eV at which the flux is desired.

EMAX is the upper energy in eV at which a Maxwellian spectrum is to be used.

T is the thermal temperature in eV of the Maxwellian spectrum.

C2 is the normalization factor for the Maxwellian spectrum.

EF is the upper limit in eV of the 1/E portion of the spectrum.

THETA is the temperature in eV of the fission spectrum used at high energies.

C1 is the normalization factor used for the fission spectrum.

IOPT selects the flux spectrum to be used. IOPT = 1 selects a ZPPR default spectrum. Otherwise, a Maxwellian-1/E-fission spectrum is used.

M2.2.39 FPUNCH

CALLING SEQUENCE:

CALL FPUNCH (N,L,LABL,IFORM)

FUNCTION:

FPUNCH is used to punch in free format the array N according to the data type specified by IFORM.

ARGUMENTS:

N is the array to be punched on unit NPU, the first variable in COMMON /PUNIT/. The default unit number is 7.

L is the length of the array.

LABL is an identifier to be punched on the output cards. If LABL<0, then the LABL and sequence number are not punched.

IFORM selects whether the data are to be punched as integers or floating-point numbers.
IFORM = 0 selects integers
IFORM = 1 selects floating point

COMMONS:

PUNIT

SUBROUTINES CALLED:

FLTFX, QZCNVT, BLANK

M2.2.40 FREAD

CALLING SEQUENCE:

WORD = FREAD(IBR,IRET)

FUNCTION:

FREAD returns a floating-point number read in free format.

ARGUMENTS:

See DREAD.

SUBROUTINES CALLED:

DREAD, Y0READ

COMMONS:

UNIT, QRDBUF

M2.2.41 FREECR

CALLING SEQUENCE:

CALL FREECR (LL)

FUNCTION:

Releases some of the array acquired by ALOCAT. This mechanism allows a program to keep only the amount of storage it needs to run. This program is currently a dummy routine.

ARGUMENTS:

LL is the negative of the number of words to be freed.

M2.2.42 GETFILE

CALLING SEQUENCE:

CALL GETFILE (NAME, FILE)

FUNCTION:

GETFILE returns the path for a given filename.

ARGUMENTS:

NAME is the given filename.

FILE is the full path to filename.

SUBROUTINES CALLED:

LNBLNK

M2.2.43 GETMS

CALLING SEQUENCE:

CALL GETMS

FUNCTION:

GETMS is used to transfer the data the SCALE driver supplies to labeled commons. It is called by SCALE control programs to isolate the communications with the driver. After the call to GETMS, the driver data are loaded into two labeled commons.

```
COMMON/CDATA/AC(40),IC(80),JPL,JDL
DOUBLE PRECISION AC
COMMON/CCDATA/JP,JD
CHARACTER JP*144,JD*96
```

AC, JC, JP, and JD are described in Sect. M1. JPL is the number of characters supplied in JP, and JDL is the number of characters supplied in JD.

COMMONS:

CDATA, CCDATA

M2.2.44 GNERGY

CALLING SEQUENCE:

CALL GNERGY (E,IGM,N6)

FUNCTION:

GNERGY sets the group boundaries of a gamma-group structure in E. It calls subroutine BDYS to access the boundaries that are expected to reside on logical 47.

ARGUMENTS:

E is the array of group boundaries.

IGM is the number of groups.

N6 is logical unit number for printed output.

SUBROUTINES CALLED:

BDYS

M2.2.45 GTISO

CALLING SEQUENCE:

CALL GTISO (U, V, W)

FUNCTION:

GTISO returns the direction cosines of an isotopically distributed random direction.

ARGUMENTS:

U is the x-direction cosine

V is the y-direction cosine

W is the z-direction cosine

SUBROUTINES CALLED:

FLTRN, SQRT, SIN, COS

M2.2.46 ICOMPA

CALLING SEQUENCE:

N = ICOMPA(S1,S2,LEN)

FUNCTION:

ICOMPA compares character string S1 of length LEN characters with string S2 and returns a value 1, 0, or -1-, depending on whether S1 is greater than, equal to, or less than S2 in the collating sequence. S1 is defined as equal to S2 if every character in S1 is equal to the corresponding character in S2. S1 is greater than S2 if the first character that is not equal to the corresponding character in S2 is further down the collating sequence.

ARGUMENTS:

S1 is the first-character string.

S2 is the second-character string.

LEN is the number of characters in S2 and S2.

M2.2.47 INQUIR

CALLING SEQUENCE:

CALL INQUIR (NUNIT,NXTREC)

FUNCTION:

INQUIR returns value of the next record on the direct-access file connected to NUNIT.

ARGUMENTS:

NUNIT FORTRAN logical unit number of the file.

NXTREC Next record on the file.

M2.2.48 INTIME,PRTIME

CALLING SEQUENCE:

CALL INTIME (IO)
CALL PRTIME (IO)

FUNCTION:

INTIME initializes the argument IO with the time left in the job step.

PRTIME computes the time used since IO and prints it in units of minutes.

ARGUMENTS:

IO is the time left in the job step in hundredths of a second at the call to INTIME.

SUBROUTINES CALLED:

JSTIME

M2.2.49 IO

CALLING SEQUENCE:

CALL IO (X,L,JUMP,NU)

FUNCTION:

IO is used to do short list input/output.

ARGUMENTS:

X is the array to be read or written.

L is the number of words in X.

JUMP selects reading or writing and whether or not the record is self-defining.
1 is a simple read.
2 is a self-defining read.
3 is a simple write.
4 is writing a self-defining record.
A self-defining record contains L as the first word.

NU is the logical unit number for the input/output.

M2.2.50 IOLEFT

CALLING SEQUENCE:

CALL IOLEFT(LEFT)

FUNCTION:

IOLEFT returns the number of input/output requests left before the system cancels the job. This routine performs a specialized function for the local Oak Ridge computer systems. A dummy routine returning a constant value of LEFT>0 is supplied with SCALE.

ARGUMENTS:

LEFT is the number of input/output requests left to the job before the system cancels it.

M2.2.51 IOWRT

CALLING SEQUENCE:

CALL IOWRT (OUTPT,PARNAM,IO,HOLLID)

FUNCTION:

IOWRT is used to print a line of information identifying the dataset connect to a logical unit number.

ARGUMENTS:

OUTPT	is the unit where the line is printed.
PARNAM	is a four-character identifier that indicates the input variable name used to set the logical unit number.
IO	is the logical unit number.
HOLLID	is a character string printed at the end of the line to further identify IO (less than 35 characters).

SUBROUTINES CALLED:

DTASET

M2.2.52 IO4

CALLING SEQUENCE:

CALL IO4 (MTX,LX,NLX,NTX,LEN,JUMP,NU)

FUNCTION:

IO4 is used to read or write the descriptor records for the transfer (2-D) arrays.

ARGUMENTS:

MTX is the array of mt numbers identifying the 2-D arrays.

LX is the array of maximum lengths of the 2-D arrays corresponding to MTX.

NLX is the array specifying the order of scattering of the 2-D arrays corresponding to MTX.

NTX is the array containing the number of temperatures of the 2-D arrays corresponding to MTX.

LEN is the number of entries in MTX, LX, NLX, and NTX.

JUMP selects whether the call is a read or a write (see IO).

NU is the logical unit number to be used.

M2.2.53 IREAD

CALLING SEQUENCE:

NUM = IREAD(IBR,IRET)

FUNCTION:

IREAD returns an integer read in free format.

ARGUMENTS:

See DREAD.

SUBROUTINES CALLED:

DREAD,Y0READ

COMMONS:

UNIT,QRDBUF

M2.2.54 ISET

CALLING SEQUENCE:

I = ISET (X)

FUNCTION:

ISET returns the integer stored at X.

ARGUMENTS:

X is the location of the integer ISET is to return.

M2.2.55 JDFJX

CALLING SEQUENCE:

CALL JDFJX (ID,NGN,NGG)

FUNCTION:

JDFJX is used to zero entries in the AMPX master library nuclide identifier record.

ARGUMENTS:

ID is the array containing control information about an AMPX master library nuclide.

NGN is the number of neutron groups.

NGG is the number of gamma groups.

M2.2.56 JLL1

CALLING SEQUENCE:

CALL JLL1 (IGM,IPM,IFTG,N,IHT)

FUNCTION:

JLL1 constructs an array, N, pointing to the beginning of each group in an expanded transfer array.

ARGUMENTS:

IGM is the number of neutron groups.

IPM is the number of gamma groups.

IFTG is the first thermal group.

N is the array of pointers returned.

IHT is the number of 1-D cross sections stored in the expanded array for each group.

M2.2.57 JOBNUM

CALLING SEQUENCE:

CALL JOBNUM (JNAME)

FUNCTION:

JOBNUM returns the eight-character jobname of the current job.

ARGUMENTS:

JNAME is the eight-character jobname.

SUBROUTINES CALLED:

GETNAM

M2.2.58 KI3

CALLING SEQUENCE:

Y = KI3(X)

FUNCTION:

KI3 returns the third-order Bickley function evaluated at its argument.

ARGUMENTS:

X is the point at which KI3 is evaluated.

M2.2.59 LABL

CALLING SEQUENCE:

CALL LABL (N,X,HEAD1,HEAD2)

FUNCTION:

LABL is used to print a page header, indexed table of an array.

ARGUMENTS:

N is the number of entries to be printed.

X is the array containing the entries to be printed.

HEAD1 and HEAD2 form the 16-character heading for each column printed.

COMMONS:

UNIT

M2.2.60 LCOMPR

CALLING SEQUENCE:

LFLAG = LCOMPR(STRING,CARRAY,NEL,INDX)

FUNCTION:

LCOMPR searches an array CARRAY for a match with STRING, and returns a value of true if a match is found. Only the number of characters supplied in STRING are compared. If a match is found, INDX is set to the index in CARRAY, where the match occurred, and STRING is set equal to CARRAY(INDX).

ARGUMENTS:

STRING is the string for which a match is checked.

CARRAY is the array of strings containing possible matches.

NEL is the number of elements in CARRAY.

INDX is the index at which a match occurred.

M2.2.61 LESTER

CALLING SEQUENCE:

CALL LESTER (E,MAXG,P,IOPT,T,THETA,AKT,FCUT)

FUNCTION:

LESTER is used to generate a flux spectrum based on the arguments in an arbitrary group structure.

ARGUMENTS:

E	is the array of energy bounds.
MAXG	is the number of groups.
P	is the array of fluxes.
IOPT	selects the basic spectrum. IOPT = 0 selects a fission to 1/E to Maxwellian spectrum. IOPT = 1 selects a fast reactor spectrum.
T	is the temperature for the Maxwellian in Kelvin.
THETA	is the temperature for the fission spectrum in eV.
AKT	is the multiplier on kT for the Maxwellian-1/E joining point.
FCUT	is the fission-1/E joining point.

SUBROUTINES CALLED:

FLUX

M2.2.62 LISTQA

CALLING SEQUENCE:

CALL LISTQA (OUTPT)

FUNCTION:

LISTQA prints a table of information useful for QA purposes.

ARGUMENTS:

OUTPT is the unit number the table will be printed on.

SUBROUTINES CALLED:

FINDQA, JOBNUM, DATE_AND_TIME, VERGET, MACHNAME

M2.2.63 LNBLNK

CALLING SEQUENCE:

L = LNBLNK (STR)

FUNCTION:

LNBLNK returns the position of the last nonblank character in a string.

ARGUMENTS:

STR is the character string to be searched.

M2.2.64 LRDERR

CALLING SEQUENCE:

LFLAG = LRDERR( )

FUNCTION:

LRDERR returns the current value of the free-form reading error flag, and resets it to false.

ARGUMENTS:

None.

COMMONS:

QRDBUF

M2.2.65 LREAD

CALLING SEQUENCE:

LFLAG = LREAD(IBR,IRET)

FUNCTION:

LREAD returns a true value if the next character in the free-form reading package buffer is a numeric digit. Otherwise, it returns a false value.

ARGUMENTS:

IRET = 2 will cause LREAD to print a message and stop. Other values of the arguments are ignored.

M2.2.66 MESAGE

CALLING SEQUENCE:

CALL MESAGE (LINE1,NOU)

FUNCTION:

MESAGE prints a banner page in block letters consisting of the eight-character LINE1, the jobname, the date, and the time of day. This page is followed by a table of information useful for QA purposes.

ARGUMENTS:

LINE1 is an eight-character name printed as the first line of block letters on the banner page.

NOU is the logical unit number of the print file.

SUBROUTINES CALLED:

FHLPR,JOBNUM,DATIM,LISTQA

M2.2.67 MGCWRD

CALLING SEQUENCE:

CALL MGCWRD (MW,IIG,IMX,IMN,M)

FUNCTION:

MGCWRD is used to either decipher or construct a magic word.

ARGUMENTS:

MW is the magic word. If it is not zero, MGCWRD sets the other arguments by deciphering it. If it is zero, MGCWRD constructs a new magic word from the other arguments: MW=IMN*1000000+IMX*1000+IIG.

IIG is the current group number.

IMX is the maximum group number that can scatter to IIG.

IMN is the minimum group number that can scatter to IIG.

M is the length of the cross-section string for IIG: M=IMX–IMN+1.

M2.2.68 MOVE

CALLING SEQUENCE:

CALL MOVE (A,B,L)

FUNCTION:

MOVE is used to move L words from B to A.

ARGUMENTS:

A is the destination of the move.

B is the source for the move.

L is the number of words to be moved.

M2.2.69 MWLIST

CALLING SEQUENCE:

CALL MWLIST (X,LA,IHT,ITRG)

FUNCTION:

MWLIST is used to print an AMPX-formatted transfer array.
All arguments must be supplied by the calling program.

ARGUMENTS:

X is the array to be printed.

LA is the length of the array.

IHT is the position of the total cross section in each group string.

ITRG is a flag selecting whether the whole array or only the 1-D cross sections will be printed. ITRG = 0 prints the whole array, ITRG = 1 prints only the 1-D cross sections in the array.

SUBROUTINES CALLED:

MGCWRD

M2.2.70 MWLS

CALLING SEQUENCE:

CALL MWLS (X,LA,IHT,TEV,MT,NOU,NL,IDR)

FUNCTION:

MWLS is used to title and print an AMPX-formatted transfer array.
All arguments must be supplied by the calling program.

ARGUMENTS:

X is the array to be printed.

LA is the length of the array.

IHT is the position of the total cross section within a group string.

TEV is the temperature of the matrix (in eV).

MT is the identifier of the array to be printed.

NOU is the logical unit number of the print file.

NL is the order of Legendre expansion for the array to be printed.

IDR is the ID record for the array to be printed.

SUBROUTINES CALLED:

MGCWRD

M2.2.71 OPENDA

CALLING SEQUENCE:

CALL OPENDA (NBLKS,LBLKS,TYPE,ASSVAR,NUNIT,BUFFER)

FUNCTION:

OPENDA is used to open a file for the random-access package and to initialize the file if necessary. It can return the length of a block when used to open an old file. Although written in FORTRAN, there are still system dependencies that must be dealt with in this routine.

ARGUMENTS:

NBLKS is the number of blocks of direct access space to be initialized. If TYPE = 'O', the number of blocks in the dataset is returned here.

LBLKS is the size of a block. If TYPE = 'O', the size is returned here in units of words.

TYPE selects the type of open to be done. TYPE = 'O' selects opening an old dataset. No initialization is done. TYPE = 'U' selects the size unit to be in words. If the dataset already exists, OPENDA deletes it and opens a new dataset. TYPE = 'L' or 'E' selects the size unit to be in bytes. Otherwise, this is the same as 'U'.

ASSVAR is the associated variable for this file.

NUNIT is the logical unit number for this file.

BUFFER is a scratch array used in initializing the file. It must be at least LBLKS long.

SUBROUTINES CALLED:

EYENIT

M2.2.72 OPNFIL

CALLING SEQUENCE:

CALL OPNFIL (NUN,STATUS,FORM,FILE)

FUNCTION:

OPNFIL is used to isolate open statements so that all system dependencies can be contained in a single subroutine.

ARGUMENTS:

NUN is the unit number to be opened.

STATUS is the status of open (i.e, 'NEW', 'OLD', 'UNKNOWN').

FORM is the format of data, 'FORMATTED' or 'UNFORMATTED'.

FILE is the filename for unit.
Not used on IBM, for other systems.
'DEFAULT' – generates a filename based on NUN.
'$XXX' - generates a unique filename, _XXXnnnn, where nnnn is a number making the name unique.
Anything else is used as a filename.

SUBROUTINES CALLED:

FILNAM

M2.2.73 PRT1D

CALLING SEQUENCE:

CALL PRT1D (X,NG,NX,NOU)

FUNCTION:

PRT1D is used to print a 1-D array of cross sections (total absorption, etc.) with their identifiers. It will compress multiple lines that are the same to reduce the amount of output.

ARGUMENTS:

X is the array of 1-D cross sections.

NG is the first dimension of X. NG is the number of groups+1.

NX is the number of 1-D cross-section sets in X.

NOU is the logical unit number of the print file.

M2.2.74 PULL

CALLING SEQUENCE:

CALL PULL (MIN,SEC,*RETN)

FUNCTION:

PULL is used to set a CPU time interval. When the interval expires, an interrupt occurs which allows execution to be continued along a different path. This is currently a dummy routine.

ARGUMENTS:

MIN refers to minutes to be set in the interval.

SEC refers to seconds to be set in the interval if MIN and SEC are 0, a previously set interval is cancelled.

*RETN is a statement where execution is to be transferred when the interval expires.

M2.2.75 QZCNVT

CALLING SEQUENCE:

CALL QZCNVT (I, LDATA, LL, PLS)

FUNCTION:

QZCNVT is used to convert a binary integer to character.

ARGUMENTS:

I is the number to be converted to character.

LDATA is the character string into which the answer is stored.

LL is the length of the answer.

PLS is the character to be used as a plus sign.

M7.2.76 QZSCAN

CALLING SEQUENCE:

CALL QZSCAN (LDATA,LL, LT, IEX)

FUNCTION:

QZSCAN is used to delete trailing zeroes by modifying the exponent.

ARGUMENTS:

LDATA is the character string into which the answer is stored.

LL is the length of the answer.

LT is the length of the string from which trailing zeroes are to be removed.

IEX is the exponent.

M2.2.77 Q0READ

CALLING SEQUENCE:

CALL Q0READ (D,LP,LOF,NER,NIN,NOU)

FUNCTION:

Q0READ is used to read a data block from a binary file with FIDO-type array identifiers.

ARGUMENTS:

D is the array into which the numbers are to be read.

LP is the array of pointers to the beginning of each array in D.

LOF is the offset to the number 1 array in LP.

NER returns the number of errors encountered in reading the data block.

NIN is the logical unit number of the binary file.

NOU is the logical unit number of the print file.

SUBROUTINES CALLED:

IO

M2.2.78 READSG

CALLING SEQUENCE:

CALL READSG (X,M,NIN,IFORM)

FUNCTION:

READSG is used to read an array of cross sections from an ANISN cross-section library.

ARGUMENTS:

X is the array of ANISN-formatted cross sections.

M is the size of the array.

NIN is the logical unit number from which the array is read.

IFORM selects the form of the ANISN cross sections on NIN.
IFORM > 0 means the cross sections are in fixed FIDO format.
IFORM = 0 means the cross sections are in free-field FIDO format.
IFORM < 0 means the cross sections are in binary form.

SUBROUTINES CALLED:

IONUMS,RCRDLN,FREAD,AREAD

COMMONS:

RETCDE

M2.2.79 RECTRY

CALLING SEQUENCE:

CALL RECTRY (X,LIM,NOU,NT1,NT2,NS,NT)

FUNCTION:

RECTRY is used to write a correct table of contents on an AMPX master library NT1 and/or an AMPX working library NT2.

ARGUMENTS:

X is a scratch array.

LIM is the length of X.

NOU is the logical unit number of the print file.

NT1 is the logical unit number of the master library (0 means skip).

NT2 is the logical unit number of the working library (0 means skip).

NS,NT are logical unit numbers of scratch files.

SUBROUTINES CALLED:

IOLEFT,JSTIME,COPY,JDFJX

M2.2.80 RESETM

CALLING SEQUENCE:

CALL RESETM

FUNCTION:

RESETM is used by control programs to reset the data communicated between the SCALE driver and the program. See GETMS.

COMMONS:

CDATA,CCDATA

M2.2.81 RMUNIT

CALLING SEQUENCE:

CALL RMUNIT (NUN)

FUNCTION:

RMUNIT deletes the dataset associated with logical unit number NUN.

ARGUMENTS:

NUN to logical unit number to delete the associated dataset.

M2.2.82 RNDIN

CALLING SEQUENCE:

CALL RNDIN (R)

FUNCTION:

RNDIN sets the seed for the next random number.

ARGUMENTS:

R is the seed. It is an eight-byte number.

M2.2.83 RNDOUT

CALLING SEQUENCE:

CALL RNDOUT (R)

FUNCTION:

RNDOUT returns the seed for the next random number.

ARGUMENTS:

R is the seed. It is an eight-byte number.

M2.2.84 SCANON

ENTRIES:

SCANON,SCANOF,ALLOWC,RESETC,SETBIN,RESETB,IONUMS,RCRDLN,GETPTR,
RSTPTR

CALLING SEQUENCE:

```
CALL SCANON
CALL SCANOF
CALL ALLOWC
CALL RESETC
CALL SETBIN
CALL RESETB
CALL IONUMS(NIN,NOU,NINOLD,NOUOLD)
CALL RCRDLN(LEN,LENOLD)
CALL GETPTR(PTR)
CALL RSTPTR(PTR)
```

FUNCTION:

SCANON turns on the feature in the free-form reading package to scan ahead to the next entry and check if it is `END'.

SCANOF turns off the scan-ahead feature.

ALLOWC turns off the invalid character check when reading numbers. With the check turned off, any character not valid in a numeric field will act as a terminator for the field.

RESETC turns the invalid character check on. With the check turned on, any character not valid in a numeric field will cause an error message to be printed and the character will be replaced by a 0.

SETBIN turns on the binary reading flag.

RESETB turns off the binary reading flag. This mode is for reading free-form character records.

IONUMS sets new input and output unit numbers and returns the previous unit numbers.

RCRDLN sets a new logical record length, and returns the previous one.

GETPTR returns the current pointer in the input buffer.

RSTPTR sets the current pointer in the input buffer.

ARGUMENTS:

NIN is the new input logical unit number.

NOU is the new output logical unit number.
If NIN or NOU is 0, the unit number is not changed.

NINOLD is where the previous input logical unit number is returned.

NOUOLD is where the previous output logical unit number is returned.

LEN is the new logical record length (LEN<253).

LENOLD is where the previous logical record length is returned.

PTR is the pointer in the input buffer.

M2.2.85 SET

CALLING SEQUENCE:

X = SET (I)

FUNCTION:

SET returns the floating point number stored at I.

ARGUMENTS:

I is the location of the floating point number SET is to return.

M2.2.86 SFLRA

CALLING SEQUENCE:

X = SFLRA ( )

FUNCTION:

SFLRA returns a double-precision random number uniformly distributed between -1.0 and 1.0.

SUBROUTINES CALLED:

FLTRN

M2.2.87 SHELC

CALLING SEQUENCE:

CALL SHELC (R,TAU,TOI,TOO)

FUNCTION:

SHELC is used to generate the transmission probabilities for a cylindrical shell.

ARGUMENT:

R is the ratio of inner radius to outer radius of the shell.

TAU is the thickness of the shell (in mean-free paths).

TOI is the transmission from the outside to the inside of the shell.

TOO is the transmission from the outside to the outside of the shell.

SUBROUTINES CALLED:

KI3,COS,SQRT

M2.2.88 SNST

CALLING SEQUENCE:

CALL SNST (CX,L,C,ITL,IHT,IHS,ITOT,GR,LL)

FUNCTION:

SNST is used to move cross-section data from an AMPX-formatted transfer array to an ANISN-formatted array. It can also make a transport correction to the within-group scatter cross section.

ARGUMENTS:

CX is the magic word 2-D array.

L is the length of CX.

C is the ANISN array.

ITL is the table length of the ANISN array.

IHT is the position of the total cross section in a cross-section string of the ANISN array.

IHS is the position of the within-group scatter cross section within a cross-section string of the ANISN array.

ITOT is the number of groups.

GR is the array containing the transport corrections to be applied to the within-group cross sections.

LL is the order of scattering of the array.

SUBROUTINES CALLED:

MGCWRD

M2.2.89 STOP

CALLING SEQUENCE:

CALL STOP (MESSAGE,STPCDE,NOU,TRCFLG,P1,...PN)

FUNCTION:

STOP is used to print a message, optionally print a trace back, print optional data, and optionally stop.

ARGUMENTS:

MESSAGE is the message to be printed. It can be no longer than 132 characters. If it is less than 132 characters, it must be terminated by a $ symbol. This argument is required, but the calling sequence can be terminated after this argument, or any subsequent argument, in which case defaults are supplied for the missing arguments.

STPCDE is a stop number, defaulted to 0. If it is greater than 0, STOP will execute a stop instead of returning to the calling program.

NOU is the logical unit number of the print file. The default is the standard error message file.

TRCFLG selects a trace back if it is greater than 0. The default is 0.

P1,...,PN are optional arguments which will be printed following MESSAGE. Printing of these arguments is not currently implemented on UNIX systems.

M2.2.90 TIMFAC

CALLING SEQUENCE:

CALL TIMFAC(FACTOR)

FUNCTION:

TIMFAC supplies a machine-dependent factor used to scale cpu times in a program so that roughly equivalent amounts of computation can be done on different machines using the same input time limit. The SCALE version sets FACTOR = 1.0.

ARGUMENTS:

FACTOR is the machine-dependent factor used to scale the time.

M2.2.91 VERGET

CALLING SEQUENCE:

L=VERGET(PGM,CDATE,CLIB,SYSTEM,SVERS,PROG,PVERS)

FUNCTION:

VERGET is used to return the system name, system version, program name, and program version for a given module created on a given date and residing in a given library.

ARGUMENTS:

PGM is the accessed name of the module.

CDATE is the date PGM was created.

CLIB is the name of the library where PGM resides.

SYSTEM is the name of the system.

SVERS is the version of the system.

PROG is the program name of PGM.

PVERS is the version of PGM.

SUBROUTINES CALLED:

STOP

M2.2.92 WOT

CALLING SEQUENCE:

CALL WOT(X,NCOL,NROW,LG,TOP1,TOP2,TOP3)

FUNCTION:

WOT is used to print a 1-, 2-, or 3-D array in a columnar output form with headings supplied as TOP1, TOP2, and TOP3. It will compress out lines that are the same to reduce the amount of output.

ARGUMENTS:

X	is the array to be printed.
NCOL	is the number of columns in X (1 if X is a vector).
NROW	is the number of rows in X.
LG	is the third dimension of X (1 if X is less than 3 dimensions).
TOP1	is the heading for the row index.
TOP2	is the heading for the columns.
TOP3	is the page heading for the third dimension.

M2.2.93 WOT8

CALLING SEQUENCE:

CALL WOT8 (A1,L1,A2,L2,A3,L3,A4,L4,A5,L5,A6,L6,A7,L7,A8,L8,NOU)

FUNCTION:

WOT8 is used to print up to eight arbitrary-length vectors as eight columns down a page. Numbers greater than a parameter, LRGINT, are assumed to be floating point, and are printed as such. Numbers less than LRGINT are printed as integers.

ARGUMENTS:

An is the n*th* vector.

Ln is the length of the n*th* vector. If Ln=0, then the n*th* vector is omitted.

NOU is the logical unit number of the print file.

M2.2.94 WRTID

CALLING SEQUENCE:

CALL WRTID (ID,N6)

FUNCTION:

WRTID is used to print a labeled table of the data in an AMPX master library nuclide identifier record.

ARGUMENTS:

ID is the ID record from an AMPX master library.

N6 is the logical unit number of the print file.

M2.2.95 WRTWID

CALLING SEQUENCE:

CALL WRTWID (ID, N6)

FUNCTION:

WRTWID is used to print a labeled table of the data in an AMPX working library nuclide identifier record.

ARGUMENTS:

ID is the nuclide identifier record from the AMPX working library.

N6 is the logical unit number of the print file.

SUBROUTINES CALLED:

SET

M2.2.96 XTENDA

CALLING SEQUENCE:

CALL XTENDA (BUFFER,NBLK,NUNIT)

FUNCTION:

XTENDA is used to add blocks to (extend) a random-access file. For a UNIX file system, this involves incrementing a limit.

ARGUMENTS:

BUFFER is a scratch array used to initialize the new blocks. BUFFER must be at least as long as a block.

NBLK is the number of new blocks to be added.

NUNIT is the logical unit number of the random-access file.

SUBROUTINES CALLED:

EYENIT

M2.2.97 XUFLOW

CALLING SEQUENCE

CALL XUFLOW (IFLAG)

FUNCTION:

XUFLOW is a dummy replacement for a deck to cause underflows to be ignored.

ARGUMENTS:

IFLAG is a flag turning underflow detection on [1] or off [0].

M2.2.98 YREAD

CALLING SEQUENCE:

CALL YREAD (DD,LD,LIM,IT,LERR)

FUNCTION:

YREAD is used to read an array using the free-form reading package while allowing interpolation, filling, skipping, multiple repeats, and arbitrary indexing. (See Sect. M3 for a more complete description.)

ARGUMENTS:

DD,LD	is the array to be read. DD is used for floating-point numbers and LD for integers.
LIM	is the number of entries in the array.
IT	selects what kind of data are being read. IT = 0 selects integers. IT = 1 selects single-precision floating-point numbers. IT = 2 selects double-precision floating-point numbers.
LERR	logical flag that is set true if an attempt is made to store data outside the DD or LD array.

SUBROUTINES CALLED:

DREAD,AREAD

COMMONS:

UNIT,QRDBUF

M2.2.99 Y0READ

CALLING SEQUENCE:

CALL Y0READ (CBUF,LBUF,IRET)

FUNCTION:

Y0READ is used to read the next logical record for the free-form reading package.

ARGUMENTS:

CBUF	is the array into which the record is read.
LBUF	is the length of the record.
IRET	is set to 2 if scan ahead is activated and an end of file is sensed.

SUBROUTINES CALLED:

ENFILE

COMMONS:

UNIT,QRDBUF

M2.2.100 Y0TRNS

CALLING SEQUENCE:

CALL Y0TRNS(CARD,LBUF)

FUNCTION:

Y0TRNS translates a character array from upper to lower case, or from lower to upper case, depending on the system it was compiled on.

ARGUMENTS:

CARD is the character array to be translated.

LBUF is the number of characters in CARD.

M2.2.101 ZREAD

CALLING SEQUENCE:

D=ZREAD(IBR,IRET)

FUNCTION:

ZREAD is used to read a hexadecimal number in free form and return it as a double-precision number.

ARGUMENTS:

See DREAD.

SUBROUTINES CALLED:

Y0READ,ENFILE

COMMONS:

UNIT,QRDBUF

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M2.A C LANGUAGE ROUTINES

The following routines are provided for UNIX systems. They may require modification to work correctly on different UNIX systems.

CALACT - A routine to provide an interface between ALOCAT and the UNIX system MALOCS routine

EXECUTE - A routine to provide an interface between a FORTRAN routine and a system call on UNIX systems.

EXIT - A routine to provide an interface to the UNIX system exit routine.

GETMTM - A routine that returns the creation date of a file

GETNAM - A routine to return the login name of the user

H7LIB - Routines for HEATING7

JSTIME - A routine to return the CPU time left to a process before it is cancelled.

MACHNAME - A routine to return the machine name of the machine being executed on.

PUTENV - A routine to set an environment variable

RETNTM - A routine to return the current *date* and *time*

M2.B AMPX SUBROUTINES

Subroutine	Used by these modules
BSQ	ALE
EBLIST	RADE
END	LAVA
FILL	
FILLY	ALE, AJAX, ALPO, RADE, WAX
LEGE	RADE
NCK	ALE, AJAX, ALPO, WAX
NOTE	AJAX, WAX
P1D	ALE
RD4	RADE
SUMX	RADE

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SCALE FREE-FORM READING ROUTINES

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ABSTRACT

The SCALE free-form reading routines are a set of subroutines for use by programs in the SCALE system to read input from cards in an unstructured manner. This document provides information for a programmer who wishes to use these routines.

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M3.1 INTRODUCTION

A set of free-form data reading routines has been developed to facilitate the use of free-formatted data input. These routines are used by the control programs to read the standard composition data and related data. Some of the functional modules such as KENO V.a and HEATING also make extensive use of these routines. This document is intended to provide guidance to a programmer desiring to use these routines in a program. Section M3.2 explains the conventions used to input data, and Sect. M3.3 contains information necessary for a programmer to use the routines.

M3.2 DATA INPUT CONSIDERATIONS

The free-form reading routines allow alphanumeric data, floating-point data, and integer data to be entered in a free-formatted manner. All columns of any record may be used; and data, with certain exceptions noted below, can start or end in any column. A single data entry cannot be started on one record and extend onto the next record, however.

Any alphanumeric data entry is terminated by one or more blanks or an equal sign, depending on the first argument supplied to the reading routine. Any numeric data entry will be terminated when a blank or a comma is encountered. The use of an E as an exponent does allow a single imbedded blank after the E. An exponent is limited to two digits, and the number being read is terminated with the second digit. Therefore, for this case only, another number can be started immediately following the second digit of the exponent without an intervening blank or comma. Decimal data may be entered as in FORTRAN input: e.g., 1.733-4, 1.733E-04, or 0.0001733 are the same as 1.733×10^{-4}; 1.733+4, 1.733E+4, 1.733E4, and 17330.0 are the same as 1.733×10^{4}. Integers may be entered for floating-point data (i.e., 10 will be interpreted as 10.0). Similarly, floating-point data may be entered for integers. Thus, 1.733E+4 would be interpreted as 17330, and 1.733E-4 would be interpreted as zero.

The free-form routines have provisions for multiple entries of the same data value. This step is done by entering the number of repeats, followed by an R, *, or $, followed by the data value to be repeated. For example, 5R2, 5*2, or 5$2 enters five successive 2s in the input data. Blanks are not allowed between the number of repeats and the repeat flag (R,*,$). However, a blank is allowed between the repeat flag and the data item to be repeated. Multiple zeros may be specified by entering nZ, where n is the number of zeros to be repeated. No blanks should be placed between the n and the Z, and the nZ must be separated from the rest of the data by one or more blanks.

All numeric data are read in double precision and are then converted to the desired form. Exponent indicators can be either a D or an E. The default method of terminating a data field is one or more blanks or a comma. A comma must immediately follow the number if it is used as a terminator (i.e., 5.6, should be used to enter the number 5.6 as data; 5.6 , results in two numbers, 5.6 and 0). Thus, commas can be used to enter zeros. 5.6,,,,,8.0 enters 6 numbers as data-5.6, four zeros, and 8.0 (the comma immediately after the 5.6 terminates that number and does not cause an entry of zero into the data). Similarly, both 5.6 ,,,,,8.0 and 5.6 , , , , , 8.0 enter seven numbers as data-5.6, five zeros and 8.0.

All data are translated to lowercase before being passed to the calling routine.

M3.3 PROGRAMMING CONSIDERATIONS

When using the free-form reading routines in a program, it is important to be aware of the different types of routines that are available in the package. Routines are available to activate desired features, to do the actual reading, and "transparent" routines that are used internally. These routines and their arguments are listed in Tables M3.1 through M3.7.

If the programmer desires to use the word END to terminate a block of data, SCANON must be called to activate the scan-ahead feature. Once SCANON has been activated, the scan-ahead feature remains in effect until it is inactivated by calling SCANOF. If the scan-ahead feature is active, the second argument, IRET, of the reading routine (see Tables M3.2 and M3.5) will be returned with a value of 1 whenever the next piece of data to be read is the word END. The argument IRET will be returned with a value of 2 if an end-of-file is the next piece of information to be read. Note: IRET should be initialized to zero before the very first read is done.

The first argument, IC, is used to communicate to the reading routine information regarding the means of reading data. This step is explained in greater detail in Tables M3.2 and M3.4. It may be advantageous to create a common that contains preset values of IC for use in the call statements.

Subroutine ALLOWC can be called to force termination of a numeric entry whenever any character that is illegal in a numeric field is encountered. Once invoked, this feature remains in effect until it is inactivated by calling RESETC.

The default record length is set at 80 columns. If it becomes desirable to set the record length at some value less than or equal to 252, this can be accomplished by calling RCRDLN. The new record length remains in effect until RCRDLN is called to set a different record length.

Under certain conditions it is desirable to be able to read unformatted data. This can be achieved by calling SETBIN. Once activated, this feature remains in effect until it is inactivated by calling RESETB. When this feature has been activated, unformatted records of the current record length are read from the input file. The reading routines then do no conversion, but simply return the next word (or two words for double precision) from the record.

Subroutine YREAD allows reading a whole array of numbers using free-form input. In addition to repeating numbers, capabilities are provided for various sequence repeats, interpolations, filling the array, and entering or overriding specific locations in the array in a manner similar to FIDO-type input (see Sect. M10). Table M3.8 lists the various data entry options.

Table M3.1 Routines to activate features

Subroutine name	Means of utilization	Purpose
SCANON	CALL SCANON	This routine is used to activate the scan-ahead feature that allows the program to scan ahead for an 'END'
SCANOF	CALL SCANOF	This disables the scan-ahead feature
IONUMS	CALL IONUMS (II,JJ,KK,LL)	This subroutine is used to change the input and output unit numbers II is the unit to be used for input (new input unit, default = 5) JJ is the unit number to be used for output (new print unit, default = 6) KK is used to return the old input unit number LL is used to return the old output unit number
RCRDLN	CALL RCRDLN (LIN,LO)	This subroutine is used to change the number of columns in a record and thereby ignore any information past column LIN LIN is the new number of columns to be considered in a record (≤ 252) LO is the previous value of the number of columns in a record (default = 80)
SETBIN	CALL SETBIN	This subroutine is used to set a flag that causes data reading to be unformatted. This feature remains in effect until RESETB is called
RESETB	CALL RESETB	This subroutine sets a flag that causes data reading to be free-form (disables the SETBIN feature)
ALLOWC	CALL ALLOWC	A call to this subroutine causes the termination of a numeric data field whenever any character that is illegal in a numeric field is encountered; i.e., it treats all such characters the way it treats a comma during normal numeric reading. This feature remains in effect until RESETC is called
RESETC	CALL RESETC	This subroutine resets a flag to disable the ALLOWC feature
GETPTR	CALL GETPTR (I)	This subroutine returns the index of the next character in the current record in I
RSTPTR	CALL RSTPTR (I)	This subroutine sets the index of the next character in the current record to I

Table M3.2 Alphanumeric reading routines

Function name	Means of utilization	Type of data
AREAD	Variable name = AREAD(IC,IRET)	Alphanumeric data, 4 characters at a time
CREAD	Variable name = CREAD(IC,IRET)	Alphanumeric data, 8 characters at a time

Table M3.3 Alphanumeric reading arguments

Value of IC	Response
-1	Returns the last character transmitted
0	Returns the next 4 characters – no scan-ahead capability
1	Read a new record and return the first 4 columns of the new record – no scan-ahead capability
2	Skip to the first nonblank character and return 4 characters – terminate at a double blank or an = If less than 4 characters were found prior to the double blank or =, the remaining characters are padded with blanks Scan ahead for END may be enabled
3	Returns the next 4 characters and terminates at either a single or double blank, depending on whether it follows an AREAD with IC=4 or 2, or an =. If less than 4 characters were read, the remaining characters are padded with blanks Scan ahead for END may be enabled
4	Skips to the first nonblank character and returns 4 characters – terminates at a single blank or an = Scan ahead for END may be enabled
Value of IRET	**A value of zero is always returned if the SCAN feature is not active**
0	Nonblank characters (not END) were found
1	END was found (SCAN feature enabled)
2	Found an end-of-file (SCAN feature enabled)

Table M3.4 Numeric data reading routines

Function name	Means of utilization	Type of data
DREAD	Variable = DREAD(IC,IRET)	Double-precision data
FREAD	Variable = FREAD(IC,IRET)	Floating-point data
IREAD	Variable = IREAD(IC,IRET)	Integer data
ZREAD	Variable = ZREAD(IC,IRET)	Double-precision hexadecimal data

Table M3.5 Numeric reading arguments

Value of IC	Response
0	Returns the next number
1	Reads a new record and returns the next number
Value of IRET	**A value of zero is always returned if the SCAN feature is not enabled**
0	Nonblank characters (not END) were found following the current number
1	END was found as the next entry after the current number
2	An end-of-file was encountered in scanning for END

Table M3.6 Miscellaneous reading routines

Name	Means of utilization	Purpose
LREAD	Variable = LREAD(IC,IRET)	This logical function returns a true if the next character is a numeric character and false if the next character is nonnumeric. It does not do any actual reading, but may cause new record(s) to be read
YREAD	CALL YREAD(A,A,NUM,ITP)	To load an array of numeric data that consists of integer or floating-point data in single or double precision. A is the array and is entered in the argument list twice. NUM is the length of the array
LRDERR	Variable = LRDERR( )	This logical function returns the current value of the reading error flag, and resets it to false

Table M3.7 Arguments for LREAD and YREAD

Argument	Explanation
IC	This argument is not used
IRET	If IRET = 2, ENFILE is called; otherwise, this argument is ignored
A	The array to be loaded by YREAD, integer, or floating point
NUM	The length of the array A
ITP	ITP = 0 indicates that integer data are to be loaded into the array A
	ITP = 1 indicates that single-precision floating-point data are to be loaded into the array A
	ITP = 2 indicates that double-precision floating-point data are to be loaded into the array A

Table M3.8 Data input options for YREAD

Count field	Option field	Data field	Function
		j	Stores j at the current position in the array
	F	j	Fills the remainder of the array with the number j, starting with the current position in the array
	A	j	Sets the current position in the array to j
i	S		Increments the current position in the array by i. (This allows skipping i positions. i may be positive or negative)
i	Q	j	Repeats the previous j entries i times. The default value of i is 1
i	N	j	Repeats the previous j entries i times inverting the sequence each time. The default value of i is 1
i	B	j	Back i entries. From that position, repeat the previous j entries in reverse order. The default value of i is 1
i	I	j k	Provides the end points, j and k, with i entries linearly interpolated between them (i.e., a total of i+2 points). At least one blank must separate j and k. When used for an integer array, the I option should only be used to generate integer steps [i.e., (k-j)/(i+1) should be a whole number]
i	L	j k	Provides the end points, j and k, with i entries logarithmically interpolated between them (i.e., a total of i+2 points). At least one blank must separate j and k
i	Z		Enters i zeros
i	R	j	Repeat j i times
i	*	j	Repeat j i times
i	$	j	Repeat j i times
i	P	j	Alternately stores j and -j in the next i positions of the array
	T		Terminates the data reading for the array

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SCALE CROSS-SECTION LIBRARIES

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ABSTRACT

This document briefly describes the cross-section libraries available in the SCALE code system. Included are the background of each library, the intended use of the library, and information relating to general experience with the library. The energy group bounds of the library are given in a manner that allows a quick comparison of the different libraries available. This document is intended as a companion document and supplement to Sect. M8, which describes the Standard Composition Library.

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M4.1 INTRODUCTION

The SCALE control modules are designed to allow complex analyses using simple input descriptions. Each shielding or criticality control module (1) uses the Standard Composition Library (see Sect. M8) for specifying the materials and mixtures used in a calculation and (2) provides automatic problem-dependent cross-section preparation prior to problem execution via the functional modules. This section describes the cross-section libraries currently available in the SCALE system. There are nine cross-section libraries distributed with SCALE, eight of which are automatically available in the SCALE system.

Six of these libraries were designed primarily for criticality analysis. The 218-group library is a fine-group library derived from ENDF/B-IV data. The library contains 140 fast groups and 78 thermal groups and includes explicit resonance data in the resolved resonance range. No unresolved resonance data are available in the library. The 27-group library (27GROUPNDF4) is the broad-group library collapsed from the 218-group library and has 14 fast and 13 thermal groups. This library has been extensively validated against critical experiments. The 27-group depletion library (27BURNUPLIB) contains the same data as 27GROUPNDF4 plus pre-release ENDF/B-V data for a large number of fission products. This was the first library designed for use with the SAS2 depletion/decay sequence. The 238-group library (238GROUPNDF5) is the most complete library in SCALE. This library contains data for all ENDF/B-V nuclides and has 148 fast and 90 thermal groups. Most resonance nuclides in the 238-group library have resonance data in the resolved resonance region and Bondarenko factors in the unresolved resonance region. The 44-group library (44GROUPNDF5) is a broad-group version of 238GROUPNDF5 designed for analysis of light-water-reactor (LWR) fresh and spent fuel systems and has been extensively validated against LWR critical experiments. The 238- and 44-group libraries are the preferred criticality safety analysis libraries in SCALE. The Hansen-Roach 16-group library (HANSEN-ROACH) is based on the original Hansen and Roach data. Important nuclides not available in the library were added by collapsing the 218-group ENDF/B-IV library to the 16-group structure. Although the library was originally developed for fast systems, a modification to the s_p data for ^{238}U has allowed it to be successfully used as a general-purpose library.

The other three libraries were developed as shielding libraries. The SCALE 18-group gamma library (18GROUPGAMMA) is based on data that were later approved as ENDF/B-IV data. The Straker-Morrison 22- neutron and 18-gamma-group coupled library (22N-18COUPLE) contains the same gamma data as 18GROUPGAMMA. The 22-neutron-group data were taken from ENDF/B-II and developed in conjunction with air-over-ground radiation transport studies done in the late 1960s. The group collapse of the cross sections was tailored for water-filled shipping cask calculations. The 27-neutron-group and 18-gamma-group coupled library (27N-18COUPLE) contains neutron data from 27GROUPNDF4 and gamma data from 18GROUPGAMMA. This library has been widely used in LWR spent fuel shielding calculations and has been validated against experimental data.

A library is selected by specifying the appropriate alphanumeric name (which in turn points to the appropriate unit number for the cross-section data). Alternative libraries can be used easily with a minimum of additional job control specifications. Table M4.1.1 lists the standard SCALE cross-section libraries, along with the alphanumeric name and associated logical unit number. Also listed is the main source of data for each library.

The SCALE control modules are designed to read AMPX master format libraries.[1] These libraries are very general and many include temperature-dependent cross-section data as well as resonance data. The master format libraries are used as a basis for creating an AMPX working format library that has

Table M4.1.1 Standard SCALE cross-section libraries

Alphanumeric name[a]	Default logical unit No.	Primary data source
HANSEN-ROACH	81	Hansen-Roach 16 group library
27GROUPNDF4	82	ENDF/B-IV 218-group library
44GROUPNDF5	83	ENDF/B-V 238-group library
238GROUPNDF5	84	ENDF/B-V
22N-18COUPLE	85	Straker-Morrison
18GROUPGAMMA	86	OGRE point-data library
27BURNUPLIB	87	ENDF/B-IV, ENDF/B-V (pre-release)
27N-18COUPLE	88	ENDF/B-IV 27-group library, 18GROUPGAMMA library
Anything else[b]	70	User-supplied library

[a]SCALE will recognize any shortened version of the alphanumeric name as long as it is unique to one name in the list. For example, "27" would not be unique because three library names begin with "27," but "27G" is unique, a shortened version of the name "27GROUPNDF4."

[b]The SCALE 218-group ENDF/B-IV library is no longer associated with a default logical unit number, but may be used via unit 70 as a user-supplied library.

problem-dependent (user-specified) temperature dependence and appropriate resonance processing. The SCALE control module sequences access BONAMI first to process nuclides with Bondarenko data. The master library output from BONAMI is input to NITAWL-II, where resonance data are processed via the Nordheim integral treatment and an AMPX working format library is produced. The SCALE criticality and shielding functional modules are all designed to use an AMPX working library format.

One significant difference between Version 4 of the SCALE system and all previous versions of SCALE is in the structure of the AMPX master format libraries. Earlier versions of SCALE used a cross-section library structure that was generated by AMPX prior to XLACS-77 and that is compatible with the NITAWL code. The current version of SCALE uses cross sections having a data structure compatible with XLACS-77 (and later versions of XLACS) and processed by NITAWL-II. The cross sections are the same in both cases; however, the data are represented in the manner that allows correct interface with the two different implementations of the Nordheim Integral Treatment found in NITAWL and NITAWL-II. This modification should be invisible to the SCALE user in most situations. However, it should be cautioned that cross sections compatible with NITAWL cannot be properly processed by NITAWL-II, and vice versa.

M4.2 DESCRIPTION OF THE SCALE CROSS-SECTION LIBRARIES

The neutron energy group structure of each of the SCALE neutron libraries other than the ENDF/B-V libraries is given in Table M4.2.1. The neutron energy group structure of the ENDF/B-V libraries is given in Table M4.2.2. Six different neutron energy group structures are available in the SCALE system: the Hansen-Roach 16-group structure, the Straker-Morrison 22-group structure, the 27-group subset of the 218-group library, the 218-group structure of the ENDF/B-IV Criticality Safety Reference Library (CSRL), the 44-group subset of the 238-group library, and the 238-group structure of the ENDF/B-V fine-group library. The energy group structure of the gamma cross-section libraries is given in Table M4.2.3. Each of the SCALE cross-section libraries is discussed in the following sections. The table of contents of each library is listed in Sect. M4.A.

M4.2.1 THE 218-GROUP ENDF/B-IV LIBRARY (218GROUPNDF4)

The 218-group ENDF/B-IV library is one of the more complete libraries available in SCALE. The source of the data was ENDF/B-IV, and the processing of the cross sections by XLACS in the AMPX system is well documented.[2,3] The weighting function used in the P_3 cross-section generation was a fission-$1/Es_t$-Maxwellian weighting (except for resonance nuclides, which were weighted 1/E instead of $1/Es_t$). One of the features of the library is that explicit resonance data carried with it can be used to generate problem-dependent, resonance-region group cross sections using NITAWL-II. This capability allows great flexibility in the use of the library as a general-purpose criticality analysis library. The library has 140 fast groups and 78 thermal groups (below 3.05 eV). The group structure was designed to fit the cross-section variation and reaction thresholds of the light and intermediate nuclides and to fit the major resonances of the intermediate and heavy nuclides. No unresolved resonance data are carried in the library. The unresolved resonance region was processed at a $s_p = 50{,}000$.

The 218-group library has not been routinely validated because of its size and the related costs. However, the 27-group ENDF/B-IV library was derived directly from the 218-group library and has been validated against a large number of critical experiments (see Sect. M4.2.2). The 218-fine-group structure of the library generally will give either the same or more precise results than its companion 27-broad-group library.

An obvious advantage of a fine-group library over a broad-group library is that the library is less sensitive to the weighting spectrum used to generate the library. The cross sections more closely represent the base data, and the group structure allows a more detailed determination of the energy dependence of the flux. In past validations, it has been found useful to compare a fine-group calculation against a broad-group calculation when bias is observed. Tables M4.2.4 and M4.2.5 show 218-group nuclides that have resonance data and thermal scattering data, respectively.

M4.2.2 THE 27-GROUP ENDF/B-IV LIBRARY (27GROUPNDF4)

The 27-group ENDF/B-IV library is the broad-group companion library to the 218-group ENDF/B-IV library. The 218-group library was flux collapsed using MALOCS and the MT 1099 flux file carried with the fine-group cross sections. (This flux file is the group representation of the original weighting spectrum used to generate the 218-group cross sections from ENDF/B-IV data.) The library has 14 fast groups and 13 thermal groups (below 3 eV). The group structure was chosen to match the 16-group Hansen-Roach structure with two additional fast groups and seven additional thermal groups. The additional groups were

Table M4.2.1 Neutron energy group structure for some SCALE libraries

CSRL 218-group	CSRL 27-group	Hansen-Roach 16-group	Straker-Morrison 22-group	Upper energy (eV)	Upper lethargy
1	1			2.0000+7[a]	(-0.693)
			1	1.4918+7	(-0.40)
			2	1.2214+7	(-0.20)
		1	3	1.0000+7	0.0
			4	8.1873+6	0.200
2	2			6.4340+6	0.441
			5	6.3600+6	0.453
			6	4.9659+6	0.70
3				4.8000+6	0.734
4				4.3040+6	0.843
			7	4.0657+6	0.90
			8	3.0119+6	1.20
5	3	2		3.0000+6	1.204
6				2.4790+6	1.395
			9	2.4660+6	1.40
7				2.3540+6	1.446
			10	2.3500+6	1.448
8	4			1.8500+6	1.687
			11	1.8268+6	1.70
9				1.5000+6	1.897
10	5	3		1.4000+6	1.966
11				1.3560+6	1.998
12				1.3170+6	2.027
13				1.2500+6	2.079
14				1.2000+6	2.120
			12	1.1080+6	2.20
15				1.1000+6	2.207
16				1.0100+6	2.293
17				9.2000+5	2.386
18	6	4		9.0000+5	2.408
19				8.7500+5	2.436
20				8.6110+5	2.452
21				8.2000+5	2.501
22				7.5000+5	2.590
23				6.7900+5	2.69
24				6.7000+5	2.703
25				6.0000+5	2.813
26				5.7300+5	2.859
			13	5.5023+5	2.90
27				5.5000+5	2.900
28				4.9952+5	2.997

Table M4.2.1 (continued)

CSRL 218-group	CSRL 27-group	Hansen-Roach 16-group	Straker-Morrison 22-group	Upper energy (eV)	Upper lethargy
29				4.7000+5	3.058
30				4.4000+5	3.124
31				4.2000+5	3.170
32	7	5		4.0000+5	3.219
33				3.3000+5	3.411
34				2.7000+5	3.612
35				2.0000+5	3.912
36				1.5000+5	4.200
37				1.2830+5	4.356
			14	1.1109+5	4.50
38	8	6		1.0000+5	4.605
39				8.5000+4	4.768
40				8.2000+4	4.804
41				7.5000+4	4.893
42				7.3000+4	4.920
43				6.0000+4	5.116
44				5.2000+4	5.259
45				5.0000+4	5.298
46				4.5000+4	5.404
47				3.0000+4	5.809
48				2.5000+4	5.991
49	9	7		1.7000+4	6.377
50				1.3000+4	6.645
51				9.5000+3	6.959
52				8.0300+3	7.127
53				6.0000+3	7.419
54				3.9000+3	7.849
55				3.7400+3	7.891
			15	3.3546+3	8.00
56	10	8		3.0000+3	8.112
57				2.5800+3	8.263
58				2.2900+3	8.382
59				2.2000+3	8.422
60				1.8000+3	8.623
61				1.5500+3	8.772
62				1.5000+3	8.805
63				1.1500+3	9.071
64				9.5000+2	9.262
65				6.8300+2	9.592

Table M4.2.1 (continued)

CSRL 218-group	CSRL 27-group	Hansen-Roach 16-group	Straker-Morrison 22-group	Upper energy (eV)	Upper lethargy
66				6.7000+2	9.611
67	11	9		5.5000+2	9.808
68				3.0500+2	10.25
			16	5.8295+2	9.75
69				2.8500+2	10.466
70				2.4000+2	10.637
71				2.1000+2	10.771
72				2.0750+2	10.783
73				1.9250+2	10.858
74				1.8600+2	10.892
75				1.2200+2	11.314
76				1.1900+2	11.339
77				1.1500+2	11.373
78				1.0800+2	11.436
			17	1.0130+2	11.50
79	12	10		1.0000+2	11.513
80				9.0000+1	11.618
81				8.2000+1	11.711
82				8.0000+1	11.736
83				7.6000+1	11.787
84				7.2000+1	11.841
85				6.7500+1	11.906
86				6.5000+1	11.944
87				6.1000+1	12.007
88				5.9000+1	12.041
89				5.3400+1	12.140
90				5.2000+1	12.167
91				5.0600+1	12.194
92				4.9200+1	12.222
93				4.8300+1	12.241
94				4.7000+1	12.268
95				4.5200+1	12.307
96				4.4000+1	12.334
97				4.2400+1	12.371
98				4.1000+1	12.405
99				3.9600+1	12.439
100				3.9100+1	12.452
101				3.8000+1	12.481
102				3.7000+1	12.507
103				3.5500+1	12.549

Table M4.2.1 (continued)

CSRL 218-group	CSRL 27-group	Hansen-Roach 16-group	Straker-Morrison 22-group	Upper energy (eV)	Upper lethargy
104				3.4600+1	12.574
105				3.3750+1	12.599
106				3.3250+1	12.614
107				3.1750+1	12.660
108				3.1250+1	12.676
109	13	11		3.0000+1	12.717
			18	2.9023+1	12.75
110				2.7500+1	12.804
111				2.5000+1	12.899
112				2.2500+1	13.005
113				2.1000+1	13.074
114				2.0000+1	13.122
115				1.9000+1	13.174
116				1.8500+1	13.200
117				1.7000+1	13.285
118				1.6000+1	13.346
119				1.5100+1	13.403
120				1.4400+1	13.451
121				1.3750+1	13.497
122				1.2900+1	13.561
123				1.1900+1	13.642
124				1.1500+1	13.676
			19	1.0677+1	13.75
125	14	12		1.0000+1	13.816
126				9.1000+0	13.910
127				8.1000+0	14.026
128				7.1500+0	14.151
129				7.0000+0	14.172
130				6.7500+0	14.209
131				6.5000+0	14.246
132				6.2500+0	14.286
133				6.0000+0	14.326
134				5.4000+0	14.432
135				5.0000+0	14.509
136				4.7500+0	14.560
137				4.0000+0	14.732
138				3.7300+0	14.802
139				3.5000+0	14.865
140				3.1500+0	14.971
			20	3.0590+0	15.00

Table M4.2.1 (continued)

CSRL 218-group	CSRL 27-group	Hansen-Roach 16-group	Straker-Morrison 22-group	Upper energy (eV)	Upper lethargy
141	15			3.0500+0[b]	15.03
142		13		3.0000+0	15.019
143				2.9700+0	15.030
144				2.8700+0	15.064
145				2.7700+0	15.099
146				2.6700+0	15.136
147				2.5700+0	15.174
148				2.4700+0	15.214
149				2.3800+0	15.251
150				2.3000+0	15.285
151				2.2100+0	15.325
152				2.1200+0	15.367
153				2.0000+0	15.425
154				1.9400+0	15.455
155				1.8600+0	15.498
156	16			1.7700+0	15.547
157				1.6800+0	15.599
158				1.5900+0	15.654
159				1.5000+0	15.713
160				1.4500+0	15.747
161				1.4000+0	15.782
162				1.3500+0	15.818
163	17			1.3000+0	15.856
164				1.2500+0	15.895
165				1.2250+0	15.915
166				1.2000+0	15.936
167				1.1750+0	15.957
168				1.1500+0	15.978
169				1.1400+0	15.987
170	18			1.1300+0	15.996
171				1.1200+0	16.005
172				1.1100+0	16.014
173				1.1000+0	16.023
174				1.0900+0	16.032
175				1.0800+0	16.041
176				1.0700+0	16.050
177				1.0600+0	16.060
178				1.0500+0	16.069
179				1.0400+0	16.079
180				1.0300+0	16.089

Table M4.2.1 (continued)

CSRL 218-group	CSRL 27-group	Hansen-Roach 16-group	Straker-Morrison 22-group	Upper energy (eV)	Upper lethargy
181				1.0200+0	16.098
182				1.0100+0	16.108
183	19	14		1.0000+0	16.118
184				9.7500-1	16.143
185				9.5000-1	16.169
186				9.2500-1	16.196
187				9.0000-1	16.223
188				8.5000-1	16.281
189	20			8.0000-1	16.341
190				7.5000-1	16.406
191				7.0000-1	16.475
192				6.5000-1	16.549
193				6.0000-1	16.629
194				5.5000-1	16.716
			21	5.3159-1	16.750
195				5.0000-1	16.811
196				4.5000-1	16.917
			22[c]	4.1400-1	17.000
197	21	15		4.0000-1	17.034
198				3.7500-1	17.099
199				3.5000-1	17.168
200	22			3.2500-1	17.242
201				3.0000-1	17.322
202				2.7500-1	17.409
203				2.5000-1	17.504
204	23			2.2500-1	17.610
205				2.0000-1	17.728
206				1.7500-1	17.861
207				1.6000-1	17.95
208				1.2500-1	18.198
209	24	16		1.0000-1	18.421
210				9.0000-2	18.526
211				8.0000-2	18.644
212				7.0000-2	18.777
213				6.0000-2	18.932
214	25			5.0000-2	19.114
215				4.0000-2	19.337
216	26			3.0000-2	19.625

Table M4.2.1 (continued)

CSRL 218-group	CSRL 27-group	Hansen-Roach 16-group	Straker-Morrison 22-group	Upper energy (eV)	Upper lethargy
217				2.5300-2	19.795
218[d]	27[d]			1.0000-2	20.723

[a]Read as 2.0000×10^{-7}.
[b]Upper energy boundary for CSRL thermal energy range.
[c]Lower energy boundary for 22-group library is 5.0000×10^{-3} eV.
[d]Lower energy boundary for CSRL 218- and 27-group libraries is 1.0000×10^{-5} eV.

Table M4.2.2 Neutron energy group structure for the SCALE ENDF/B-V libraries

238 group	44 group	Upper energy (eV)	238 group	44 group	Upper energy (eV)	238 group	44 group	Upper energy (eV)	238 group	44 group	Upper energy (eV)
1	1	2.0000E+07	41		2.7000E+05	81		1.8600E+02	121		2.0000E+01
2		1.7333E+07	42		2.0000E+05	82		1.2200E+02	122		1.9000E+01
3		1.5683E+07	43		1.5000E+05	83		1.1900E+02	123		1.8500E+01
4		1.4550E+07	44		1.2830E+05	84		1.1500E+02	124		1.7000E+01
5		1.3840E+07	45	12	1.0000E+05	85		1.0800E+02	125		1.6000E+01
6		1.2840E+07	46		8.5000E+04	86	17	1.0000E+02	126		1.5100E+01
7		1.0000E+07	47		8.2000E+04	87		9.0000E+01	127		1.4400E+01
8	2	8.1873E+06	48		7.5000E+04	88		8.2000E+01	128		1.3750E+01
9	3	6.4340E+06	49		7.3000E+04	89		8.0000E+01	129		1.2900E+01
10	4	4.8000E+06	50		6.0000E+04	90		7.6000E+01	130		1.1900E+01
11		4.3040E+06	51		5.2000E+04	91		7.2000E+01	131		1.1500E+01
12	5	3.0000E+06	52		5.0000E+04	92		6.7500E+01	132	19	1.0000E+01
13	6	2.4790E+06	53		4.5000E+04	93		6.5000E+01	133		9.1000E+00
14	7	2.3540E+06	54		3.0000E+04	94		6.1000E+01	134	20	8.1000E+00
15	8	1.8500E+06	55	13	2.5000E+04	95		5.9000E+01	135		7.1500E+00
16		1.5000E+06	56	14	1.7000E+04	96		5.3400E+01	136		7.0000E+00
17	9	1.4000E+06	57		1.3000E+04	97		5.2000E+01	137		6.7500E+00
18		1.3560E+06	58		9.5000E+03	98		5.0600E+01	138		6.5000E+00
19		1.3170E+06	59		8.0300E+03	99		4.9200E+01	139		6.2500E+00
20		1.2500E+06	60		6.0000E+03	100		4.8300E+01	140	21	6.0000E+00
21		1.2000E+06	61		3.9000E+03	101		4.7000E+01	141		5.4000E+00
22		1.1000E+06	62		3.7400E+03	102		4.5200E+01	142		5.0000E+00
23		1.0100E+06	63	15	3.0000E+03	103		4.4000E+01	143	22	4.7500E+00
24		9.2000E+05	64		2.5800E+03	104		4.2400E+01	144		4.0000E+00
25	10	9.0000E+05	65		2.2900E+03	105		4.1000E+01	145		3.7300E+00
26		8.7500E+05	66		2.2000E+03	106		3.9600E+01	146		3.5000E+00
27		8.6110E+05	67		1.8000E+03	107		3.9100E+01	147		3.1500E+00
28		8.2000E+05	68		1.5500E+03	108		3.8000E+01	148		3.0500E+00
29		7.5000E+05	69		1.5000E+03	109		3.7000E+01	149	23	3.0000E+00[a]
30		6.7900E+05	70		1.1500E+03	110		3.5500E+01	150		2.9700E+00
31		6.7000E+05	71		9.5000E+02	111		3.4600E+01	151		2.8700E+00
32		6.0000E+05	72		6.8300E+02	112		3.3750E+01	152		2.7700E+00
33		5.7300E+05	73		6.7000E+02	113		3.3250E+01	153		2.6700E+00
34		5.5000E+05	74	16	5.5000E+02	114		3.1750E+01	154		2.5700E+00
35		4.9952E+05	75		3.0500E+02	115		3.1250E+01	155		2.4700E+00
36		4.7000E+05	76		2.8500E+02	116	18	3.0000E+01	156		2.3800E+00
37		4.4000E+05	77		2.4000E+02	117		2.7500E+01	157		2.3000E+00
38		4.2000E+05	78		2.1000E+02	118		2.5000E+01	158		2.2100E+00
39	11	4.0000E+05	79		2.0750E+02	119		2.2500E+01	159		2.1200E+00
40		3.3000E+05	80		1.9250E+02	120		2.1000E+01	160		2.0000E+00

Table M4.2.2 (continued)

238 group	44 group	Upper energy (eV)	238 group	44 group	Upper energy (eV)	238 group	44 group	Upper energy (eV)	238 group	44 group	Upper energy (eV)
161		1.9400E+00	181		1.0900E+00	201		6.0000E-01	221		6.0000E-02
162		1.8600E+00	182		1.0800E+00	202		5.5000E-01	222	38	5.0000E-02
163	24	1.7700E+00	183		1.0700E+00	203		5.0000E-01	223	39	4.0000E-02
164		1.6800E+00	184		1.0600E+00	204		4.5000E-01	224	40	3.0000E-02
165		1.5900E+00	185		1.0500E+00	205	27	4.0000E-01	225	41	2.5300E-02
166		1.5000E+00	186		1.0400E+00	206	28	3.7500E-01	226	42	1.0000E-02
167		1.4500E+00	187		1.0300E+00	207	29	3.5000E-01	227	43	7.5000E-03
168		1.4000E+00	188		1.0200E+00	208	30	3.2500E-01	228		5.0000E-03
169		1.3500E+00	189		1.0100E+00	209		3.0000E-01	229		4.0000E-03
170		1.3000E+00	190	25	1.0000E+00	210	31	2.7500E-01	230	44	3.0000E-03
171		1.2500E+00	191		9.7500E-01	211	32	2.5000E-01	231		2.5000E-03
172		1.2250E+00	192		9.5000E-01	212	33	2.2500E-01	232		2.0000E-03
173		1.2000E+00	193		9.2500E-01	213	34	2.0000E-01	233		1.5000E-03
174		1.1750E+00	194		9.0000E-01	214		1.7500E-01	234		1.2000E-03
175		1.1500E+00	195		8.5000E-01	215	35	1.5000E-01	235		1.0000E-03
176		1.1400E+00	196		8.0000E-01	216		1.2500E-01	236		7.5000E-04
177		1.1300E+00	197		7.5000E-01	217	36	1.0000E-01	237		5.0000E-04
178		1.1200E+00	198		7.0000E-01	218		9.0000E-02	238		1.0000E-04
179		1.1100E+00	199		6.5000E-01	219		8.0000E-02			1.0000E-05[b]
180		1.1000E+00	200	26	6.2500E-01	220	37	7.0000E-02			

[a]Upper energy boundary for ENDF/B-V libraries thermal range.

[b]Lower energy boundary for ENDF/B-V libraries.

Table M4.2.3 SCALE gamma energy group structure

SCALE 18-group gamma structure	Upper energy (eV)
1	1.0000+7
2	8.0000+6
3	6.5000+6
4	5.0000+6
5	4.0000+6
6	3.0000+6
7	2.5000+6
8	2.0000+6
9	1.6600+6
10	1.3300+6
11	1.0000+6
12	8.0000+5
13	6.0000+5
14	4.0000+5
15	3.0000+5
16	2.0000+5
17	1.0000+5
18	5.0000+4
	1.0000+4[a]

[a]Lower energy boundary of gamma libraries.

Table M4.2.4 Resonance nuclides in the ENDF/B-IV libraries

Standard composition alphanumeric name	Nuclide ID No.
Na	11023
Mn	25055
Fe	26000
Co	27059
Co-59	27059
Cu	29000
Br-79	35079
Br-81	35081
ZIRCALLOY	40302
Nb-93	41093
Mo	42000
Ag-107	47107
Ag-109	47109
In-113	49113
In-115	49115
Cs-133	55133
Gd	64000
Dy-164	66164
Lu-175	71175
Lu-176	71176
Ta-181	73181
W-182	74182
W-183	74183
W-184	74184
W-186	74186
Re-185	75185
Re-187	75187
Au	79197
Th-232	90232
Pa-233	91233
U-233	92233
U-234	92234
U-235	92235
U-236	92236
U-238	92238
Np-237	93237
Pu-238	94238
Pu-239	94239
Pu-240	94240
Pu-241	94241
Pu-242	94242
Am-241	95241
Am-243	95423
Cm-244	96244

Table M4.2.5 Nuclides in ENDF/B-IV libraries with multiple sets of thermal-scattering data

Standard composition alphanumeric name	Nuclide ID No.	Temperatures (K) for which thermal-scattering cross-section data are available
H	1001	293, 550
D	1002	293, 550
Be	4009	296, 900, 1000, 1200
B-10	5010	293, 550
B-11	5011	293, 550
C	6012	293, 900, 1000, 1200

chosen such that, for the systems considered, the broad-group calculations meet an acceptance criterion of $? k_{eff}/k_{eff} < 0.3\%$ when compared with the reference 218-group calculation using the XSDRN code.[4] This criterion was relaxed to 1% for ^{238}U in systems where the median fission energy was greater than 1 eV and less than 100 eV. The resonance data and the thermal scattering data carried with the 27-group library and the 218-group library are the same and are processed by NITAWL-II. The library was conceived as a general-purpose criticality analysis library with a special interest in applicability toward shipping cask analysis and thermal neutron systems.

The 27-group library has been extensively validated against critical experiments.[5-13] Areas of validation include highly enriched uranium-metal, compound and solution systems, moderated low-enriched uranium, heterogeneous and homogeneous systems, and plutonium metal and solution systems. The 27-group ENDF/B-IV cross-section set is known to have a 1 to 2% positive bias for highly thermal ^{239}Pu systems. Negative bias of 1 to 2% has been observed for light-water-reactor (LWR) fuel lattice depending on the degree of lattice moderation. Other areas of bias tend to be geometry and composition dependent (the reader is referred to the various validation reports for specific areas of applicability). Refer to Sect. M4.B for more information on ORNL experience with the 27-group ENDF/B-IV library.

M4.2.3 THE 27-GROUP DEPLETION LIBRARY (27BURNUPLIB)

The 27-group depletion library is a criticality library originally developed for use in the SAS2 depletion/shielding control module. The library consists of the 27-group ENDF/B-IV library discussed in Sect. M4.2.2 supplemented with data from a pre-release version of ENDF/B-V for a large number of fission products. Prior to the release of the 44-group library, this library was the preferred library for use with SAS2 (Shielding Analysis Sequence 2, Sect. S2) because of the large number of nuclides that can be processed explicitly in XSDRNPM for use in the ORIGEN-S depletion code. This processing eliminates the cross-section dependence on the ORIGEN-S library for those nuclides that are treated in XSDRNPM. Because the base library was the 27-group ENDF/B-IV library, all the comments in Sects. M4.2.2 and M4.2.9 are directly applicable here.

M4.2.4 THE 238-GROUP ENDF/B-V LIBRARY (238GROUPNDF5)

The 238-group ENDF/B-V library is a general-purpose criticality analysis library and the most complete library available in SCALE. This library is also known as the LAW (Library to Analyze Radioactive Waste) Library. The library contains data for all nuclides (more than 300) available in ENDF/B-V processed by the AMPX-77 systems.[14] It also contains data for ENDF/B-VI evaluations of ^{14}N, ^{15}N, ^{16}O, ^{154}Eu, and ^{155}Eu, as discussed in Sect. M4.2.5.

A special nuclide set, identified by nuclide ID number 900, contains dose factors based on the ANSI/ANS 6.1.1-1977 standard (dose factor ID 9029) and on the more recent ANSI/ANS 6.1.1-1991 standard (dose factor ID 9031).

The library has 148 fast groups and 90 thermal groups (below 3 eV). The group structure is listed in Table M4.2.2.

Most resonance nuclides in the 238 group and 44 group have resonance data (to be processed by NITAWL-II) in the resolved resonance range and Bondarenko factors (to be processed by BONAMI) for the unresolved range. Both libraries contain resolved resonance data for s-wave, p-wave, and d-wave resonances ($\ell = 0$, $\ell = 1$, and $\ell = 2$, respectively) as shown in Table M4.2.6. These data can have a significant effect on results for undermoderated, intermediate-energy problems. Resonance structures in several light-to-intermediate mass "nonresonance" ENDF nuclides (i.e., ^{7}Li, ^{19}F, ^{27}Al, ^{28}Si) are accounted for using Bondarenko shielding factors. These structures can also be important in intermediate energy problems. Nuclides with thermal scattering data are listed in Table M4.2.7.

All nuclides in the 238-group LAW Library use the same weighting spectrum, consisting of

1. Maxwellian spectrum (peak at 300 K) from 10^{-5} to 0.125 eV,
2. a 1/E spectrum from 0.125 eV to 67.4 keV,
3. a fission spectrum (effective temperature at 1.273 MeV) from 67.4 keV to 10 MeV, and
4. a 1/E spectrum from 10 to 20 MeV.

A plot of this spectrum is shown in Fig. M4.2.1.

All nuclides use a P_5 Legendre expansion to fit the elastic and discrete level inelastic scattering processes in the fast range, thereby making the library suitable for both reactor and shielding applications. A P_3 fit was used for thermal-scattering. All other scattering processes use P_0 fits.

A special material is included in the library with an identifier of 99, which contains 238-group weighting spectra for collapsing the 238-group library using the MALOCS module to produce an application-specific collapsed library.

Several spectra are included, as listed below:

1. spectrum based on a fuel cell from a 17 × 17 Westinghouse LWR assembly and identified by 9001,
2. spectrum designed for use with the Molten Salt Reactor Experiment (MSRE) fuel storage tanks at ORNL and identified by 9002,
3. average spectrum in a 27-cm carbon steel shield for use in cask shielding studies and identified by 9003,
4,5. average spectra in an 18.6-cm lead/13-cm resin shield for use in shielding cask studies (the flux in the lead region is identified by 9004 and that in the resin region by 9005), and
6. average spectrum in a 50-cm concrete shield for cask shielding studies and identified by 9006.
7. spectrum in an infinite medium of hydrogen and ^{235}U with H/X = 300.

Table M4.2.6 Resonance nuclides in the ENDF/B-V libraries

Standard composition alphanumeric name	Nuclide ID No.	Highest order resonance (ℓ value)
NA	11023	0
S	16000	0
CR	24000	0
CR (1/EsigT)	24301	0
CRSS	24304	0
MN	25055	0
FE	26000	1
FE (1/EsigT)	26301	0
FESS	26304	0
CO-59	27059	1
NI	28000	0
NI (1/EsigT)	28301	0
NISS	28304	0
CU	29000	1
GE-72	32072	1
GE-73	32073	1
GE-74	32074	1
GE-76	32076	0
AS-75	33075	1
SE-74	34074	1
SE-76	34076	2
SE-77	34077	1
SE-78	34078	1
SE-80	34080	1
SE-82	34082	1
BR-79	35079	1
BR-81	35081	1
KR-78	36078	1
KR-80	36080	1
KR-82	36082	2
KR-83	36083	1
KR-84	36084	1
KR-86	36086	0
RB-85	37085	0
RB-87	37087	0
SR-84	38084	0
SR-86	38086	0
SR-87	38087	0
SR-88	38088	0
Y-89	39089	0
ZR	40000	0
ZR-90	40090	0
ZR-91	40091	0
ZR-92	40092	0
ZR-94	40094	0
ZR-96	40096	0
NB-93	41093	0
NB-94	41094	0
MO	42000	0
MO-92	42092	0
MO-94	42094	0
MO-95	42095	0
MO-96	42096	0

Table M4.2.6 (continued)

Standard composition alphanumeric name	Nuclide ID No.	Highest order resonance (ℓ value)
MO-97	42097	0
MO-98	42098	0
MO-100	42100	0
TC-99	43099	0
RU-99	44099	0
RU-100	44100	0
RU-101	44101	0
RU-102	44102	0
RU-104	44104	0
RH-103	45103	0
PD-104	46104	0
PD-105	46105	0
PD-106	46106	0
PD-108	46108	0
AG-107	47107	0
AG-109	47109	0
CD-110	48110	0
CD-111	48111	0
CD-112	48112	0
CD-113	48113	0
CD-114	48114	0
CD-116	48116	0
IN-113	49113	0
IN-115	49115	0
SN-112	50112	0
SN-114	50114	0
SN-115	50115	0
SN-116	50116	0
SN-117	50117	0
SN-118	50118	0
SN-119	50119	0
SN-120	50120	0
SN-122	50122	0
SN-124	50124	0
SB-121	51121	0
SB-123	51123	0
TE-122	52122	0
TE-123	52123	0
TE-124	52124	0
TE-125	52125	0
TE-126	52126	0
TE-128	52128	0
TE-130	52130	0
I-127	53127	0
I-129	53129	0
XE-124	54124	0
XE-126	54126	0
XE-128	54128	0
XE-129	54129	0
XE-130	54130	0
XE-131	54131	0
XE-132	54132	0
XE-134	54134	0

Table M4.2.6 (continued)

Standard composition alphanumeric name	Nuclide ID No.	Highest order resonance (ℓ value)
CS-133	55133	0
CS-136	55136	0
BA-134	56134	0
BA-135	56135	0
BA-136	56136	0
BA-137	56137	0
LA-139	57139	0
PR-141	59141	0
ND-142	60142	0
ND-143	60143	0
ND-144	60144	0
ND-145	60145	0
ND-146	60146	0
ND-148M	60148	0
ND-150	60150	0
PM-147	61147	0
PM-148	61601	0
SM-147	62147	0
SM-149	62149	0
SM-150	62150	0
SM-151	62151	0
SM-152	62152	0
SM-154	62154	0
EU	63000	0
EU-151	63151	0
EU-152	63152	0
EU-153	63153	0
EU-154[a]	63154	0
EU-155[a]	63155	0
GD-152	64152	0
GD-154	64154	0
GD-155	64155	0
GD-156	64156	0
GD-157	64157	0
GD-158	64158	0
GD-160	64160	0
TB-159	65159	0
DY-160	66160	0
DY-161	66161	0
DY-162	66162	0
DY-163	66163	0
DY-164	66164	0
HO-165	67165	0
ER-166	68166	0
ER-167	68167	0
LU-175	71175	0
LU-176	71176	0
HF	72000	0
HF-174	72174	0

Table M4.2.6 (continued)

Standard composition alphanumeric name	Nuclide ID No.	Highest order resonance (ℓ value)
HF-180	72180	0
TA-181	73181	0
TA-182	73182	0
W	74000	0
W-182	74182	0
W-183	74183	0
W-184	74184	0
W-186	74186	0
RE-185	75185	0
RE-187	75187	0
AU	79197	0
TH-230	90230	0
TH-232	90232	0
PA-231	91231	0
PA-233	91233	0
U-232	92232	0
U-234	92234	0
U-235	92235	0
U-236	92236	0
U-237	92237	0
U-238	92238	0
NP-237	93237	0
PU-236	94236	0
PU-238	94238	0
PU-239	94239	0
PU-240	94240	0
PU-242	94242	0
PU-243	94243	0
PU-244	94244	0
AM-241	95241	0
AM-243	95243	0
AM-242M	95601	0
CM-242	96242	0
CM-243	96243	0
CM-244	96244	0
CM-245	96245	0
CM-246	96246	0
CM-247	96247	0
CM-248	96248	0
BK-249	97249	0
CF-249	98249	0
CF-250	98250	0
CF-251	98251	0
CF-252	98252	0
ES-253	99253	0
EU-154 (ENDF/B-V)	631541	0
EU-155 (ENDF/B-V)	631551	0

[a] ENDF/B-VI data.

Table M4.2.7 Nuclides in ENDF/B-V libraries with multiple sets of thermal-scattering data

Standard composition alphanumeric name	Nuclide ID No.	Temperatures (K) for which thermal-scattering cross-section data are available
H	1001	296, 500, 900
D	1002	296, 500, 900
H-3	1003	296, 500, 900
HFREEGAS	1801	296, 500, 900
DFREEGAS	1802	296, 500, 900
H-POLY	1901	296, 500, 900
HE-3	2003	296, 400, 500, 600, 700, 800, 1000, 1200
HE	2004	296, 400, 500, 600, 700, 800, 1000, 1200
LI-6	3006	296, 500, 900
LI-7	3007	296, 500, 900
BE	4009	296, 500, 900
BEBOUND	4309	296, 500, 900
B-10	5010	296, 500, 900
B-11	5011	296, 500, 900
C-12	6012	296, 500, 900
C-GRAPHITE	6312	296, 500, 900
N-14	7014	296, 500, 900
N-15	7015	296, 500, 900
O-16[a]	8016	296, 500, 900
O-17	8017	296, 500, 900
F	9019	296, 500, 900
NA	11023	300, 500, 900
MG	12000	296, 500, 900
AL	13027	296, 500, 900
SI	14000	296, 500, 900
P	15031	296, 500, 900
S	16000	296, 500, 900
S-32	16032	296, 500, 900
CL	17000	300, 500, 900, 2100.1
K	19000	300, 500, 900, 2100.1
CA	20000	296, 500, 900
TI	22000	296, 500, 900
V	23000	296, 500, 900
CR	24000	296, 500, 900
CR (1/EsigT)	24301	296, 500, 900
CRSS	24304	296, 500, 900
MN	25055	296, 500, 900
FE	26000	296, 500, 900
FE (1/EsigT)	26301	296, 500, 900
FESS	26304	296, 500, 900
CO-59	27059	296, 500, 900
NI	28000	296, 500, 900
NI (1/EsigT)	28301	296, 500, 900
NISS	28304	296, 500, 900
CU	29000	296, 500, 900
GA	31000	296, 500, 900
GE-72	32072	296, 500, 900
GE-73	32073	296, 500, 900
GE-74	32074	296, 500, 900
GE-76	32076	296, 500, 900
AS-75	33075	296, 500, 900
SE-74	34074	296, 400, 500, 600, 700, 800, 1000, 1200, 1600, 2000

Table M4.2.7 (continued)

Standard composition alphanumeric name	Nuclide ID No.	Temperatures (K) for which thermal-scattering cross-section data are available
SE-76	34076	296, 500, 900
SE-77	34077	296, 500, 900
SE-78	34078	296, 350
SE-80	34080	296, 350, 400, 450, 500, 600, 800, 1000
SE-82	34082	296, 350, 400, 450, 500, 600, 800, 1000
BR-79	35079	296, 500, 900
BR-81	35081	296, 500, 900
KR-78	36078	296, 500, 900
KR-80	36080	296, 500, 900
KR-82	36082	296, 500, 900
KR-83	36083	296, 500, 900
KR-84	36084	296, 500, 900
KR-85	36085	296, 500, 900
KR-86	36086	296, 500, 900
RB-85	37085	296, 500, 900
RB-86	37086	296, 500, 900
RB-87	37087	296, 500, 900
SR-84	38084	296, 500, 900
SR-86	38086	296, 500, 900
SR-87	38087	296, 500, 900
SR-88	38088	296, 500, 900
SR-89	38089	296, 500, 900
SR-90	38090	296, 500, 900
Y-89	39089	296, 500, 900
Y-90	39090	296, 500, 900
Y-91	39091	296, 500, 900
ZR	40000	296, 500, 900
ZR-90	40090	296, 500, 900
ZR-91	40091	296, 500, 900
ZR-92	40092	296, 500, 900
ZR-93	40093	296, 500, 900
ZR-94	40094	296, 500, 900
ZR-95	40095	296, 500, 900
ZR-96	40096	296, 500, 900
NB-93	41093	296, 500, 900
NB-94	41094	296, 500, 900
NB-95	41095	296, 500, 900
MO	42000	296, 500, 900
MO-92	42092	296, 500, 900
MO-94	42094	296, 500, 900
MO-95	42095	296, 500, 900
MO-96	42096	296, 500, 900
MO-97	42097	296, 500, 900
MO-98	42098	296, 500, 900
MO-99	42099	296, 500, 900
MO-100	42100	296, 500, 900
TC-99	43099	296, 500, 900
RU-96	44096	296, 500, 900
RU-98	44098	296, 500, 900
RU-99	44099	296, 500, 900
RU-100	44100	296, 500, 900
RU-101	44101	296, 500, 900
RU-102	44102	296, 500, 900

Table M4.2.7 (continued)

Standard composition alphanumeric name	Nuclide ID No.	Temperatures (K) for which thermal-scattering cross-section data are available
RU-103	44103	295, 500, 900
RU-104	44104	296, 500, 900
RU-105	44105	296, 500, 900
RU-106	44106	296, 500, 900
RH-103	45103	296, 500, 900
RH-105	45105	296, 500, 900
PD-102	46102	296, 500, 900
PD-104	46104	296, 500, 900
PD-105	46105	296, 500, 900
PD-106	46106	296, 500, 900
PD-107	46107	296, 500, 900
PD-108	46108	296, 500, 900
PD-110	46110	296, 500, 900
AG-107	47107	296, 500, 900
AG-109	47109	296, 500, 900
AG-111	47111	296, 500, 900
CD	48000	296, 500, 900
CD-106	48106	296, 500, 900
CD-108	48108	296, 500, 900
CD-110	48110	296, 500, 900
CD-111	48111	296, 500, 900
CD-112	48112	296, 500, 900
CD-113	48113	296, 500, 900
CD-114	48114	296, 500, 900
CD-116	48116	296, 500, 900
CD-115M	48601	296, 500, 900
IN-113	49113	296, 500, 900
IN-115	49115	296, 500, 900
SN-112	50112	296, 500, 900
SN-114	50114	296, 500, 900
SN-115	50115	296, 500, 900
SN-116	50116	296, 500, 900
SN-117	50117	296, 500, 900
SN-118	50118	296, 500, 900
SN-119	50119	296, 500, 900
SN-120	50120	296, 500, 900
SN-122	50122	296, 500, 900
SN-123	50123	296, 500, 900
SN-124	50124	296, 500, 900
SN-125	50125	296, 500, 900
SN-126	50126	296, 500, 900
SB-121	51121	296, 500, 900
SB-123	51123	296, 500, 900
SB-124	51124	296, 500, 900
SB-125	51125	296, 500, 900
SB-126	52126	296, 500, 900

Table M4.2.7 (continued)

Standard composition alphanumeric name	Nuclide ID No.	Temperatures (K) for which thermal-scattering cross-section data are available
TE-120	52120	296, 500, 900
TE-122	52122	296, 500, 900
TE-123	52123	296, 500, 900
TE-124	52124	296, 500, 900
TE-125	52125	296, 500, 900
TE-126	52126	296, 500, 900
TE-130	52130	296, 500, 900
TE-132	52132	296, 500, 900
TE-127M	52601	296, 500, 900
TE-129M	52611	296, 500, 900
I-127	53127	296, 500, 900
I-129	53129	296, 500, 900
I-130	53130	296, 500, 900
I-131	53131	296, 500, 900
I-135	53135	296, 500, 900
XE-124	54124	296, 500, 900
XE-126	54126	296, 500, 900
XE-128	54128	296, 500, 900
XE-129	54129	296, 500, 900
XE-130	54130	296, 500, 900
XE-131	54131	296, 500, 900
XE-132	54132	296, 500, 900
XE-133	54133	296, 500, 900
XE-134	54134	296, 500, 900
XE-135	54135	296, 500, 900
XE-136	54136	296, 500, 900
CS-133	55133	296, 500, 900
CS-134	55134	296, 500, 900
CS-135	55135	296, 500, 900
CS-136	55136	296, 500, 900
CS-137	55137	296, 500, 900
BA-134	56134	296, 500, 900
BA-135	56135	296, 500, 900
BA-136	56136	296, 500, 900
BA-137	56137	296, 500, 900
BA-138	56138	296, 500, 900
BA-140	56140	296, 500, 900
LA-139	57139	296, 500, 900
LA-140	57140	296, 500, 900
CE-140	58140	296, 500, 900
CE-141	58141	296, 500, 900
CE-142	58142	296, 500, 900
CE-143	58143	296, 500, 900
CE-144	58144	296, 500, 900
PR-141	59141	296, 500, 900
PR-142	59142	296, 500, 900
PR-143	59143	296, 500, 900
ND-142	60142	296, 500, 900
ND-143	60143	296, 500, 900
ND-144	60144	296, 500, 900
ND-145	60145	296, 500, 900
ND-146	60146	296, 500, 900
ND-147	60147	296, 500, 900
ND-148	60148	296, 500, 900
ND-150	60150	296, 500, 900
PM-147	61147	296, 500, 900
PM-148	61148	296, 500, 900

Table M4.2.7 (continued)

Standard composition alphanumeric name	Nuclide ID No.	Temperatures (K) for which thermal-scattering cross-section data are available
PM-149	61149	296, 500, 900
PM-148M	61601	296, 500, 900
SM-144	62144	296, 500, 900
SM-147	62147	296, 500, 900
SM-148	62148	296, 500, 900
SM-149	62149	296, 500, 900
SM-150	62150	296, 500, 900
SM-151	62151	296, 500, 900
SM-152	62152	296, 500, 900
SM-153	62153	296, 500, 900
SM-154	62154	296, 500, 900
EU	63000	296, 500, 900
EU-151	63151	296, 500, 900
EU-152	63152	296, 500, 900
EU-153	63153	296, 500, 900
EU-154[a]	63154	296, 500, 900
EU-155[a]	63155	296, 500, 900
EU-156	63156	296, 500, 900
EU-157	63157	296, 500, 900
GD-152	64152	296, 500, 900
GD-154	64154	296, 500, 900
GD-155	64155	296, 500, 900
GD-156	64156	296, 500, 900
GD-157	64157	296, 500, 900
GD-158	64158	296, 500, 900
GD-160	64160	296, 500, 900
TB-159	65159	296, 500, 900
TB-160	65160	296, 500, 900
DY-160	66160	296, 500, 900
DY-161	66161	296, 500, 900
DY-162	66162	296, 500, 900
DY-163	66163	296, 500, 900
DY-164	66164	296, 500, 900
HO-165	67165	296, 500, 900
ER-166	68166	296, 500, 900
ER-167	68167	296, 500, 900
LU-175	71175	296, 500, 900
LU-176	71176	296, 500, 900
HF	72000	296, 500, 900
HF-174	72174	296, 500, 900
HF-176	72176	296, 500, 900
HF-177	72177	296, 500, 900
HF-178	72178	296, 500, 900
HF-179	72179	296, 500, 900
HF-180	72180	296, 500, 900
TA-181	73181	296, 500, 900
TA-182	73182	296, 500, 900
W	74000	296, 500, 900
W-182	74182	296, 500, 900
W-183	74183	296, 500, 900
W-184	74184	296, 500, 900
W-186	74186	296, 500, 900
RE-185	75185	296, 500, 900

Table M4.2.7 (continued)

Standard composition alphanumeric name	Nuclide ID No.	Temperatures (K) for which thermal-scattering cross-section data are available
RE-187	75187	296, 500, 900
AU	79197	296, 500, 900
PB	82000	296, 500, 900
BI-209	83209	296, 500, 900
TH-230	90230	296, 500, 900
TH-232	90232	296, 500, 900
PA-231	91231	296, 500, 900
PA-233	91233	296, 500, 900
U-232	92232	296, 500, 900
U-233	92233	296, 500, 900
U-234	92234	296, 500, 900
U-235	92235	296, 500, 900
U-236	92236	296, 500, 900
U-237	92237	296, 500, 900
U-238	92238	296, 500, 900
NP-237	93237	296, 500, 900
PU-236	94236	296, 500, 900
PU-237	94237	296, 500, 900
PU-238	94238	296, 500, 900
PU-239	94239	296, 500, 900
PU-240	94240	296, 500, 900
PU-241	94241	296, 500, 900
PU-242	94242	296, 500, 900
PU-243	94243	296, 500, 900
PU-244	94244	296, 500, 900
AM-241	95241	296, 500, 900
AM-242M	95243	296, 500, 900
AM-243	95601	296, 500, 900
CM-241	96241	296, 500, 900
CM-242	96242	296, 500, 900
CM-243	96243	296, 500, 900
CM-244	96244	296, 500, 900
CM-245	96245	296, 500, 900
CM-246	96246	296, 500, 900
CM-247	96247	296, 500, 900
CM-248	96248	296, 500, 900
BK-249	97249	296, 500, 900
CF-249	98249	296, 500, 900
CF-250	98250	296, 500, 900
CF-251	98251	296, 500, 900
CF-252	98252	296, 500, 900
ES-253	99253	296, 500, 900
EU-154 (ENDF/B-V)	631541	296, 500, 900
EU-155 (ENDF/B-V)	631551	296, 500, 900
N-14 (ENDF/B-VI)	701401	296, 500, 900
N-15 (ENDF/B-VI)	701501	296, 500, 900
O-16 (ENDF/B-V)	801601	296, 500, 900

[a] ENDF/B-VI data.

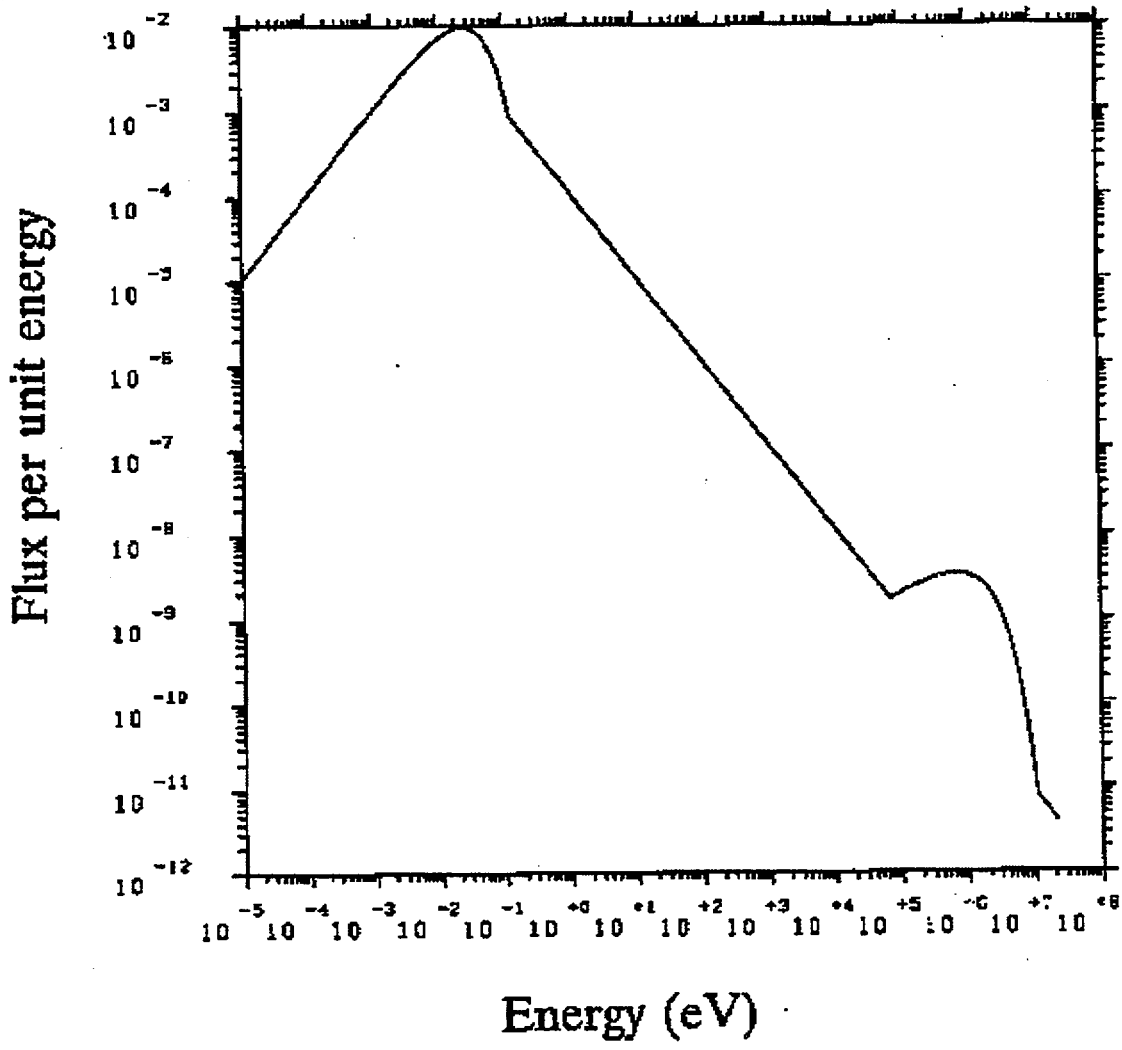

Figure M4.2.1 Weighting function for 238-group LAW Library

In cases 3 through 6, the spent fuel source was a 15 × 15 Westinghouse LWR assembly with initial enrichment of 3.0 wt % and burned to 30 GWd/MTU and cooled for 5 years.

Data testing has been performed for 33 benchmarks, including 28 Cross Section Evaluation Working Group (CSEWG) benchmarks. Results obtained for these benchmarks are very close to those obtained by other data testers using different ENDF/B-V-based cross-section libraries. There is considerable improvement in the trend of k_{eff} vs leakage obtained with the use of the ENDF/B-VI oxygen evaluation. The LAW-238 library appears to be acceptable for general use in criticality and reactor physics applications. The library has had minimal testing for shielding applications and should be evaluated by the user for applicability.

M4.2.5 THE 44-GROUP ENDF/B-V LIBRARY (44GROUPNDF5)

The 44-group ENDF/B-V library has been developed for use in the analysis of fresh and spent fuel and radioactive waste systems. Collapsed from the fine-group 238GROUPNDF5 cross-section library, this broad-group library contains all nuclides (more than 300) from the ENDF/B-V data files. Broad-group boundaries were chosen as a subset of the parent 238GROUPNDF5 boundaries, emphasizing the key spectral aspects of a typical LWR fuel package. Specifically, the broad-group structure was designed to accommodate the following features: two windows in the oxygen cross-section spectrum; a window in the cross section of iron; the Maxwellian peak in the thermal range; and the 0.3-eV resonance in ^{239}Pu (which, due to its low energy, cannot be properly modeled via the SCALE Nordheim Integral Treatment module NITAWL-II). The resulting boundaries represent 22 fast and 22 thermal energy groups; the full group structure is compared to that of the 238-group library in Table M.4.2.2. The fine-group 238GROUPNDF5 cross sections were collapsed into this broad-group structure using a fuel cell spectrum calculated based on a 17 × 17 Westinghouse pressurized-water reactor (PWR) assembly.

Because of the significantly improved and conservative behavior of the ENDF/B-VI ^{16}O evaluation under conditions where higher-order scattering terms are important (e.g., high leakage geometries), this cross section has been included in the 238-group and 44-group libraries as the default for ^{16}O. The ENDF/B-V evaluation is available within the library as cross-section number 801601, and may be copied into an AMPX working library using AJAX for subsequent use in calculations. Similarly, ENDF/B-VI evaluations of ^{14}N and ^{15}N are included in the library; however, ENDF/B-V versions remain the default for these isotopes. The ENDF/B-VI nitrogen data were processed using the same methods used for ^{16}O, and, like oxygen, were tested to see if significant differences between ENDF/B-V and ENDF/B-VI could be identified. No significant differences have been identified; however, because they had already been processed into AMPX master library format and were readily available, ENDF/B-VI ^{14}N and ^{15}N cross sections are included in the library as cross sections 701401 and 701501, respectively. Finally, ENDF/B-VI evaluations of ^{154}Eu and ^{155}Eu are also included in the library as default cross sections 63154 and 63155, respectively. The more recent ENDF/B-VI evaluations include resonance parameters not included in previous evaluations and yield energy-dependent cross sections significantly different from those obtained using ENDF/B-V cross sections. Comparisons of depletion/decay calculations to experimental isotopic measurements have indicated that the ENDF/B-VI europium evaluations are more accurate than those available in ENDF/B-V. However, as with ^{16}O, ENDF/B-V cross sections are available within the library, as isotopes 631541 and 631551.

The 44GROUPNDF5 library was tested against its parent library[15] using a set of 33 benchmark problems in order to demonstrate that the collapsed set was an acceptable representation of 238GROUPNDF5, except for intermediate energy systems. Validation of the library within the SCALE system was based on a comparison of calculated values of k_{eff} with that of 93 experiments: 92 critical and 1 subcritical experiments.[15] The experiments primarily consisted of various configurations of light-water-reactor-type fuel representative

of transportation and storage conditions. Additional experiments were included to allow comparison with results obtained in earlier validation of the 27GROUPNDF4 library.

Results show that the broad 44-group structure is an acceptable representation of its parent 238-group library for thermal as well as hard fast spectrum systems. Accurate broad-group analyses of intermediate spectrum systems will require either a more detailed group structure in this energy range or a more appropriate collapsing spectrum. Further, validation calculations indicate that the 44-group library is an accurate tool in the prediction of criticality for arrays of light-water-reactor-type fuel assemblies, as would be encountered in fresh or spent fuel transportation or storage environments. Validation results for LWR-type UO_2 fuel show virtually no bias. A positive bias of 0.5 to 1% has been observed for very thermal mixed-oxide systems. The bias is caused by inadequate representation of plutonium cross sections, possibly in the ENDF/B-V data. These validation results are consistently better than those seen for the same cases using the 27GROUPNDF4 library and make the 44GROUPNDF5 library the recommended library for thermal and many hard fast spectrum systems. For intermediate energy systems, the parent 238GROUPNDF5 library is recommended.

M4.2.6 THE HANSEN-ROACH LIBRARY (HANSEN-ROACH)

The Hansen-Roach 16-group library is based on the original Los Alamos report by Hansen and Roach.[16] Important nuclides not available in the original library were added by collapsing the 218-group ENDF/B-IV library to the 16-group structure. Table M4.A.6 in Appendix M4.A gives a complete list of the nuclides available in this library and the source of the data.

Resonance nuclides in the original Hansen-Roach library had cross sections tabulated at several s_p values. To make these cross sections compatible with the SCALE system, an infinite dilution library was defined for each resonance nuclide and Bondarenko data were generated for the remaining values of s_p. The implementation of the Hansen-Roach library in SCALE departs significantly from historical use of the Hansen-Roach library. In the past the shielded cross-section set used in a Hansen-Roach calculation was determined by calculating a s_p value using a single value of the potential scatter cross section for each nuclide. As implemented in SCALE, s_p is calculated on a group-wise basis using the total cross-section. Cross-section shielding is then done on a group-wise basis. The original Hansen-Roach library did not carry total cross sections, per se, but had a total cross section that included a transport correction. In order to implement the Hansen-Roach library in SCALE, an infinite dilute 16-group total cross-section was generated from the SCALE 27-group library and added to the Hansen-Roach library as MT-201. The Bondarenko iteration in BONAMI automatically uses MT-201 when it is present in a library. The addition of the 16-group total cross sections allowed the original SCALE control modules to perform automatic problem-dependent cross-section processing using BONAMI.

The Hansen-Roach library was developed primarily for fast systems. There are 12 fast groups and 4 thermal groups (groups below 3 eV). However, thermal upscatter is not included in the original Hansen-Roach data. The cross sections are generally P_0 cross sections that are transport corrected to account for leakage. The exceptions are hydrogen and deuterium, which are P_1 transport-corrected cross sections. All of the nuclides added to the original library were generated to P_3. One significant modification was made to ^{238}U in the original library such that the library more accurately calculated low-enriched uranium systems. This was the Knight modification to the s_p data for ^{238}U such that the 2% enriched green block experiments were accurately calculated.[17]

While the library was originally developed for fast systems, the Knight modification has allowed it to be successfully used as a general-purpose library. The areas of applicability have been periodically documented at the Oak Ridge facilities in validations against critical experiments.[5-11,18-20] The library continues to be widely

used because it is well known. Areas of validation include highly enriched uranium-metal, compounds and solutions, moderated low-enriched uranium systems, and plutonium-metal and solution systems. The Hansen-Roach cross-section set is known to have a 1.5 to 2% negative bias for some highly enriched uranyl nitrate systems and to have a 1 to 1.5% positive bias for highly thermal ^{239}Pu systems. Other areas of bias tend to be geometry and composition dependent (the reader is referred to the various validation reports for specific areas of applicability). Tables M4.2.8 and M4.2.9 show Hansen-Roach nuclides that have resonance and thermal scattering data, respectively.

M4.2.7 THE 18-GROUP GAMMA LIBRARY (18GROUPGAMMA)

The 18-group gamma energy group structure available in SCALE is given in Table M4.2.3. The SCALE gamma energy group structure is available in the stand-alone 18-group gamma library (18GROUPGAMMA), the 27n-18g coupled library (27N-18COUPLE), and the 22n-18g coupled library (22N-18COUPLE).

The standard SCALE 18-group gamma library was originally based on the OGRE point-data library.[21] The OGRE library, in turn, was originally based on photon cross sections available through the National Bureau of Standards. The OGRE library was periodically updated as ENDF/B data became available. The group cross sections were generated by the SMUG1 code. At the time the data were generated for the 18-group gamma cross sections, the OGRE library contained the same data as the HPICE library, DLC-7E.[22] Subsequently, data in the HPICE library were approved as ENDF/B-IV by the Cross Section Evaluation Working Group (CSEWG). In SCALE-4, the gamma data released in the 22n-18g Straker-Morrison library are ENDF/B-V data processed by SMUG. Both of these libraries have been widely used in shielding applications. No formal validation has been done for these libraries against experiments or analytic benchmarks.

M4.2.8 THE 22n-18g STRAKER-MORRISON LIBRARY (22N-18COUPLE)

The 22-group neutron library was developed and introduced in conjunction with air-over-ground radiation transport studies done in the late 1960s.[23] The library is a P_3 radiation shielding library with secondary gamma-ray production data coupled to an 18-group gamma library. The source of the neutron cross sections was the ENDF/B-II library. The neutron cross sections were generated at infinite dilution (1/E weighting) into a 104 fine-group structure using SUPERTOG.[24] The 104-group structure was then collapsed to the 22 broad-group structure using the flux from a fine-group ANISN[25] calculation for a uranium-water mixture.[26] There are 19 fast groups, tailored to weapons radiation transport, and 3 thermal groups (below 3 eV). The 18-group gamma data are discussed in Sect. M4.2.5. The gamma-ray data were generated for SCALE 4 so as to preserve the pair-production cross section. This cross section is needed by the Klein-Nishina estimator in MORSE-SGC.

The 22n-18g library is a widely used radiation shielding library. No resonance data are located in the library, and the group collapse of the cross sections has tailored the cross sections to water-filled shipping-cask-type calculations. The library used in SCALE was converted from an ANISN working format to an AMPX master format library. The library should not be expected to give good results for general criticality calculations or in shielding calculations where fission neutrons are important.

Table M4.2.8 Resonance nuclides found on the Hansen-Roach library

Standard composition alphanumeric name	Nuclide ID No.
Mn	25055
Ag-107	47107
Ag-109	47109
In-113	49113
In-115	49115
Dy-164	66164
Lu-175	71175
Lu-176	71176
W-182	74182
W-183	74183
W-184	74184
W-186	74186
Re-185	75185
Re-187	75187
Au	79197
Th-232	90232[a]
Pa-233	91233
U-233	92233[a]
U-234	92234
U-235	92235[a]
U-236	92236
U-238	92238[a]
Np-237	93237
Pu-238	94338[a]
Pu-239	94239[a]
Pu-240	94240[a]
Pu-241	94241
Pu-242	94242
Am-241	95241
Am-243	95243
Cm-244	96244

[a]Denotes nuclides having Bondarenko data in lieu of resonance parameters.

Table M4.2.9 Nuclides in Hansen-Roach library with multiple sets of thermal scattering data

Standard composition alphanumeric name	Nuclide ID No.	Temperature (K) for which different sets of thermal scattering cross-section data are available
B-10	5010	293,550
B-11	5011	293,550

M4.2.9 THE 27n-18g COUPLED LIBRARY (27N-18COUPLE)

The 27n-18g library is a coupled 27 neutron group, 18 gamma-ray group library for shielding calculations. The neutron data were taken from the 27-group ENDF/B-IV library discussed in Sect. M4.2.8, and the gamma-ray data were taken from the standard SCALE gamma library discussed in Sect. M4.2.5. Secondary gamma production data from ENDF/B-IV were processed by LAPHNGAS and added to the library. As shown in Table M4.2.10, several potentially important nuclides have no gamma-ray production matrices because ENDF/B-IV provided no production data for these nuclides. For many problems in which these nuclides occur, this will not cause a problem, but the user should be aware that these nuclides have no gamma production matrices and should verify that this is not important for the particular problem of interest. The neutron library used in this coupled library is primarily a criticality analysis library and has only one group in the 6- to 20-MeV range. Thus the user should determine that the group structure is adequate for the particular shielding application being considered. A recent shielding analyses study[27] that compared the 27n-18g library structure against other group structures indicated that the 27n-18g library performs satisfactorily for LWR spent fuel sources. This library has been widely used in LWR spent fuel shielding applications and has been validated against experimental data in Ref. 28.

Table M4.2.10 List of nuclides in the 27n-18g library with no gamma-ray production cross sections

Standard composition alphanumeric name	Nuclide ID No.
He	2004
B-11	5011
Br-79	35079
Br-81	35081
Ag-107	47107
Ag-109	47109
Cd	48000
In-113	49113
In-115	49115
Sn	50000
Xe-135	54135
Cs-133	55133[a]
Gd	64000
Dy-164	66164
Lu-175	71175
Lu-176	71176
Hf	72000
Re-185	75185
Re-187	75187
Au-197	79197
Th-232	90232
Pa-233	91233[a]
U-233	92233
U-234	92234
U-236	92236
Np-237	93237[a]
Pu-238	94238
Pu-241	94241
Pu-242	94242
Am-241	95241[a]
Am-243	95243[a]
Cm-244	96244[a]

[a]These nuclides have no gamma-ray data at all.

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M4.A TABLE OF CONTENTS LISTING FOR SCALE LIBRARIES

M4.A.1 THE 218-GROUP ENDF/B-IV LIBRARY

```
table of contents for /scale4.4/data/scale.rev04.xn218          on logical unit  1
 tape id                          4321
 number of nuclides                 79
 number of neutron groups          218
 first thermal group               141
 number of gamma groups              0
        scale 4.2 - 218 group neutron library
           based on endf-b version 4 data
              compiled for nrc     1/27/89
                 last updated                                          08/12/94
                    l.m.petrie   -   ornl
      999          1/v cross sections normalized to 1.0 at 0.0253 ev      updated 08/12/94
     1001           hydrogen        endf/b-iv mat 1269/thrm1002           updated 08/12/94
     1002           deuterium       endf/b-iv mat 1120                    updated 08/12/94
     2004           helium-4        endf/b-iv mat 1270                    updated 08/12/94
     3006           lithium-6       endf/b-iv mat 1271                    updated 08/12/94
     3007           lithium-7       endf/b-iv mat 1272                    updated 08/12/94
     4009           beryllium-9     endf/b-iv mat 1289/thrm1064           updated 08/12/94
     5010          b-10 1273 218ngp 042375 p-3 293k                       updated 08/12/94
     5011           boron-11        endf/b-iv mat 1160                    updated 08/12/94
     6012          c-12 1274f,1065t 218 gp 030476(7)                      updated 08/12/94
     7014          n-14 1275 218 gp 030476(7)                             updated 08/12/94
     8016           oxygen-16       endf/b-iv mat 1276                    updated 08/12/94
     9019          f 1277 218gp 030476(7)                                 updated 08/12/94
    11023           sodium-23       endf/b-iv mat 1156                    updated 08/12/94
    12000          mg 1280 218 gp 1/e*sigt 040375(5)                      updated 08/12/94
    13027          al-27 1193 218 gp 040375(5)                            updated 08/12/94
    14000           silicon         endf/b-iv mat 1194                    updated 08/12/94
    15031           phosphorus-31   endf/b-iv mat 7019                    updated 08/12/94
    16000          sulfur  lendl mat 7020                                 updated 08/12/94
    19000          potassium endf/b-iv mat 1150                           updated 08/12/94
    20000          calcium endf/b-iv mat 1195                             updated 08/12/94
    22000          ti 1286 218 gp wt 1/est 042375 p3 293k                 updated 08/12/94
    23051          v 1196 218 gp 1/e*sigt 040375(5)                       updated 08/12/94
    24000          cr 1191 218ngp wt 1/e p-3 293k sigp=5+4 re(042375)     updated 08/12/94
    24304          cr 1191 wt ss-304(1/est) p-3 293k sp=5+4(42375)'       updated 08/12/94
    24404           cr (inconel)    endf/b-iv mat 1191                    updated 08/12/94
    25055           manganese-55    endf/b-iv mat 1197                    updated 08/12/94
    26000           iron            endf/b-iv mat 1192                    updated 08/12/94
    26304          fe 1192 wt ss-304(1/est) p-3 293k sp=5+4(42375)'       updated 08/12/94
    26404          fe 1192 wt inconl(1/est) p-3 293k sp=5+4(42375)'       updated 08/12/94
    27059           cobalt-59       endf/b-iv mat 1199                    updated 08/12/94
    28000          ni 1190 218ngp wt 1/e p-3 293k sigp=5+4 re(042375)     updated 08/12/94
    28304           nickel (ss304) endf/b-iv mat 1190                     updated 08/12/94
    28404          ni 1190 wt inconl(1/est) p-3 293k sp=5+4(42375)'       updated 08/12/94
    29000           copper          endf/b-iv mat 1295                    updated 08/12/94
    35079           bromine-79      endf/b-iv mat 108                     updated 08/12/94
    35081           bromine-81      endf/b-iv mat 112                     updated 08/12/94
    40000           zirconium       endf/b-iv mat 7141                    updated 08/12/94
    40302           zircalloy       endf/b-iv mat 1284                    updated 08/12/94
    41093           niobium-93      endf/b-iv mat 1189                    updated 08/12/94
    42000           molybdenum      endf/b-iv mat 1287                    updated 08/12/94
    47107           silver-107      endf/b-iv mat 1138                    updated 08/12/94
    47109           silver-109      endf/b-iv mat 1139                    updated 08/12/94
    48000           cadmium         endf/b-iv mat 1281                    updated 08/12/94
    49113           indium-113      endf/b-iv mat 445                     updated 08/12/94
    49115           indium-115      endf/b-iv mat 449                     updated 08/12/94
    50000          sn 7039 wt 1/est 218ngp p-3 293k re(042375)            updated 08/12/94
    56138           barium-138      endf/b-iv mat 7040                    updated 08/12/94
    64000          gd (1030) sig0=1.+5p3 293k f-1/e-m vb 61479            updated 08/12/94
    66164           dyprosium-164   endf/b-iv mat 1031                    updated 08/12/94
    71175           lutetium-175    endf/b-iv mat 1032                    updated 08/12/94
```

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71176          lutetium-176   endf/b-iv mat 1033                          updated 08/12/94
72000         hf(nat) 1034 218ngp wt 1/e p-3 sigp=5+4 293k re(042375)  updated 08/12/94
73181          tantalum-181   endf/b-iv mat 1285                          updated 08/12/94
74182         w-182  1128 sigp=5+4 newxlacs 218ngp p-3 293k             updated 08/12/94
74183          tungsten-183   endf/b-iv mat 1129                          updated 08/12/94
74184          tungsten-184   endf/b-iv mat 1130                          updated 08/12/94
74186          tungsten-186   endf/b-iv mat 1131                          updated 08/12/94
75185          rhenium-185    endf/b-iv mat 1083                          updated 08/12/94
75187          rhenium-187    endf/b-iv mat 1084                          updated 08/12/94
79197          gold-197       endf/b-iv mat 1283                          updated 08/12/94
82000         pb   1288 218ngp 042375 p-3 293k                           updated 08/12/94
90232          thorium-232    endf/b-iv mat 1296                          updated 08/12/94
91233          paladium-231   endf/b-iv mat 1297                          updated 08/12/94
92233         u-233  1260 sigp=5+4 newxlacs 218ngp p-3 293k              updated 08/12/94
92234         u-234 1043 sigo=5+4 newxlacs p-3 293k f-1/e-m(1.+5)       updated 08/12/94
92235          uranium-235    endf/b-iv mat 1261                          updated 08/12/94
92236          uranium-236    endf/b-iv mat 1163                          updated 08/12/94
92238          uranium-238    endf/b-iv mat 1262                          updated 08/12/94
93237          neptunium-237  endf/b-iv mat 1263                          updated 08/12/94
94238          plutonium-238  endf/b-iv mat 1050                          updated 08/12/94
94239          plutonium-239  endf/b-iv mat 1264                          updated 08/12/94
94240          plutonium-240  endf/b-iv mat 1265                          updated 08/12/94
94241          plutonium-241  endf/b-iv mat 1266                          updated 08/12/94
94242          plutonium-242  endf/b-iv mat 1161                          updated 08/12/94
95241         am-241 1056 sigp=5+4 newxlacs 218ngp p-3 293k             updated 08/12/94
95243         am-243 1057 218 gp wt f-1/e-m 090376 p3 293k              updated 08/12/94
96244          curium-244     endf/b-iv mat 1162                          updated 08/12/94
17000         chlorine (mat 1149 from version iv) using 1/sigt weightiupdated 08/12/94
```

M4.A.2 THE 27-GROUP ENDF/B-IV LIBRARY

```
table of contents for /scale4.4/data/scale.rev04.xn27            on logical unit  1
tape id                          4321
number of nuclides                 83
number of neutron groups           27
first thermal group                15
number of gamma groups              0
        scale 4.2 - 27 group neutron group library
           based on endf-b version 4 data
              compiled for nrc     1/27/89
                 last updated                                              08/12/94
                    l.m.petrie   -   ornl
    900           dose factors from ansi/ans-6.1.1-1977          updated 9/07/89
    999           1/v cross sections normalized to 1.0 at 0.0253 ev       updated 08/12/94
   1001            hydrogen       endf/b-iv mat 1269/thrm1002             updated 08/12/94
   1002            deuterium      endf/b-iv mat 1120                      updated 08/12/94
   2004            helium-4       endf/b-iv mat 1270                      updated 08/12/94
   3006           li-6 1271 218 gp 1/e*sigt 040375(5)                     updated 08/12/94
   3007           li-7 1272 218 gp 1/e*sigt 040375(5)                     updated 08/12/94
   4009            beryllium-9    endf/b-iv mat 1289/thrm1064             updated 08/12/94
   5010           b-10 1273 218ngp 042375 p-3 293k                        updated 08/12/94
   5011            boron-11       endf/b-iv mat 1160                      updated 08/12/94
   6012            carbon-12      endf/b-iv mat 1274/thrm1065             updated 08/12/94
   7014            nitrogen-14    endf/b-iv mat 1275                      updated 08/12/94
   8016            oxygen-16      endf/b-iv mat 1276                      updated 08/12/94
   9019            fluorine       endf/b-iv mat 1277                      updated 08/12/94
  11023            sodium-23      endf/b-iv mat 1156                      updated 08/12/94
  12000           mg 1280 218 gp 1/e*sigt 040375(5)                       updated 08/12/94
  13027           al-27 1193 218 gp 040375(5)                             updated 08/12/94
  14000            silicon        endf/b-iv mat 1194                      updated 08/12/94
  15031           p-31 7019 218ngp wt 1/est 042375 p3 293k                updated 08/12/94
  16000           sulfur  lendl mat 7020                                  updated 08/12/94
  19000            potassium      endf/b-iv mat 1150                      updated 08/12/94
  20000           calcium endf/b-iv mat 1195                              updated 08/12/94
  22000            titanium       endf/b-iv mat 1286                      updated 08/12/94
  23051           v 1196 218 gp 1/e*sigt 040375(5)                        updated 08/12/94
  24000           cr 1191 218ngp wt 1/e p-3 293k sigp=5+4 re(042375)      updated 08/12/94
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```
 24304          cr 1191 wt ss-304(1/est) p-3 293k sp=5+4(42375)'        updated 08/12/94
 24404          cr 1191 wt inconl(1/est) p-3 293k sp=5+4(42375)'        updated 08/12/94
 25055           manganese-55   endf/b-iv mat 1197                      updated 08/12/94
 26000           iron           endf/b-iv mat 1192                      updated 08/12/94
 26304          fe 1192 wt ss-304(1/est) p-3 293k sp=5+4(42375)'        updated 08/12/94
 26404          fe 1192 wt inconl(1/est) p-3 293k sp=5+4(42375)'        updated 08/12/94
 27059           cobalt-59      endf/b-iv mat 1199                      updated 08/12/94
 28000          ni 1190 218ngp wt 1/e p-3 293k sigp=5+4 re(042375)      updated 08/12/94
 28304          ni 1190 wt ss-304(1/est) p-3 293k sp=5+4(42375)'        updated 08/12/94
 28404          ni 1190 wt inconl(1/est) p-3 293k sp=5+4(42375)'        updated 08/12/94
 29000           copper         endf/b-iv mat 1295                      updated 08/12/94
 35079           bromine-79     endf/b-iv mat 108                       updated 08/12/94
 35081           bromine-81     endf/b-iv mat 112                       updated 08/12/94
 40000           zirconium      endf/b-iv mat 7141                      updated 08/12/94
 40302           zircalloy      endf/b-iv mat 1284                      updated 08/12/94
 41093           niobium-93     endf/b-iv mat 1189                      updated 08/12/94
 42000          mo (1287) sigp=5+4 newxlacs 218ngp f-1/e-m p-3 293k     updated 08/12/94
 47107           silver-107     endf/b-iv mat 1138                      updated 08/12/94
 47109           silver-109     endf/b-iv mat 1139                      updated 08/12/94
 48000          cd 1281 wt 1/est 218ngp p-3 293k re(042375)             updated 08/12/94
 49113           indium-113     endf/b-iv mat 445                       updated 08/12/94
 49115           indium-115     endf/b-iv mat 449                       updated 08/12/94
 50000          sn 7039 wt 1/est 218ngp p-3 293k re(042375)             updated 08/12/94
 54135           xenon-135      endf/b-iv mat 1294                      updated 08/12/94
 55133           cesium-133     endf/b-iv mat 1141                      updated 08/12/94
 56138          ba-138 7040 218ngp wt 1/est 042375 p3 293k              updated 08/12/94
 64000          gd (1030) sig0=1.+5p3 293k f-1/e-m vb 61479             updated 08/12/94
 66164           dyprosium-164  endf/b-iv mat 1031                      updated 08/12/94
 71175           lutetium-175   endf/b-iv mat 1032                      updated 08/12/94
 71176           lutetium-176   endf/b-iv mat 1033                      updated 08/12/94
 72000          hf(nat) 1034 218ngp wt 1/e p-3 sigp=5+4 293k re(042375) updated 08/12/94
 73181           tantalum-181   endf/b-iv mat 1285                      updated 08/12/94
 74182           tungsten-182   endf/b-iv mat 1128                      updated 08/12/94
 74183           tungsten-183   endf/b-iv mat 1129                      updated 08/12/94
 74184           tungsten-184   endf/b-iv mat 1130                      updated 08/12/94
 74186           tungsten-186   endf/b-iv mat 1131                      updated 08/12/94
 75185           rhenium-185    endf/b-iv mat 1083                      updated 08/12/94
 75187           rhenium-187    endf/b-iv mat 1084                      updated 08/12/94
 79197           gold-197       endf/b-iv mat 1283                      updated 08/12/94
 82000          pb   1288 218ngp 042375 p-3 293k                        updated 08/12/94
 90232           thorium-232    endf/b-iv mat 1296                      updated 08/12/94
 91233          pa-233 1297 218 gp wt f-1/e-m 090376 p3 293k            updated 08/12/94
 92233          u-233  1260 sigp=5+4 newxlacs 218ngp p-3 293k            updated 08/12/94
 92234           uranium-234    endf/b-iv mat 1043                      updated 08/12/94
 92235           uranium-235    endf/b-iv mat 1261                      updated 08/12/94
 92236          u-236 1163 sigo=5+4 newxlacs p-3 293k f-1/e-m(1.+5)     updated 08/12/94
 92238           uranium-238    endf/b-iv mat 1262                      updated 08/12/94
 93237           neptunium-237  endf/b-iv mat 1263                      updated 08/12/94
 94238          pu-238 1050 sigo=5+4 newxlacs p-3 293k f-1/e-m(1.+5)    updated 08/12/94
 94239           plutonium-239  endf/b-iv mat 1264                      updated 08/12/94
 94240           plutonium-240  endf/b-iv mat 1265                      updated 08/12/94
 94241           plutonium-241  endf/b-iv mat 1266                      updated 08/12/94
 94242           plutonium-242  endf/b-iv mat 1161                      updated 08/12/94
 95241          am-241 1056 sigp=5+4 newxlacs 218ngp p-3 293k           updated 08/12/94
 95243          am-243 1057 218 gp wt f-1/e-m 090376 p3 293k            updated 08/12/94
 96244           curium-244     endf/b-iv mat 1162                      updated 08/12/94
500000          jrk's neutron(9029) dose factors from ansi/ans-6.1.1-1977.
 17000          chlorine (mat 1149 from version iv) using 1/sigt weightiupdated 08/12/94
```

M4.A.3 THE 27-GROUP BURNUP LIBRARY

```
table of contents for /scale4.4/data/scale.rev05.xn27burn          on logical unit  1
tape id                          27
number of nuclides              252
number of neutron groups         27
first thermal group              15
number of gamma groups            0
```

```
    scale - 27 group neutron burnup library
       based on endf-b version 4 data with endf-b version 5 fission products
          compiled for nrc     1/27/89
             last updated      1/14/98
                l.m.petrie   -   ornl
  900          dose factors from ansi/ans-6.1.1-1977          updated 9/15/89
  999          1/v cross sections normalized to 1.0 at 0.0253 ev       updated 08/12/94
 1001           hydrogen       endf/b-iv mat 1269/thrm1002             updated 08/12/94
 1002           deuterium      endf/b-iv mat 1120                      updated 08/12/94
 2004          he-4 1270 218 gp wt f-1/est-m 042375 p3 293k            updated 08/12/94
 3006          li-6 1271 218 gp 1/e*sigt 040375(5)                     updated 08/12/94
 3007          li-7 1272 218 gp 1/e*sigt 040375(5)                     updated 08/12/94
 4009           beryllium-9    endf/b-iv mat 1289/thrm1064             updated 08/12/94
 5010          b-10 1273 218ngp 042375 p-3 293k                        updated 08/12/94
 5011           boron-11       endf/b-iv mat 1160                      updated 08/12/94
 6012           carbon-12      endf/b-iv mat 1274/thrm1065             updated 08/12/94
 7014           nitrogen-14    endf/b-iv mat 1275                      updated 08/12/94
 8016           oxygen-16      endf/b-iv mat 1276                      updated 08/12/94
 9019           fluorine       endf/b-iv mat 1277                      updated 08/12/94
11023           sodium-23      endf/b-iv mat 1156                      updated 08/12/94
12000          mg 1280 218 gp 1/e*sigt 040375(5)                       updated 08/12/94
13027          al-27 1193 218 gp 040375(5)                             updated 08/12/94
14000           silicon        endf/b-iv mat 1194                      updated 08/12/94
15031          p-31 7019 218ngp wt 1/est 042375 p3 293k                updated 08/12/94
16000          sulfur    lendl     mat 7020                            updated 08/12/94
19000           potassium      endf/b-iv mat 1150                      updated 08/12/94
20000          calcium   endf/b-iv mat 1195                            updated 08/12/94
22000           titanium       endf/b-iv mat 1286                      updated 08/12/94
23051          v 1196 218 gp 1/e*sigt 040375(5)                        updated 08/12/94
24000          cr 1191 218ngp wt 1/e p-3 293k sigp=5+4 re(042375)      updated 08/12/94
24304          cr 1191 wt ss-304(1/est) p-3 293k sp=5+4(42375)'        updated 08/12/94
24404          cr 1191 wt inconl(1/est) p-3 293k sp=5+4(42375)'        updated 08/12/94
25055           manganese-55   endf/b-iv mat 1197                      updated 08/12/94
26000           iron           endf/b-iv mat 1192                      updated 08/12/94
26304          fe 1192 wt ss-304(1/est) p-3 293k sp=5+4(42375)'        updated 08/12/94
26404          fe 1192 wt inconl(1/est) p-3 293k sp=5+4(42375)'        updated 08/12/94
27059           cobalt-59      endf/b-iv mat 1199                      updated 08/12/94
28000          ni 1190 218ngp wt 1/e p-3 293k sigp=5+4 re(042375)      updated 08/12/94
28304          ni 1190 wt ss-304(1/est) p-3 293k sp=5+4(42375)'        updated 08/12/94
28404          ni 1190 wt inconl(1/est) p-3 293k sp=5+4(42375)'        updated 08/12/94
29000           copper         endf/b-iv mat 1295                      updated 08/12/94
32072           ge-72          mt=102                                  updated 08/12/94
32073           ge-73          mt=102                                  updated 08/12/94
32074           ge-74          mt=102                                  updated 08/12/94
32076           ge-76          mt=102                                  updated 08/12/94
33075           as-75          mt=102                                  updated 08/12/94
34076           se-76          mt=102                                  updated 08/12/94
34077           se-77          mt=102                                  updated 08/12/94
34078           se-78          mt=102                                  updated 08/12/94
34080           se-80             mt=  102                             updated 08/12/94
34082           se-82          mt=102                                  updated 08/12/94
35079           bromine-79     endf/b-iv mat 108                       updated 08/12/94
35081           bromine-81     endf/b-iv mat 112                       updated 08/12/94
36080           kr-80             mt=  102, 103, 104, 105, 106, 107    updated 08/12/94
36082           kr-82             mt=  102, 103, 104, 105, 106, 107    updated 08/12/94
36083           kr-83          mt=102,103,103,105,106,107              updated 08/12/94
36084           kr-84             mt=  102, 103, 104, 105, 106, 107    updated 08/12/94
36085           kr-85             mt=  102                             updated 08/12/94
36086           kr-86             mt=  102, 103, 104, 105, 107         updated 08/12/94
37085           rb-85          mt=102                                  updated 08/12/94
37086           rb-86          mt=102                                  updated 08/12/94
37087           rb-87          mt=102                                  updated 08/12/94
38086           sr-86             mt=  102                             updated 08/12/94
38087           sr-87          mt=102                                  updated 08/12/94
38088           sr-88             mt=  102                             updated 08/12/94
38089           sr-89          mt=102                                  updated 08/12/94
38090           sr-90          mt=102                                  updated 08/12/94
39089            y-89          mt=102                                  updated 08/12/94
39090            y-90             mt=  102                             updated 08/12/94
39091            y-91          mt=102                                  updated 08/12/94
```

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40000          zirconium       endf/b-iv mat 7141                          updated 08/12/94
40090          zr-90              mt=  102                                 updated 08/12/94
40091          zr-91              mt=  102                                 updated 08/12/94
40092          zr-92           mt=102                                      updated 08/12/94
40093          zr-93              mt=  102                                 updated 08/12/94
40094          zr-94           mt=102                                      updated 08/12/94
40095          zr-95           mt=102                                      updated 08/12/94
40096          zr-96              mt=  102                                 updated 08/12/94
40302          zircalloy       endf/b-iv mat 1284                          updated 08/12/94
41093          niobium-93      endf/b-iv mat 1189                          updated 08/12/94
41094          nb-94           mt=102                                      updated 08/12/94
41095          nb-95           mt=102                                      updated 08/12/94
42000         mo (1287) sigp=5+4 newxlacs 218ngp f-1/e-m p-3 293k          updated 08/12/94
42094          mo-94              mt=  102                                 updated 08/12/94
42095          mo-95           mt=102                                      updated 08/12/94
42096          mo-96           mt=102                                      updated 08/12/94
42097          mo-97           mt=102                                      updated 08/12/94
42098          mo-98           mt=102                                      updated 08/12/94
42099          mo-99           mt=102                                      updated 08/12/94
42100          mo-100          mt=102                                      updated 08/12/94
43099          tc-99           mt=102                                      updated 08/12/94
44099          ru-99           mt=102                                      updated 08/12/94
44100          ru-100          mt=102                                      updated 08/12/94
44101          ru-101          mt=102                                      updated 08/12/94
44102          ru-102          mt=102                                      updated 08/12/94
44103          ru-103          mt=102                                      updated 08/12/94
44104          ru-104          mt=102                                      updated 08/12/94
44105          ru-105          mt=102                                      updated 08/12/94
44106          ru-106          mt=102                                      updated 08/12/94
45105          rh-105             mt=  102                                 updated 08/12/94
46104          pd-104          mt=102                                      updated 08/12/94
46105          pd-105          mt=102                                      updated 08/12/94
46106          pd-106          mt=102                                      updated 08/12/94
46107          pd-107          mt=102                                      updated 08/12/94
46108          pd-108          mt=102                                      updated 08/12/94
46110          pd-110          mt=102                                      updated 08/12/94
47107          silver-107      endf/b-iv mat 1138                          updated 08/12/94
47109          silver-109      endf/b-iv mat 1139                          updated 08/12/94
47111          ag-111          mt=102                                      updated 08/12/94
48000          cadmium         endf/b-iv mat 1281                          updated 08/12/94
48108          cd-108          mt=102                                      updated 08/12/94
48110          cd-110          mt=102                                      updated 08/12/94
48111          cd-111          mt=102                                      updated 08/12/94
48112          cd-112          mt=102                                      updated 08/12/94
48113          cd-113             mt=  102, 103, 107                       updated 08/12/94
48114          cd-114          mt=102                                      updated 08/12/94
48601          cd-115m            mt=  102                                 updated 08/12/94
48116          cd-116             mt=  102                                 updated 08/12/94
49113          indium-113      endf/b-iv mat 445                           updated 08/12/94
49115          indium-115      endf/b-iv mat 449                           updated 08/12/94
50000         sn 7039 wt 1/est 218ngp p-3 293k re(042375)                  updated 08/12/94
50115          sn-115          mt=102                                      updated 08/12/94
50116          sn-116             mt=  102                                 updated 08/12/94
50117          sn-117             mt=  102                                 updated 08/12/94
50118          sn-118          mt=102                                      updated 08/12/94
50119          sn-119          mt=102                                      updated 08/12/94
50120          sn-120          mt=102                                      updated 08/12/94
50122          sn-122          mt=102                                      updated 08/12/94
50123          sn-123          mt=102                                      updated 08/12/94
50124          sn-124          mt=102                                      updated 08/12/94
50125          sn-125          mt=102                                      updated 08/12/94
50126          sn-126          mt=102                                      updated 08/12/94
51121          sb-121          mt=102                                      updated 08/12/94
51123          sb-123          mt=102                                      updated 08/12/94
51124          sb-124          mt=102                                      updated 08/12/94
51125          sb-125          mt=102                                      updated 08/12/94
51126          sb-126          mt=102                                      updated 08/12/94
52122          te-122          mt=102                                      updated 08/12/94
52123          te-123          mt=102                                      updated 08/12/94
52124          te-124          mt=102                                      updated 08/12/94
```

52125	te-125	mt=102	updated 08/12/94
52126	te-126	mt=102	updated 08/12/94
52601	te-127m	mt= 102	updated 08/12/94
52128	te-128	mt=102	updated 08/12/94
52611	te-129m	mt= 102	updated 08/12/94
52130	te-130	mt=102	updated 08/12/94
52132	te-132	mt=102	updated 08/12/94
53127	i-127	mt=102	updated 08/12/94
53129	i-129	mt=102	updated 08/12/94
53130	i-130	mt= 102	updated 08/12/94
53131	i-131	mt= 102	updated 08/12/94
53135	i-135	mt= 102	updated 08/12/94
54128	xe-128	mt=102,103,104,105,106,107	updated 08/12/94
54129	xe-129	mt=102,103,104,105,106	updated 08/12/94
54130	xe-130	mt=102,103,104,105,106	updated 08/12/94
54131	xe-131	mt=102,103,104,105,106	updated 08/12/94
54132	xe-132	mt=102,103,104,105,106	updated 08/12/94
54133	xe-133	mt= 102	updated 08/12/94
54134	xe-134	mt=102,103,104,105,106	updated 08/12/94
54135	xenon-135	endf/b-iv mat 1294	updated 08/12/94
54136	xe-136	mt= 102, 103, 104, 105, 107	updated 08/12/94
55133	cesium-133	endf/b-iv mat 1141	updated 08/12/94
55134	cs-134	mt=102	updated 08/12/94
55135	cs-135	mt= 102	updated 08/12/94
55136	cs-136	mt= 102	updated 08/12/94
55137	cs-137	mt=102	updated 08/12/94
56134	ba-134	mt=102	updated 08/12/94
56135	ba-135	mt= 102	updated 08/12/94
56136	ba-136	mt=102	updated 08/12/94
56137	ba-137	mt= 102	updated 08/12/94
56138	ba-138 7040 218ngp wt 1/est 042375 p3 293k		updated 08/12/94
56140	ba-140	mt= 102	updated 08/12/94
57139	la-139	mt=102	updated 08/12/94
57140	la-140	mt=102	updated 08/12/94
58140	ce-140	mt=102	updated 08/12/94
58141	ce-141	mt=102	updated 08/12/94
58142	ce-142	mt=102	updated 08/12/94
58143	ce-143	mt= 102	updated 08/12/94
58144	ce-144	mt= 102	updated 08/12/94
59141	pr-141	mt=102,103,104,105,106,107	updated 08/12/94
59142	pr-142	mt= 102	updated 08/12/94
59143	pr-143	mt=102	updated 08/12/94
60142	nd-142	mt=102	updated 08/12/94
60143	nd-143	mt=102	updated 08/12/94
60144	nd-144	mt=102	updated 08/12/94
60145	nd-145	mt=102	updated 08/12/94
60146	nd-146	mt= 102, 103, 104, 105, 106, 107	updated 08/12/94
60147	nd-147	mt=102	updated 08/12/94
60148	nd-148	mt=102	updated 08/12/94
60150	nd-150	mt=102	updated 08/12/94
61147	pm-147	mt=102	updated 08/12/94
61148	pm-148	mt= 102	updated 08/12/94
61149	pm-149	mt=102	updated 08/12/94
61151	pm-151	mt=102	updated 08/12/94
62147	sm-147	endf/b-v fission product	updated 08/12/94
62148	sm-148	mt= 102	updated 08/12/94
62149	sm-149	mt=102,103,107	updated 08/12/94
62150	sm-150	mt=102	updated 08/12/94
62151	sm-151	mt=102,103,104,105,106,107	updated 08/12/94
62152	sm-152	mt=102,103,104,105,106,107	updated 08/12/94
62153	sm-153	mt=102	updated 08/12/94
62154	sm-154	mt=102	updated 08/12/94
63151	eu-151	mt=102,103,104,105,106,107	updated 08/12/94
63152	eu-152	mt=102,103,104,105,106,107	updated 08/12/94
63153	eu-153	mt=102,103,104,105,106,107	updated 08/12/94
63154	eu-154	mt=102,103,104,105,106,107	updated 08/12/94
63155	eu-155	mt=102,103,104,105,106,107	updated 08/12/94
63156	eu-156	mt=102	updated 08/12/94
63157	eu-157	mt= 102	updated 08/12/94
64000	gd (1030) sig0=1.+5p3 293k f-1/e-m vb 61479		updated 08/12/94

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 64154          gd-154          mt=102                                  updated 08/12/94
 64155          gd-155          mt=102                                  updated 08/12/94
 64156          gd-156          mt=102                                  updated 08/12/94
 64157          gd-157          mt=102                                  updated 08/12/94
 64158          gd-158          mt=102                                  updated 08/12/94
 64160          gd-160          mt=102                                  updated 08/12/94
 65159          tb-159          mt=102                                  updated 08/12/94
 65160          tb-160             mt=  102                             updated 08/12/94
 66160          dy-160          mt=102                                  updated 08/12/94
 66161          dy-161          mt=102                                  updated 08/12/94
 66162          dy-162          mt=102                                  updated 08/12/94
 66163          dy-163          mt=102                                  updated 08/12/94
 66164          dyprosium-164   endf/b-iv mat 1031                      updated 08/12/94
 67165          ho-165          mt=102                                  updated 08/12/94
 68166          er-166          mt=102                                  updated 08/12/94
 68167          er-167          mt=102                                  updated 08/12/94
 71175          lutetium-175    endf/b-iv mat 1032                      updated 08/12/94
 71176          lutetium-176    endf/b-iv mat 1033                      updated 08/12/94
 72000         hf(nat) 1034 218ngp wt 1/e p-3 sigp=5+4 293k re(042375)  updated 08/12/94
 73181          tantalum-181    endf/b-iv mat 1285                      updated 08/12/94
 74182          tungsten-182    endf/b-iv mat 1128                      updated 08/12/94
 74183          tungsten-183    endf/b-iv mat 1129                      updated 08/12/94
 74184          tungsten-184    endf/b-iv mat 1130                      updated 08/12/94
 74186          tungsten-186    endf/b-iv mat 1131                      updated 08/12/94
 75185         re-185 1083 sigp=5+4 newxlacs 218ngp p-3 293k            updated 08/12/94
 75187          rhenium-187     endf/b-iv mat 1084                      updated 08/12/94
 79197          gold-197        endf/b-iv mat 1283                      updated 08/12/94
 82000         pb   1288 218ngp 042375 p-3 293k                         updated 08/12/94
 90232         th-232 1296 sigp=5+4 newxlacs 218ngp p-3 293k            updated 08/12/94
 91233         pa-233 1297 218 gp wt f-1/e-m 090376 p3 293k             updated 08/12/94
 92233         u-233  1260 sigp=5+4 newxlacs 218ngp p-3 293k            updated 08/12/94
 92234         u-234 1043 sigo=5+4 newxlacs p-3 293k f-1/e-m(1.+5)      updated 08/12/94
 92235          uranium-235     endf/b-iv mat 1261                      updated 08/12/94
 92236         u-236 1163 sigo=5+4 newxlacs p-3 293k f-1/e-m(1.+5)      updated 08/12/94
 92238          uranium-238     endf/b-iv mat 1262                      updated 08/12/94
 93237          neptunium-237   endf/b-iv mat 1263                      updated 08/12/94
 94238         pu-238 1050 sigo=5+4 newxlacs p-3 293k f-1/e-m(1.+5)     updated 08/12/94
 94239          plutonium-239   endf/b-iv mat 1264                      updated 08/12/94
 94240          plutonium-240   endf/b-iv mat 1265                      updated 08/12/94
 94241          plutonium-241   endf/b-iv mat 1266                      updated 08/12/94
 94242          plutonium-242   endf/b-iv mat 1161                      updated 08/12/94
 95241         am-241 1056 sigp=5+4 newxlacs 218ngp p-3 293k            updated 08/12/94
 95243         am-243 1057 218 gp wt f-1/e-m 090376 p3 293k             updated 08/12/94
 96244          curium-244      endf/b-iv mat 1162                      updated 08/12/94
500000         jrk's neutron(9029) dose factors from ansi/ans-6.1.1-1977.
 17000         chlorine (mat 1149 from version iv) using 1/sigt weightiupdated 08/12/94
 45103          45rh103 hedl baw evalnov78 schenter livols       mod1 01/09/98
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M4.A.4 THE 238-GROUP ENDF/B-V LIBRARY

```
table of contents for  scale.rev08.xn238                        on logical unit  1
tape id                          238
number of nuclides               315
number of neutron groups         238
first thermal group              149
number of gamma groups             0
        scale - 238 neutron group library           based on endf-b version 5 data
          generated with a chi-1/e-maxwellian weight spectrum
            compiled for doe        8/18/94
              last updated          7/29/99
                n.m.greene & l.m.petrie    nuclear eng. appl. - cped - ornl
 24301           24CR BNL EVALDEC77 A.PRINCE AND T.     (1/esigt)  MOD2 11/18/91
 24304           24CR BNL EVALDEC77 A.PRINCE AND T.     (1/esigtSS304)  MOD2 11/18/91
 26301           26FE 0 ORNL EVALOCT77 C.Y.FU F.G.PE  (1/esigt)   MOD3 11/18/91
 26304           26FE 0 ORNL EVALOCT77 C.Y.FU F.G.PE  (1/esigtSS304)   MOD3 11/18/91
 28301           28NI 0 BNL NNDC EVALMAR77 M.DIVADEENAM (1/esigt) MOD2 11/18/91
 28304           28NI 0 BNL NNDC EVALMAR77 M.DIVADEENAM (1/esigtSS304) MOD2 11/18/91
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  1701          smiler for h-1 (hzrh)  tape 132, mat 7   5-14-98
 40701          smiler for zr (in zrh)  tape 133, mat 58   5-15-98
 19000          19k gga evalfeb67 m.k.drake                          mod1 lupdated 01/18/95
 92232          92u232 hedl evalnov77 mann                           mod1 11/14/97
 33075          33as 75 hedl evalapr74 r.e.schenter an               mod1 04/02/97
 56135          56ba135 hedl evalapr74 r.e.schenter an               mod1 04/02/97
 48110          48cd110 hedl evalapr74 r.e.schenter an               mod1 04/02/97
 48114          48cd114 hedl evalapr74 r.e.schenter an               mod1 04/02/97
 96244          96cm244 hedlsrllll evalapr78 mann benjamin h         mod2 11/14/97
 96248          96cm248 hedlsrllll evalapr78 mann benjamin h         mod1 11/14/97
 66160          66dy160 hedl evalapr74 r.e.schenter an               mod1 04/08/97
 66163          66dy163 hedl evalapr74 r.e.schenter an               mod1 04/09/97
 68166          68er166 hedl evalapr74 r.e.schenter an               mod1 04/23/97
 32074          32ge 74 hedl evalapr74 r.e.schenter an               mod1 04/23/97
 42096          42mo 96 hedl rcn evalfeb80 r.e.schenter an           mod1 04/23/97
 60145          60nd145 hedl bnl+ evalfeb80 schenter schmit          mod1 04/23/97
 60146          60nd146 hedl bnl+ evalfeb80 schenter schmit          mod1 04/24/97
 60150          60nd150 hedl bnl+ evalfeb80 schenter schmit          mod1 04/24/97
 46108          46pd108 hedl rcn evalfeb80 r.e.schenter an           mod1 04/24/97
 34076          34se 76 hedl evalapr74 r.e.schenter an               mod1 04/24/97
 34078          34se 78 hedl evalapr74 r.e.schenter an               mod1 04/24/97
 62152          62sm152 hedl bnl+ evalfeb80 schenter schmit          mod1 04/29/97
 62154          62sm154 hedl evalapr74 r.e.schenter an               mod1 04/29/97
 52122          52te122 hedl evalapr74 r.e.schenter an               mod1 04/29/97
  4309          be metal 13041064                                    mod2 04/29/97
 60143          60nd143 hedl bnl+ evalfeb80 schenter schmit          mod1 04/23/97
 62147          62sm147 hedl bnl+ evalfeb80 schenter + man           mod2 04/24/97
    99          collected weight functions for use in collapsing     updated 5/12/95
   900          neutron dose factors from ansl/ans 6.1.1-1977        updated 5/12/95
  1802          1d 20lasl eval nov67 l.stewart lasl mod2 12/11/92 free gas
  2003          2he 30lasl evaljun68 leona stewart mod1 12/23/92 free gas
  2004          2he 40lasl evaloct73 nisley hale young mod0 12/23/92 free gas
  3006          3li0060lasl eval sep77 g.hale l.stewart mod1 12/11/92 free gas
  3007          3li 7 lanl evaldec81 p.g.young mod1 12/11/92 free gas
  4009          4be 9 free gas. lll evaloct76 howerton/perkins   mod 08/17/94
  5010          5b 100lasl evaldec76 g.hale l.stewart mod1 12/11/92 free gas
  5011          5b11 gebnl evalsep71 c.cowan mod1 12/11/92 free gas
  6012          6c ornl evaldec73 c.y.fu and f.g. perey mod2 12/11/92 free gas
  7015          7n 15 lasl evalmar77 e.arthur p.youn                 mod1 12/16/88
 40096          40zr 96 sai evalapr76 m.drake d.sa                   mod2 01/04/89
 74183          74w183 las anl brcevaldec80 arthur young sm          mod2 01/04/89
 74184          74w184 las anl brcevaldec80 arthur young sm          mod2 01/05/89
 92238          92U 238 ANL+ EVALJUN77 E.PENNINGTON A.               MOD3 02/13/92
701501          7n 15 from version 6 evaluation
 14000          14si 0 ornl evalfeb74 larson perey dr                mod3 12/20/88
 63154          EU-154 FROM VERSION 6 OF ENDFB (2/9/93)
 63155          EU-155 FROM VERSION 6 OF ENDFB (6/30/93)
631541          63eu154 bnl evaldec73 h.takahashi                    mod1 12/28/88
631551          63eu155 bnl hedl + evaldec79 princeschenter          mod1 01/16/89
 94241          AMPX MASTER FILE FOR ENDF MAT 1381  ***  PU-241 ***
 92233          AMPX MASTER FILE FOR ENDF MAT 1393  ***  U-233  ***
 43099          43TC 99 HEDL BAW EVALNOV78 SCHENTER LIVOLS           MOD2 01/18/91
 40091          40ZR 91 SAI EVALAPR76 M.DRAKE D.SA                   MOD2 01/18/91
 13027          13al 270lasl evaldec73 p.g. young d.g                mod1 11/29/88
 27059          27co 59 bnl evaljun77 s.mughabghab                   mod3 12/20/88
 24000          24cr bnl evaldec77 a.prince and t.                   mod2 11/29/88
  9019          9f 19 ornl evaljul74 c.y.fu d.c.lars                 mod3 12/16/88
 26000          26fe 0 ornl evaloct77 c.y.fu f.g.pe                  mod3 11/29/88
 25055          25mn 55 bnl evalmar77 s.f. mughabghab                mod2 12/20/88
 42000          42mo 111 hedl evalfeb79 howerton schmit              mod1 02/17/89
 11023          11na 23 ornl evaldec77 d. c. larson                  mod3 11/29/88
 41093          41nb 93 anl lll evalmay74 r.howerton lll             mod1 12/28/88
 28000          28ni 0 bnl nndc evalmar77 m.divadeenam               mod2 11/29/88
 37085          37rb 85 bnlbrc evaloct79 a. prince                   mod1 01/03/89
 37087          37rb 87 bnlbrc evaloct79 a. prince                   mod1 12/29/88
 45103          45rh103 hedl baw evalnov78 schenter livols           mod1 12/28/88
 16000          16 s 0 bnl evalapr79 divadeenam                      mod1 12/20/88
 90232          90th232 bnl-evaldec77 bhat smith leon                mod2 01/05/89
 40000          40zr sai evalapr76 m.drake d.sa                      mod2 01/03/89
 40090          40zr 90 sai evalapr76 m.drake d.sa                   mod2 01/04/89
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40092          40zr 92 sai evalapr76 m.drake d.sa                mod2 01/04/89
40094          40zr 94 sai evalapr76 m.drake d.sa                mod2 01/04/89
 6312          graphite 1306/1065 96 angles 10/21/92 jpr eval.
61601          61PM148MHEDL INEL EVALDEC79 SCHENTER SCHMIT       MOD1 01/22/91
 8016          80 16 from version 6 evaluation
 1901          hydrogen in ch2   1301/1114          11/25/92
 1002          deuterium in d2o  1302/1004   96 angles    11/13/92
 1001          hydrogen in water 1301/1002    mod1   11/23/92
  999         1/v function (normalized to 1.0 at 2200m/s<==>0.0253ev)
96242          96CM242 HEDLSRLLLL EVALAPR78 MANN BENJAMIN H      MOD1 01/18/91
66164          66DY164 BNW EVALJUN67 B.R.LEONARD JR.             MOD1 01/18/91
63151          63EU151 BNL EVALDEC77 S.F. MUGHABGHAB             MOD1 01/21/91
64155          64GD155 BNL EVALJAN77 B.A.MAGURNO                 MOD1 01/21/91
64157          64GD157 BNL EVALJAN77 B.A.MAGURNO                 MOD1 01/18/91
72176          72HF176 SAI EVALAPR76 M.DRAKE D.SA                MOD1 01/18/91
72179          72HF179 SAI EVALAPR76 M.DRAKE D.SA                MOD1 01/18/91
60144          60ND144 HEDL EVALFEB80 SCHENTER SCHMIT            MOD1 01/22/91
93237          93NP237 HEDL SRL + EVALAPR78 MANN BENJAMIN S      MOD2 01/23/91
91231          91PA231 HEDL EVALNOV77 MANN                       MOD1 01/18/91
94236          94PU236 HEDL SRL EVALAPR78 MANN SCHENTER B        MOD1 01/18/91
94237          94PU237 HEDL EVALAPR78 MANN AND SCHENT            MOD1 01/18/91
94238          94PU238 HEDL AI + EVALAPR78 MANN SCHENTER A       MOD3 01/18/91
94242          94PU242 HEDL SRL + EVALOCT78 MANN BENJAMIN M      MOD2 01/21/91
94243          94PU243 BNL SRL LLLEVALJUL76 KINSEYASSEMBLE       MOD1 01/18/91
94244          94PU244 HEDL SRL EVALAPR78 MANN SCHENTER B        MOD1 01/18/91
73181          73TA181 LLL EVALJAN72 HOWERTON PERKI              MOD2 01/22/91
90230          90TH230 HEDL EVALNOV77 MANN                       MOD1 01/18/91
92234          92U 234 BNL HEDL + EVALJUL78 DIVADEENAM MANN      MOD3 01/10/91
92236          92U 236 BNL HEDL + EVALJUL78 DIVADEENAM MANN      MOD3 01/23/91
47107          47ag107 bnl hedl evaljun83 a.prince r.e.sc        mod2 01/04/89
47109          47ag109 bnl hedl evaljun83 a.prince r.e.sc        mod2 01/04/89
47111          47ag111 hedl inel evaldec79 schenter schmit       mod1 01/12/89
95241          95am241 hedl ornl evalapr78 mann schenter         mod2 01/10/90
95601          95am242mhedlsrllll evalapr78 mann benjamin h      mod1 01/16/90
95243          95am243 hedlsrllll evalapr78 mann benjamin h      mod2 01/10/90
79197          79au197 bnl evalfeb77 s.f.mughabghab              mod3 01/04/89
56134          56ba134 hedl evalapr74 r.e.schenter an            mod1 01/13/89
56136          56ba136 hedl evalapr74 r.e.schenter an            mod1 01/13/89
56137          56ba137 hedl evalapr74 r.e.schenter an            mod1 01/13/89
56138          56ba138 lll evalaug78 howerton                    mod1 01/03/89
56140          56ba140 hedl inel evaldec79 schenter schmit       mod1 01/13/89
83209          83bi209 anl lll evalapr80 d.smith a.smith         mod1 01/04/89
35079          35br 79 hedl evalapr74 r.e.schenter an            mod1 01/11/89
35081          35br 81 hedl evalapr74 r.e.schenter an            mod1 01/11/89
20000          20ca ornl evalaug71 c.y.fu and d.m.               mod3 12/20/88
48000          48cd bnl evalmay74 s.pearlstein tr                mod1 01/03/89
48106          48cd106 hedl evalfeb80 f.m.mann                   mod2 01/12/89
48108          48cd108 hedl evalapr74 r.e.schenter an            mod1 01/12/89
48111          48cd111 hedl evalapr74 r.e.schenter an            mod1 01/12/89
48112          48cd112 hedl evalapr74 r.e.schenter an            mod1 01/12/89
48113          48cd113 bnl hedl evalnov78 pearlstein mann        mod1 01/03/89
48601          48cd115mhedl inel evaldec79 schenter schmit       mod1 01/12/89
48116          48cd116 hedl evalapr74 r.e.schenter an            mod1 01/12/89
58140          58ce140 hedl evalapr74 r.e.schenter an            mod1 01/13/89
58141          58ce141 hedl inel evaldec79 schenter schmit       mod1 01/13/89
58142          58ce142 hedl evalapr74 r.e.schenter an            mod1 01/13/89
58143          58ce143 hedl inel evaldec79 schenter schmit       mod1 01/13/89
58144          58ce144 hedl inel evaldec79 schenter schmit       mod1 01/16/89
98249          cf249 bnl srl lllevaljul76 kinseyassemble         mod1 01/12/89
98251          98cf251 bnl srl lllevaljul76 kinseyassemble        mod1 01/10/89
98252          98cf252 bnl srl lllevaljul76 kinseyassemble        mod1 01/10/89
17000          17cl gga evalfeb67 m.s.allen and m                 mod1 03/14/89
96241          96cm241 hedl evalapr78 mann and schent            mod1 01/10/90
96243          96cm243 hedlsrllll evalapr78 mann benjamin h      mod1 01/10/90
96245          96cm245 srl lll evaljan79 benjamin and ho         mod2 01/05/89
96246          96cm246 bnl srl lllevaljul76 kinseyassemble        mod1 01/10/90
96247          96cm247 bnl srl lllevaljul76 kinseyassemble        mod1 01/10/89
55133          55cs133 hedl bnl evalnov78 schenter bhat p         mod1 01/03/89
55134          55cs134 hedl inel evaldec79 schenter schmit        mod1 01/13/89
55135          55cs135 hedl inel evaldec79 schenter schmit        mod1 01/13/89
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55136	55cs136 hedl inel evaldec79 schenter schmit	mod1 01/13/89
55137	55cs137 hedl inel evaldec79 schenter schmit	mod1 01/13/89
29000	29cu ornl sai evaldec73 fu drake fricke	mod1 12/20/88
66161	66dy161 hedl evalapr74 r.e.schenter an	mod1 01/16/89
66162	66dy162 hedl evalapr74 r.e.schenter an	mod1 04/03/89
68167	68er167 hedl evalapr74 r.e.schenter an	mod1 04/03/89
99253	99es253 bnl srl evaljul76 kinsey benjamin	mod1 01/10/89
63000	63eu nndc evalaug81 autocombined	mod1 01/04/89
63152	63eu152 bnl evaldec73 h.takahashi	mod2 02/28/89
63153	63eu153 bnl evalfeb78 s.mughabghab	mod1 01/03/89
63156	63eu156 hedl inel evaldec79 schenter schmit	mod1 01/16/89
63157	63eu157 hedl evalfeb80 r.e.schenter an	mod1 01/17/89
31000	31ga lll lasl evalmay80 howerton young	mod1 12/21/88
64152	64gd152 bnl evaljan77 b.a.magurno	mod2 01/03/89
64154	64gd154 bnl evaljan77 b.a.magurno	mod1 01/03/89
64156	64gd156 bnl evaljan77 b.a.magurno	mod2 01/04/89
64158	64gd158 bnl evaljan77 b.a.magurno	mod1 01/04/89
64160	64gd160 bnl evaljan77 b.a.magurno	mod1 01/04/89
32072	32ge 72 hedl evalapr74 r.e.schenter an	mod1 01/11/89
32073	32ge 73 hedl evalapr74 r.e.schenter an	mod1 01/11/89
32076	32ge 76 hedl evalapr74 r.e.schenter an	mod1 01/11/89
1801	1h 101asl evalaug70 l.stewart r.j.	mod1 12/16/88
72000	72hf sai evalapr76 m.drake d.sa	mod1 01/04/89
72174	72hf174 sai evalapr76 m.drake d.sa	mod1 03/21/89
72177	72hf177 sai evalapr76 m.drake d.sa	mod1 03/21/89
72178	72hf178 sai evalapr76 m.drake d.sa	mod1 03/21/89
72180	72hf180 sai evalapr76 m.drake d.sa	mod1 01/04/89
67165	67ho165 hedl evalapr74 r.e.schenter an	mod1 01/16/89
53127	53i 127 hedl rcn evalfeb80 r.e.schenter an	mod1 01/13/89
53129	53i 129 hedl inel+ evalfeb80 schenter schmit	mod1 01/13/89
53130	53i 130 hedl inel evaldec79 schenter schmit	mod1 01/13/89
53131	53i 131 hedl inel evaldec79 schenter schmit	mod1 01/13/89
53135	53i 135 hedl inel evaldec79 schenter schmit	mod1 01/13/89
49113	49in113 hedl evalapr74 r.e.schenter an	mod1 01/12/89
49115	49in115 hedl inel evaldec79 schenter schmit	mod1 01/12/89
36078	36kr 78 bnl evalapr78 a.prince	mod1 12/29/88
36080	36kr 80 bnl evalapr78 a.prince	mod1 12/29/88
36082	36kr 82 bnl evalapr78 a.prince	mod1 12/29/88
36083	36kr 83 bnl evalapr78 a.prince	mod1 12/29/88
36084	36kr 84 bnl evalapr78 a.prince	mod1 12/29/88
36085	36kr 85 hedl inel evaldec79 schenter schmit	mod1 01/11/89
36086	36kr 86 bnl evaljul72 a.prince	mod1 12/30/88
57139	57la139 hedl rcn evalfeb80 r.e.schenter an	mod1 01/13/89
57140	57la140 hedl inel evaldec79 schenter schmit	mod1 01/13/89
71175	71lu175 bnw evaljun67 b.r.leonard jr.	mod1 12/22/88
71176	71lu176 bnw evaljun67 b.r.leonard jr.	mod1 12/22/88
12000	12mg ornl evalfeb78 d.c.larson	mod1 12/16/88
42092	42mo 92 hedl evalfeb80 f.m.mann	mod1 01/12/89
42094	42mo 94 hedl rcn evalfeb80 r.e.schenter an	mod1 01/11/89
42095	42mo 95 hedl rcn evalfeb80 r.e.schenter an	mod1 01/11/89
42097	42mo 97 hedl rcn evalfeb80 r.e.schenter an	mod1 01/12/89
42098	42mo 98 hedl rcn evalfeb80 r.e.schenter an	mod1 01/12/89
42099	42mo 99 hedl inel evaldec79 schenter schmit	mod1 01/12/89
42100	42mo100 hedl rcn evalfeb80 r.e.schenter an	mod1 01/12/89
7014	7n 14 lasl evaljul73 p.young d.fost	mod2 11/28/88
41094	41nb 94 hedl inel evaldec79 schenter schmit	mod1 01/11/89
41095	41nb 95 hedl inel evaldec79 schenter schmit	mod1 01/11/89
60142	60nd142 hedl evalapr74 r.e.schenter an	mod1 01/16/89
60147	60nd147 hedl inel evaldec79 schenter schmit	mod1 01/16/89
60148	60nd148 hedl bnl+ evalfeb80 schenter schmit	mod1 03/21/89
8017	8o 17 bnl evaljan78 b.a.magurno	mod1 12/20/88
15031	15p 31 lll evaloct77 howerton	mod1 12/20/88
82000	82pb ornl evaljul71 c.y.fu and f.g.	mod2 01/04/89
46102	46pd102 hedl evalfeb80 f.m.mann	mod2 01/12/89
46104	46pd104 hedl rcn evalfeb80 r.e.schenter an	mod1 01/12/89
46105	46pd105 hedl rcn evalfeb80 r.e.schenter an	mod1 01/12/89
46106	46pd106 hedl rcn evalfeb80 r.e.schenter an	mod1 01/12/89
46107	46pd107 hedl inel+ evalfeb80 schenter schmit	mod1 01/12/89
46110	46pd110 hedl rcn evalfeb80 r.e.schenter an	mod1 01/12/89
61147	61pm147 hedl inel +evalfeb80 schenter + rei	mod1 01/16/89

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61148    61pm148 hedl inel evaldec79 schenter schmit      mod1 01/16/89
61149    61pm149 hedl inel evaldec79 schenter schmit      mod1 01/16/89
61151    61pm151 hedl inel evaldec79 schenter schmit      mod1 01/16/89
59141    59pr141 hedl bnl+ evalfeb80 schenter schmit      mod1 03/21/89
59142    59pr142 hedl inel evaldec79 schenter schmit      mod1 01/16/89
59143    59pr143 hedl inel evaldec79 schenter schmit      mod1 01/16/89
94239    94pu239 lanl jun83 e.arthur p.you                mod2 02/28/89
94240    94pu240 ornl evalapr77 l.w. weston               mod3 12/12/88
37086    37rb 86 hedl inel evaldec79 schenter schmit      mod1 01/11/89
75185    75re185 ge nmpo evaljan68 w.b.henderson a        mod1 12/22/88
75187    75re187 ge nmpo evaljan68 w.b.henderson a        mod1 12/22/88
45105    45rh105 hedl inel evaldec79 schenter schmit      mod2 01/12/89
44096    44ru 96 hedl evalfeb80 f.m.mann                  mod2 01/12/89
44098    44ru 98 hedl evalfeb80 f.m.mann                  mod2 01/12/89
44099    44ru 99 hedl evalapr74 r.e.schenter an           mod1 01/12/89
44100    44ru100 hedl rcn evalfeb80 r.e.schenter an       mod1 01/12/89
44101    44ru101 hedl rcn evalfeb80 r.e.schenter an       mod1 01/12/89
44102    44ru102 hedl rcn evalfeb80 r.e.schenter an       mod1 01/12/89
44103    44ru103 hedl inel evaldec79 schenter schmit      mod1 01/12/89
44104    44ru104 hedl rcn evalfeb80 r.e.schenter an       mod1 01/12/89
44105    44ru105 hedl inel evaldec79 schenter schmit      mod1 01/12/89
44106    44ru106 hedl inel evaldec79 schenter schmit      mod1 01/12/89
16032    16s 32 lll evaloct77 howerton                    mod1 12/20/88
51121    51sb121 hedl rcn evalfeb80 r.e.schenter an       mod1 01/13/89
51123    51sb123 hedl rcn evalfeb80 r.e.schenter an       mod1 01/13/89
51124    51sb124 hedl inel evaldec79 schenter schmit      mod1 01/13/89
51125    51sb125 hedl inel evaldec79 schenter schmit      mod1 01/13/89
51126    51sb126 hedl inel evaldec79 schenter schmit      mod1 01/13/89
34074    34se 74 hedl evalfeb80 f.m.mann                  mod2 03/21/89
34077    34se 77 hedl evalapr74 r.e.schenter an           mod1 01/11/89
34080    34se 80 hedl evalapr74 r.e.schenter an           mod1 03/21/89
34082    34se 82 hedl evalapr74 r.e.schenter an           mod1 01/11/89
62144    62sm144 hedl evalfeb80 f.m.mann                  mod2 01/16/89
62148    62sm148 hedl evalfeb80 schenter schmit           mod1 01/16/89
62149    62sm149 hedl bnw evalnov78 schenter leonar       mod1 01/03/89
62150    62sm150 hedl evalapr74 r.e.schenter an           mod1 03/21/89
62151    62sm151 hedl inel +evalfeb80 schenter + rei      mod1 01/16/89
62153    62sm153 hedl inel evaldec79 schenter schmit      mod1 01/16/89
50112    50sn112 hedl evalfeb80 f.m.mann                  mod2 01/12/89
50114    50sn114 hedl evalfeb80 f.m.mann                  mod2 01/12/89
50115    50sn115 hedl evalapr74 r.e.schenter an           mod1 01/12/89
50116    50sn116 hedl evalapr74 r.e.schenter an           mod1 01/12/89
50117    50sn117 hedl evalapr74 r.e.schenter an           mod1 01/12/89
50118    50sn118 hedl evalapr74 r.e.schenter an           mod1 01/12/89
50119    50sn119 hedl evalapr74 r.e.schenter an           mod1 01/12/89
50120    50sn120 hedl evalapr74 r.e.schenter an           mod1 01/12/89
50122    50sn122 hedl evalapr74 r.e.schenter an           mod1 01/12/89
50123    50sn123 hedl inel evaldec79 schenter schmit      mod1 01/12/89
50124    50sn124 hedl evalapr74 r.e.schenter an           mod1 01/12/89
50125    50sn125 hedl inel evaldec79 schenter schmit      mod1 01/13/89
50126    50sn126 hedl inel evaldec79 schenter schmit      mod1 01/12/89
38084    38sr 84 hedl evalfeb80 f.m.mann                  mod2 01/11/89
38086    38sr 86 hedl evalapr74 r.e.schenter an           mod1 01/11/89
38087    38sr 87 hedl evalapr74 r.e.schenter an           mod1 01/11/89
38088    38sr 88 hedl evalapr74 r.e.schenter an           mod1 01/11/89
38089    38sr 89 hedl inel evaldec79 schenter schmit      mod1 01/11/89
38090    38sr 90 hedl inel evaldec79 schenter schmit      mod1 01/11/89
 1003    1t 30lasl evalfeb65 leona stewart                mod2 12/16/88
73182    73ta182 ai evalapr71 j.otter c.dunfo             mod1 12/22/88
65159    65tb159 hedl rcn evalfeb80 r.e.schenter an       mod1 01/16/89
65160    65tb160 hedl inel evaldec79 schenter schmit      mod1 01/16/89
52120    52te120 hedl evalfeb80 f.m.mann                  mod2 01/13/89
52123    52te123 hedl evalapr74 r.e.schenter an           mod1 03/21/89
52124    52te124 hedl evalapr74 r.e.schenter an           mod1 01/13/89
52125    52te125 hedl evalapr74 r.e.schenter an           mod1 01/13/89
52126    52te126 hedl evalapr74 r.e.schenter an           mod1 01/13/89
52601    52te127mhedl inel evaldec79 schenter schmit      mod1 01/13/89
52128    52te128 hedl evalapr74 r.e.schenter an           mod1 01/13/89
52611    52te129mhedl inel evaldec79 schenter schmit      mod1 01/13/89
52130    52te130 hedl evalapr74 r.e.schenter an           mod1 01/13/89
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 52132          52te132 hedl inel evaldec79 schenter schmit      mod1 01/13/89
 22000          22ti buranllll evalaug77 c.philis a.smit        mod1 12/20/88
 92235          92u 235 bnl evalapr77 m.r.bhat                  mod3 02/28/89
 92237          92u237 bnl srl lllevaljul76 kinseyassemble       mod1 01/10/89
 23000          23v anllllhedl evaljan77 a.smith+ h.howe        mod1 12/20/88
 74000          74w lanl evalmar82 e.d.arthur                   mod1 01/04/89
 74182          74w182 las anl brcevaldec80 arthur young sm     mod2 01/04/89
 74186          74w186 las anl brcevaldec80 arthur young sm     mod2 01/05/89
 54124          54xe124 bnl evalmar78 m.r.bhat and s.           mod1 12/29/88
 54126          54xe126 bnl evalmar78 m.r.bhat and s.           mod1 12/29/88
 54128          54xe128 bnl evalmar78 m.r.bhat and s.           mod1 12/30/88
 54129          54xe129 bnl evalmar78 m.r.bhat and s.           mod1 01/03/89
 54130          54xe130 bnl evalmar78 m.r.bhat and s.           mod1 12/30/88
 54131          54xe131 bnl evalmar78 m.r.bhat and s.           mod1 01/03/89
 54132          54xe132 bnl evalmar78 m.r.bhat and s.           mod2 01/03/89
 54133          54xe133 hedl inel evaldec79 schenter schmit     mod1 01/13/89
 54134          54xe134 bnl evalmar78 m.r.bhat and s.           mod1 01/03/89
 54135          54xe135 bnw evaljun67 b.r.leonard jr.           mod1 12/28/88
 54136          54xe136 bnl evalmar78 m.r.bhat and s.           mod1 01/03/89
 39089          39y 89 hedl evalapr74 r.e.schenter an           mod1 01/11/89
 39090          39y 90 hedl inel evaldec79 schenter schmit      mod1 01/11/89
 39091          39y 91 hedl inel evaldec79 schenter schmit      mod1 01/11/89
 40093          40zr 93 hedl inel evaldec79 schenter schmit     mod1 01/11/89
 40095          40zr 95 hedl inel evaldec79 schenter schmit     mod1 01/11/89
801601          8o 16 lasl evalaug73 p.young d.fost             mod2 12/16/88
701401          7n 14 from version 6 evaluation
 98250          98cf250 bnl srl lllevaljul76 kinseyassemble     mod1 11/14/97
 91233          91PA233 HEDL INEL EVALMAY78 MANN SCHENTER R     MOD2 01/18/91
 97249          97bk249 bnl srl lllevaljul76 kinseyassemble     mod1 01/11/89
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M4.A.5 THE 44-GROUP ENDF/B-V LIBRARY

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table of contents for  scale.rev10.xn44                        on logical unit  1
tape id                          44
number of nuclides              315
number of neutron groups         44
first thermal group              23
number of gamma groups            0
        scale - 44 neutron group library           based on endf-b version 5 data
          collapsed with a light water reactor cell flux spectrum from 238 groups
            compiled for nrc        9/01/94
              last updated          7/29/99
                m.d.dehart & l.m.petrie    nuclear eng. appl. - cped - ornl
 24301          24CR BNL EVALDEC77 A.PRINCE AND T.    (1/esigt)  MOD2 11/18/91
 24304          24CR BNL EVALDEC77 A.PRINCE AND T.    (1/esigtSS304)  MOD2 11/18/91
 26301          26FE 0 ORNL EVALOCT77 C.Y.FU F.G.PE  (1/esigt)   MOD3 11/18/91
 26304          26FE 0 ORNL EVALOCT77 C.Y.FU F.G.PE  (1/esigtSS304)   MOD3 11/18/91
 28301          28NI 0 BNL NNDC EVALMAR77 M.DIVADEENAM (1/esigt) MOD2 11/18/91
 28304          28NI 0 BNL NNDC EVALMAR77 M.DIVADEENAM (1/esigtSS304) MOD2 11/18/91
  1701            smiler for h-1 (hzrh)  tape 132, mat 7   5-14-98
 40701            smiler for zr (in zrh)  tape 133, mat 58   5-15-98
 19000          19k gga evalfeb67 m.k.drake                      mod1 1updated 01/18/95
 92232          92u232 hedl evalnov77 mann                       mod1 11/14/97
 33075          33as 75 hedl evalapr74 r.e.schenter an           mod1 04/02/97
 56135          56ba135 hedl evalapr74 r.e.schenter an           mod1 04/02/97
 48110          48cd110 hedl evalapr74 r.e.schenter an           mod1 04/02/97
 48114          48cd114 hedl evalapr74 r.e.schenter an           mod1 04/02/97
 96244          96cm244 hedlsrllll evalapr78 mann benjamin h     mod2 11/14/97
 96248          96cm248 hedlsrllll evalapr78 mann benjamin h     mod1 11/14/97
 66160          66dy160 hedl evalapr74 r.e.schenter an           mod1 04/08/97
 66163          66dy163 hedl evalapr74 r.e.schenter an           mod1 04/09/97
 68166          68er166 hedl evalapr74 r.e.schenter an           mod1 04/23/97
 32074          32ge 74 hedl evalapr74 r.e.schenter an           mod1 04/23/97
 42096          42mo 96 hedl rcn evalfeb80 r.e.schenter an       mod1 04/23/97
 60145          60nd145 hedl bnl+ evalfeb80 schenter schmit      mod1 04/23/97
 60146          60nd146 hedl bnl+ evalfeb80 schenter schmit      mod1 04/24/97
 60150          60nd150 hedl bnl+ evalfeb80 schenter schmit      mod1 04/24/97
 46108          46pd108 hedl rcn evalfeb80 r.e.schenter an       mod1 04/24/97
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 34076          34se 76 hedl evalapr74 r.e.schenter an                mod1 04/24/97
 34078          34se 78 hedl evalapr74 r.e.schenter an                mod1 04/24/97
 62152          62sm152 hedl bnl+ evalfeb80 schenter schmit           mod1 04/29/97
 62154          62sm154 hedl evalapr74 r.e.schenter an                mod1 04/29/97
 52122          52te122 hedl evalapr74 r.e.schenter an                mod1 04/29/97
  4309          be metal 13041064                                     mod2 04/29/97
 60143          60nd143 hedl bnl+ evalfeb80 schenter schmit           mod1 04/23/97
 62147          62sm147 hedl bnl+ evalfeb80 schenter + man            mod2 04/24/97
    99          collected weight functions for use in collapsing    updated 5/12/95
   900          neutron dose factors from ansl/ans 6.1.1-1977       updated 5/12/95
  1802          1d 20lasl eval nov67 l.stewart lasl mod2 12/11/92 free gas
  2003          2he 30lasl evaljun68 leona stewart mod1 12/23/92 free gas
  2004          2he 40lasl evaloct73 nisley hale young mod0 12/23/92 free gas
  3006          3li0060lasl eval sep77 g.hale l.stewart mod1 12/11/92 free gas
  3007          3li 7 lanl evaldec81 p.g.young mod1 12/11/92 free gas
  4009          4be 9 free gas. lll evaloct76 howerton/perkins   mod 08/17/94
  5010          5b 100lasl evaldec76 g.hale l.stewart mod1 12/11/92 free gas
  5011          5b11 gebnl evalsep71 c.cowan mod1 12/11/92 free gas
  6012          6c ornl evaldec73 c.y.fu and f.g. perey mod2 12/11/92 free gas
  7015           7n 15 lasl evalmar77 e.arthur p.youn                 mod1 12/16/88
 40096           40zr 96 sai evalapr76 m.drake d.sa                   mod2 01/04/89
 74183           74w183 las anl brcevaldec80 arthur young sm          mod2 01/04/89
 74184           74w184 las anl brcevaldec80 arthur young sm          mod2 01/05/89
 92238           92U 238 ANL+ EVALJUN77 E.PENNINGTON A.               MOD3 02/13/92
701501           7n 15 from version 6 evaluation
 14000           14si 0 ornl evalfeb74 larson perey dr                mod3 12/20/88
 63154          EU-154 FROM VERSION 6 OF ENDFB (2/9/93)
 63155          EU-155 FROM VERSION 6 OF ENDFB (6/30/93)
631541           63eu154 bnl evaldec73 h.takahashi                    mod1 12/28/88
631551           63eu155 bnl hedl + evaldec79 princeschenter          mod1 01/16/89
 94241          AMPX MASTER FILE FOR ENDF MAT 1381  ***  PU-241 ***
 92233          AMPX MASTER FILE FOR ENDF MAT 1393  ***  U-233  ***
 43099           43TC 99 HEDL BAW EVALNOV78 SCHENTER LIVOLS           MOD2 01/18/91
 40091           40ZR 91 SAI EVALAPR76 M.DRAKE D.SA                   MOD2 01/18/91
 13027           13al 270lasl evaldec73 p.g. young d.g                mod1 11/29/88
 27059           27co 59 bnl evaljun77 s.mughabghab                   mod3 12/20/88
 24000           24cr bnl evaldec77 a.prince and t.                   mod2 11/29/88
  9019           9f 19 ornl evaljul74 c.y.fu d.c.lars                 mod3 12/16/88
 26000           26fe 0 ornl evaloct77 c.y.fu f.g.pe                  mod3 11/29/88
 25055           25mn 55 bnl evalmar77 s.f. mughabghab                mod2 12/20/88
 42000           42mo lll hedl evalfeb79 howerton schmit              mod1 02/17/89
 11023           11na 23 ornl evaldec77 d. c. larson                  mod3 11/29/88
 41093           41nb 93 anl lll evalmay74 r.howerton lll             mod1 12/28/88
 28000           28ni 0 bnl nndc evalmar77 m.divadeenam               mod2 11/29/88
 37085           37rb 85 bnlbrc evaloct79 a. prince                   mod1 01/03/89
 37087           37rb 87 bnlbrc evaloct79 a. prince                   mod1 12/29/88
 45103           45rh103 hedl baw evalnov78 schenter livols           mod1 12/28/88
 16000           16 s 0 bnl evalapr79 divadeenam                      mod1 12/20/88
 90232           90th232 bnl evaldec77 bhat smith leon                mod2 01/05/89
 40000           40zr sai evalapr76 m.drake d.sa                      mod2 01/03/89
 40090           40zr 90 sai evalapr76 m.drake d.sa                   mod2 01/04/89
 40092           40zr 92 sai evalapr76 m.drake d.sa                   mod2 01/04/89
 40094           40zr 94 sai evalapr76 m.drake d.sa                   mod2 01/04/89
  6312          graphite 1306/1065 96 angles 10/21/92 jpr eval.
 61601           61PM148MHEDL INEL EVALDEC79 SCHENTER SCHMIT          MOD1 01/22/91
  8016           8O 16 from version 6 evaluation
  1901          hydrogen in ch2   1301/1114          11/25/92
  1002          deuterium in d2o  1302/1004   96 angles    11/13/92
  1001          hydrogen in water 1301/1002    mod1   11/23/92
   999          1/v function (normalized to 1.0 at 2200m/s<==>0.0253ev)
 96242           96CM242 HEDLSRLLLL EVALAPR78 MANN BENJAMIN H         MOD1 01/18/91
 66164           66DY164 BNW EVALJUN67 B.R.LEONARD JR.                MOD1 01/18/91
 63151           63EU151 BNL EVALDEC77 S.F. MUGHABGHAB                MOD1 01/21/91
 64155           64GD155 BNL EVALJAN77 B.A.MAGURNO                    MOD1 01/21/91
 64157           64GD157 BNL EVALJAN77 B.A.MAGURNO                    MOD1 01/18/91
 72176           72HF176 SAI EVALAPR76 M.DRAKE D.SA                   MOD1 01/18/91
 72179           72HF179 SAI EVALAPR76 M.DRAKE D.SA                   MOD1 01/18/91
 60144           60ND144 HEDL EVALFEB80 SCHENTER SCHMIT               MOD1 01/22/91
 93237           93NP237 HEDL SRL + EVALAPR78 MANN BENJAMIN S         MOD2 01/23/91
 91231           91PA231 HEDL EVALNOV77 MANN                          MOD1 01/18/91
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94236	94PU236 HEDL SRL EVALAPR78 MANN SCHENTER B	MOD1 01/18/91
94237	94PU237 HEDL EVALAPR78 MANN AND SCHENT	MOD1 01/18/91
94238	94PU238 HEDL AI + EVALAPR78 MANN SCHENTER A	MOD3 01/18/91
94242	94PU242 HEDL SRL + EVALOCT78 MANN BENJAMIN M	MOD2 01/21/91
94243	94PU243 BNL SRL LLLEVALJUL76 KINSEYASSEMBLE	MOD1 01/18/91
94244	94PU244 HEDL SRL EVALAPR78 MANN SCHENTER B	MOD1 01/18/91
73181	73TA181 LLL EVALJAN72 HOWERTON PERKI	MOD2 01/22/91
90230	90TH230 HEDL EVALNOV77 MANN	MOD1 01/18/91
92234	92U 234 BNL HEDL + EVALJUL78 DIVADEENAM MANN	MOD3 01/10/91
92236	92U 236 BNL HEDL + EVALJUL78 DIVADEENAM MANN	MOD3 01/23/91
47107	47ag107 bnl hedl evaljun83 a.prince r.e.sc	mod2 01/04/89
47109	47ag109 bnl hedl evaljun83 a.prince r.e.sc	mod2 01/04/89
47111	47ag111 hedl inel evaldec79 schenter schmit	mod1 01/12/89
95241	95am241 hedl ornl evalapr78 mann schenter	mod2 01/10/90
95601	95am242mhedlsrllll evalapr78 mann benjamin h	mod1 01/16/90
95243	95am243 hedlsrllll evalapr78 mann benjamin h	mod2 01/10/90
79197	79au197 bnl evalfeb77 s.f.mughabghab	mod3 01/04/89
56134	56ba134 hedl evalapr74 r.e.schenter an	mod1 01/13/89
56136	56ba136 hedl evalapr74 r.e.schenter an	mod1 01/13/89
56137	56ba137 hedl evalapr74 r.e.schenter an	mod1 01/13/89
56138	56ba138 lll evalaug78 howerton	mod1 01/03/89
56140	56ba140 hedl inel evaldec79 schenter schmit	mod1 01/13/89
83209	83bi209 anl lll evalapr80 d.smith a.smith	mod1 01/04/89
35079	35br 79 hedl evalapr74 r.e.schenter an	mod1 01/11/89
35081	35br 81 hedl evalapr74 r.e.schenter an	mod1 01/11/89
20000	20ca ornl evalaug71 c.y.fu and d.m.	mod3 12/20/88
48000	48cd bnl evalmay74 s.pearlstein tr	mod1 01/03/89
48106	48cd106 hedl evalfeb80 f.m.mann	mod2 01/12/89
48108	48cd108 hedl evalapr74 r.e.schenter an	mod1 01/12/89
48111	48cd111 hedl evalapr74 r.e.schenter an	mod1 01/12/89
48112	48cd112 hedl evalapr74 r.e.schenter an	mod1 01/12/89
48113	48cd113 bnl hedl evalnov78 pearlstein mann	mod1 01/03/89
48601	48cd115mhedl inel evaldec79 schenter schmit	mod1 01/12/89
48116	48cd116 hedl evalapr74 r.e.schenter an	mod1 01/12/89
58140	58ce140 hedl evalapr74 r.e.schenter an	mod1 01/13/89
58141	58ce141 hedl inel evaldec79 schenter schmit	mod1 01/13/89
58142	58ce142 hedl evalapr74 r.e.schenter an	mod1 01/13/89
58143	58ce143 hedl inel evaldec79 schenter schmit	mod1 01/13/89
58144	58ce144 hedl inel evaldec79 schenter schmit	mod1 01/16/89
98249	cf249 bnl srl lllevaljul76 kinseyassemble	mod1 01/12/89
98251	98cf251 bnl srl lllevaljul76 kinseyassemble	mod1 01/10/89
98252	98cf252 bnl srl lllevaljul76 kinseyassemble	mod1 01/10/89
17000	17cl gga evalfeb67 m.s.allen and m	mod1 03/14/89
96241	96cm241 hedl evalapr78 mann and schent	mod1 01/10/90
96243	96cm243 hedlsrllll evalapr78 mann benjamin h	mod1 01/10/90
96245	96cm245 srl lll evaljan79 benjamin and ho	mod2 01/05/89
96246	96cm246 bnl srl lllevaljul76 kinseyassemble	mod1 01/10/90
96247	96cm247 bnl srl lllevaljul76 kinseyassemble	mod1 01/10/89
55133	55cs133 hedl bnl evalnov78 schenter bhat p	mod1 01/03/89
55134	55cs134 hedl inel evaldec79 schenter schmit	mod1 01/13/89
55135	55cs135 hedl inel evaldec79 schenter schmit	mod1 01/13/89
55136	55cs136 hedl inel evaldec79 schenter schmit	mod1 01/13/89
55137	55cs137 hedl inel evaldec79 schenter schmit	mod1 01/13/89
29000	29cu ornl sai evaldec73 fu drake fricke	mod1 12/20/88
66161	66dy161 hedl evalapr74 r.e.schenter an	mod1 01/16/89
66162	66dy162 hedl evalapr74 r.e.schenter an	mod1 04/03/89
68167	68er167 hedl evalapr74 r.e.schenter an	mod1 04/03/89
99253	99es253 bnl srl evaljul76 kinsey benjamin	mod1 01/10/89
63000	63eu nndc evalaug81 autocombined	mod1 01/04/89
63152	63eu152 bnl evaldec73 h.takahashi	mod2 02/28/89
63153	63eu153 bnl evalfeb78 s.mughabghab	mod1 01/03/89
63156	63eu156 hedl inel evaldec79 schenter schmit	mod1 01/16/89
63157	63eu157 hedl evalfeb80 r.e.schenter an	mod1 01/17/89
31000	31ga lll lasl evalmay80 howerton young	mod1 12/21/88
64152	64gd152 bnl evaljan77 b.a.magurno	mod2 01/03/89
64154	64gd154 bnl evaljan77 b.a.magurno	mod1 01/03/89
64156	64gd156 bnl evaljan77 b.a.magurno	mod2 01/04/89
64158	64gd158 bnl evaljan77 b.a.magurno	mod1 01/04/89
64160	64gd160 bnl evaljan77 b.a.magurno	mod1 01/04/89
32072	32ge 72 hedl evalapr74 r.e.schenter an	mod1 01/11/89

32073	32ge 73 hedl evalapr74 r.e.schenter an	mod1 01/11/89
32076	32ge 76 hedl evalapr74 r.e.schenter an	mod1 01/11/89
1801	1h 10lasl evalaug70 l.stewart r.j.	mod1 12/16/88
72000	72hf sai evalapr76 m.drake d.sa	mod1 01/04/89
72174	72hf174 sai evalapr76 m.drake d.sa	mod1 03/21/89
72177	72hf177 sai evalapr76 m.drake d.sa	mod1 03/21/89
72178	72hf178 sai evalapr76 m.drake d.sa	mod1 03/21/89
72180	72hf180 sai evalapr76 m.drake d.sa	mod1 01/04/89
67165	67ho165 hedl evalapr74 r.e.schenter an	mod1 01/16/89
53127	53i 127 hedl rcn evalfeb80 r.e.schenter an	mod1 01/13/89
53129	53i 129 hedl inel+ evalfeb80 schenter schmit	mod1 01/13/89
53130	53i 130 hedl inel evaldec79 schenter schmit	mod1 01/13/89
53131	53i 131 hedl inel evaldec79 schenter schmit	mod1 01/13/89
53135	53i 135 hedl inel evaldec79 schenter schmit	mod1 01/13/89
49113	49in113 hedl evalapr74 r.e.schenter an	mod1 01/12/89
49115	49in115 hedl inel evaldec79 schenter schmit	mod1 01/12/89
36078	36kr 78 bnl evalapr78 a.prince	mod1 12/29/88
36080	36kr 80 bnl evalapr78 a.prince	mod1 12/29/88
36082	36kr 82 bnl evalapr78 a.prince	mod1 12/29/88
36083	36kr 83 bnl evalapr78 a.prince	mod1 12/29/88
36084	36kr 84 bnl evalapr78 a.prince	mod1 12/29/88
36085	36kr 85 hedl inel evaldec79 schenter schmit	mod1 01/11/89
36086	36kr 86 bnl evaljul72 a.prince	mod1 12/30/88
57139	57la139 hedl rcn evalfeb80 r.e.schenter an	mod1 01/13/89
57140	57la140 hedl inel evaldec79 schenter schmit	mod1 01/13/89
71175	71lu175 bnw evaljun67 b.r.leonard jr.	mod1 12/22/88
71176	71lu176 bnw evaljun67 b.r.leonard jr.	mod1 12/22/88
12000	12mg ornl evalfeb78 d.c.larson	mod1 12/16/88
42092	42mo 92 hedl evalfeb80 f.m.mann	mod1 01/12/89
42094	42mo 94 hedl rcn evalfeb80 r.e.schenter an	mod1 01/11/89
42095	42mo 95 hedl rcn evalfeb80 r.e.schenter an	mod1 01/11/89
42097	42mo 97 hedl rcn evalfeb80 r.e.schenter an	mod1 01/12/89
42098	42mo 98 hedl rcn evalfeb80 r.e.schenter an	mod1 01/12/89
42099	42mo 99 hedl inel evaldec79 schenter schmit	mod1 01/12/89
42100	42mo100 hedl rcn evalfeb80 r.e.schenter an	mod1 01/12/89
7014	7n 14 lasl evaljul73 p.young d.fost	mod2 11/28/88
41094	41nb 94 hedl inel evaldec79 schenter schmit	mod1 01/11/89
41095	41nb 95 hedl inel evaldec79 schenter schmit	mod1 01/11/89
60142	60nd142 hedl evalapr74 r.e.schenter an	mod1 01/16/89
60147	60nd147 hedl inel evaldec79 schenter schmit	mod1 01/16/89
60148	60nd148 hedl bnl+ evalfeb80 schenter schmit	mod1 03/21/89
8017	8o 17 bnl evaljan78 b.a.magurno	mod1 12/20/88
15031	15p 31 lll evaloct77 howerton	mod1 12/20/88
82000	82pb ornl evaljul71 c.y.fu and f.g.	mod2 01/04/89
46102	46pd102 hedl evalfeb80 f.m.mann	mod2 01/12/89
46104	46pd104 hedl rcn evalfeb80 r.e.schenter an	mod1 01/12/89
46105	46pd105 hedl rcn evalfeb80 r.e.schenter an	mod1 01/12/89
46106	46pd106 hedl rcn evalfeb80 r.e.schenter an	mod1 01/12/89
46107	46pd107 hedl inel+ evalfeb80 schenter schmit	mod1 01/12/89
46110	46pd110 hedl rcn evalfeb80 r.e.schenter an	mod1 01/12/89
61147	61pm147 hedl inel +evalfeb80 schenter + rei	mod1 01/16/89
61148	61pm148 hedl inel evaldec79 schenter schmit	mod1 01/16/89
61149	61pm149 hedl inel evaldec79 schenter schmit	mod1 01/16/89
61151	61pm151 hedl inel evaldec79 schenter schmit	mod1 01/16/89
59141	59pr141 hedl bnl+ evalfeb80 schenter schmit	mod1 03/21/89
59142	59pr142 hedl inel evaldec79 schenter schmit	mod1 01/16/89
59143	59pr143 hedl inel evaldec79 schenter schmit	mod1 01/16/89
94239	94pu239 lanl jun83 e.arthur p.you	mod2 02/28/89
94240	94pu240 ornl evalapr77 l.w. weston	mod3 12/12/88
37086	37rb 86 hedl inel evaldec79 schenter schmit	mod1 01/11/89
75185	75re185 ge nmpo evaljan68 w.b.henderson a	mod1 12/22/88
75187	75re187 ge nmpo evaljan68 w.b.henderson a	mod1 12/22/88
45105	45rh105 hedl inel evaldec79 schenter schmit	mod2 01/12/89
44096	44ru 96 hedl evalfeb80 f.m.mann	mod2 01/12/89
44098	44ru 98 hedl evalfeb80 f.m.mann	mod2 01/12/89
44099	44ru 99 hedl evalapr74 r.e.schenter an	mod1 01/12/89
44100	44ru100 hedl rcn evalfeb80 r.e.schenter an	mod1 01/12/89
44101	44ru101 hedl rcn evalfeb80 r.e.schenter an	mod1 01/12/89
44102	44ru102 hedl rcn evalfeb80 r.e.schenter an	mod1 01/12/89
44103	44ru103 hedl inel evaldec79 schenter schmit	mod1 01/12/89

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44104          44ru104 hedl rcn evalfeb80 r.e.schenter an       mod1 01/12/89
44105          44ru105 hedl inel evaldec79 schenter schmit      mod1 01/12/89
44106          44ru106 hedl inel evaldec79 schenter schmit      mod1 01/12/89
16032          16s 32 lll evaloct77 howerton                    mod1 12/20/88
51121          51sb121 hedl rcn evalfeb80 r.e.schenter an       mod1 01/13/89
51123          51sb123 hedl rcn evalfeb80 r.e.schenter an       mod1 01/13/89
51124          51sb124 hedl inel evaldec79 schenter schmit      mod1 01/13/89
51125          51sb125 hedl inel evaldec79 schenter schmit      mod1 01/13/89
51126          51sb126 hedl inel evaldec79 schenter schmit      mod1 01/13/89
34074          34se 74 hedl evalfeb80 f.m.mann                  mod2 03/21/89
34077          34se 77 hedl evalapr74 r.e.schenter an           mod1 01/11/89
34080          34se 80 hedl evalapr74 r.e.schenter an           mod1 03/21/89
34082          34se 82 hedl evalapr74 r.e.schenter an           mod1 01/11/89
62144          62sm144 hedl evalfeb80 f.m.mann                  mod2 01/16/89
62148          62sm148 hedl evalfeb80 schenter schmit           mod1 01/16/89
62149          62sm149 hedl bnw evalnov78 schenter leonar       mod1 01/03/89
62150          62sm150 hedl evalapr74 r.e.schenter an           mod1 03/21/89
62151          62sm151 hedl inel +evalfeb80 schenter + rei      mod1 01/16/89
62153          62sm153 hedl inel evaldec79 schenter schmit      mod1 01/16/89
50112          50sn112 hedl evalfeb80 f.m.mann                  mod2 01/12/89
50114          50sn114 hedl evalfeb80 f.m.mann                  mod2 01/12/89
50115          50sn115 hedl evalapr74 r.e.schenter an           mod1 01/12/89
50116          50sn116 hedl evalapr74 r.e.schenter an           mod1 01/12/89
50117          50sn117 hedl evalapr74 r.e.schenter an           mod1 01/12/89
50118          50sn118 hedl evalapr74 r.e.schenter an           mod1 01/12/89
50119          50sn119 hedl evalapr74 r.e.schenter an           mod1 01/12/89
50120          50sn120 hedl evalapr74 r.e.schenter an           mod1 01/12/89
50122          50sn122 hedl evalapr74 r.e.schenter an           mod1 01/12/89
50123          50sn123 hedl inel evaldec79 schenter schmit      mod1 01/12/89
50124          50sn124 hedl evalapr74 r.e.schenter an           mod1 01/12/89
50125          50sn125 hedl inel evaldec79 schenter schmit      mod1 01/13/89
50126          50sn126 hedl inel evaldec79 schenter schmit      mod1 01/12/89
38084          38sr 84 hedl evalfeb80 f.m.mann                  mod2 01/11/89
38086          38sr 86 hedl evalapr74 r.e.schenter an           mod1 01/11/89
38087          38sr 87 hedl evalapr74 r.e.schenter an           mod1 01/11/89
38088          38sr 88 hedl evalapr74 r.e.schenter an           mod1 01/11/89
38089          38sr 89 hedl inel evaldec79 schenter schmit      mod1 01/11/89
38090          38sr 90 hedl inel evaldec79 schenter schmit      mod1 01/11/89
 1003          1t 301asl evalfeb65 leona stewart                mod2 12/16/88
73182          73ta182 ai evalapr71 j.otter c.dunfo             mod1 12/22/88
65159          65tb159 hedl rcn evalfeb80 r.e.schenter an       mod1 01/16/89
65160          65tb160 hedl inel evaldec79 schenter schmit      mod1 01/16/89
52120          52te120 hedl evalfeb80 f.m.mann                  mod2 01/13/89
52123          52te123 hedl evalapr74 r.e.schenter an           mod1 03/21/89
52124          52te124 hedl evalapr74 r.e.schenter an           mod1 01/13/89
52125          52te125 hedl evalapr74 r.e.schenter an           mod1 01/13/89
52126          52te126 hedl evalapr74 r.e.schenter an           mod1 01/13/89
52601          52te127mhedl inel evaldec79 schenter schmit      mod1 01/13/89
52128          52te128 hedl evalapr74 r.e.schenter an           mod1 01/13/89
52611          52te129mhedl inel evaldec79 schenter schmit      mod1 01/13/89
52130          52te130 hedl evalapr74 r.e.schenter an           mod1 01/13/89
52132          52te132 hedl inel evaldec79 schenter schmit      mod1 01/13/89
22000          22ti buranllll evalaug77 c.philis a.smit         mod1 12/20/88
92235          92u 235 bnl evalapr77 m.r.bhat                   mod3 02/28/89
92237          92u237 bnl srl lllevaljul76 kinseyassemble       mod1 01/10/89
23000          23v anllllhedl evaljan77 a.smith+ h.howe         mod1 12/20/88
74000          74w lanl evalmar82 e.d.arthur                    mod1 01/04/89
74182          74w182 las anl brcevaldec80 arthur young sm      mod2 01/04/89
74186          74w186 las anl brcevaldec80 arthur young sm      mod2 01/05/89
54124          54xe124 bnl evalmar78 m.r.bhat and s.            mod1 12/29/88
54126          54xe126 bnl evalmar78 m.r.bhat and s.            mod1 12/29/88
54128          54xe128 bnl evalmar78 m.r.bhat and s.            mod1 12/30/88
54129          54xe129 bnl evalmar78 m.r.bhat and s.            mod1 01/03/89
54130          54xe130 bnl evalmar78 m.r.bhat and s.            mod1 12/30/88
54131          54xe131 bnl evalmar78 m.r.bhat and s.            mod1 01/03/89
54132          54xe132 bnl evalmar78 m.r.bhat and s.            mod2 01/03/89
54133          54xe133 hedl inel evaldec79 schenter schmit      mod1 01/13/89
54134          54xe134 bnl evalmar78 m.r.bhat and s.            mod1 01/03/89
54135          54xe135 bnw evaljun67 b.r.leonard jr.            mod1 12/28/88
54136          54xe136 bnl evalmar78 m.r.bhat and s.            mod1 01/03/89
```

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 39089          39y 89 hedl evalapr74 r.e.schenter an          mod1 01/11/89
 39090          39y 90 hedl inel evaldec79 schenter schmit     mod1 01/11/89
 39091          39y 91 hedl inel evaldec79 schenter schmit     mod1 01/11/89
 40093          40zr 93 hedl inel evaldec79 schenter schmit    mod1 01/11/89
 40095          40zr 95 hedl inel evaldec79 schenter schmit    mod1 01/11/89
801601          8o 16 lasl evalaug73 p.young d.fost            mod2 12/16/88
701401          7n 14 from version 6 evaluation
 98250          98cf250 bnl srl lllevaljul76 kinseyassemble    mod1 11/14/97
 91233          91PA233 HEDL INEL EVALMAY78 MANN SCHENTER R    MOD2 01/18/91
 97249          97bk249 bnl srl lllevaljul76 kinseyassemble    mod1 01/11/89
```

M4.A.6 THE 16-GROUP HANSEN-ROACH LIBRARY

```
table of contents for /scale4.4/data/scale.rev03.xn16            on logical unit  1
tape id                       4016000
number of nuclides                 84
number of neutron groups           16
first thermal group                13
number of gamma groups              0
        scale 4 - 16 neutron group criticality safety library
          hansen-roach data with knight modifications and some endf/b 4 data
            compiled for nrc       1/27/89
              last updated                                                08/12/94
                l.m.petrie       ornl
   999          1/v cross sections normalized to 1.0 at 0.0253 ev
  1001          hydrogen de/e                    hansen-roach          updated 08/12/94
  1301          hydrogen x(e)                    hansen roach          updated 08/12/94
  1002          deuterium x(e)                   hansen roach          updated 08/12/94
  2004           helium-4 endf/b-iv mat 1270                          updated 08/12/94
  3006          lithium-6                        hansen roach          updated 08/12/94
  3007          lithium-7                        hansen roach          updated 08/12/94
  4009          beryllium                        hansen roach          updated 08/12/94
  5000          boron                            hansen roach          updated 08/12/94
  5010           boron-10 endf/b-iv mat 1273                          updated 08/12/94
  5011           boron-11       endf/b-iv mat 1160                    updated 08/12/94
  6012          carbon                           hansen roach          updated 08/12/94
  7014          nitrogen                         hansen roach          updated 08/12/94
  8016          oxygen                           hansen roach          updated 08/12/94
  9019          fluorine                         hansen roach          updated 08/12/94
 11023          sodium                           hansen roach          updated 08/12/94
 12000           magnesium endf/b-iv mat 1280                         updated 08/12/94
 13027          aluminum                         hansen roach          updated 08/12/94
 14000           silicon        endf/b-iv mat 1194                    updated 08/12/94
 15031           phosphorus-31 lendl mat 7019                         updated 08/12/94
 16000          sulfur  lendl mat 7020                                updated 08/12/94
 17000          chlorine                         hansen roach          updated 08/12/94
 19000          potassium                        hansen-roach          updated 08/12/94
 20000          calcium endf/b-iv mat 1195                            updated 08/12/94
 22000           titanium       endf/b-iv mat 1286                    updated 08/12/94
 23051           vanadium endf/b-iv mat 1196                          updated 08/12/94
 24000          chromium                         aerojet               updated 08/12/94
 24304           chromium endf/b-iv mat 1191 ss-304 wt                updated 08/12/94
 24404           chromium endf/b-iv mat 1191 inconel wt               updated 08/12/94
 25055           manganese-55 endf/b-iv mat 1197                      updated 08/12/94
 26000          iron                             hansen roach          updated 08/12/94
 26304           iron endf/b-iv mat 1192 ss-304 wt                    updated 08/12/94
 26404           iron endf/b-iv mat 1192 inconel wt                   updated 08/12/94
 27059          cobalt                           hansen roach          updated 08/12/94
 28000          nickel                           hansen roach          updated 08/12/94
 28304           nickel endf/b-iv mat 1190 ss-304 wt                  updated 08/12/94
 28404           nickel endf/b-iv mat 1190 inconel wt                 updated 08/12/94
 29000           copper endf/b-iv mat 1295                            updated 08/12/94
 30000          zinc                             gam-2                 updated 08/12/94
 40000          zirconium                        hansen roach          updated 08/12/94
 40302           zircalloy-2 endf/b-iv mat 1284                       updated 08/12/94
 41093          niobium                          hansen roach          updated 08/12/94
 42000          molybdenum                       hansen roach          updated 08/12/94
```

```
47107          silver-107     endf/b-iv mat 1138                    updated 08/12/94
47109          silver-109 endf/b-iv mat 1139                        updated 08/12/94
48000          cadmium        endf/b-iv mat 1281                    updated 08/12/94
49113          indium-113     endf/b-iv mat 445                     updated 08/12/94
49115          indium-115 endf/b-iv mat 449                         updated 08/12/94
50000          tin lendl mat 7039                                   updated 08/12/94
56138          barium-138 lendl mat 7040                            updated 08/12/94
58000          cerium                          hansen roach
62000          samarium                        gam-2
63000          europium                        gam-2                updated 08/12/94
64000          gadolinium endf/b-iv mat 1030                        updated 08/12/94
66164          dyprosium-164  endf/b-iv mat 1031                    updated 08/12/94
71175          lutetium-175   endf/b-iv mat 1032                    updated 08/12/94
71176          lutetium-176 endf/b-iv mat 1033                      updated 08/12/94
72000          hafnium endf/b-iv mat 1034                           updated 08/12/94
73181          tantalum                        hansen roach         updated 08/12/94
74182          tungsten-182   endf/b-iv mat 1128                    updated 08/12/94
74183          tungsten-183   endf/b-iv mat 1129                    updated 08/12/94
74184          tungsten-184   endf/b-iv mat 1130                    updated 08/12/94
74186          tungsten-186   endf/b-iv mat 1131                    updated 08/12/94
75185          rhenium-185 endf/b-iv mat 1083                       updated 08/12/94
75187          rhenium-187    endf/b-iv mat 1084                    updated 08/12/94
79197          gold-197       endf/b-iv mat 1283                    updated 08/12/94
82000          lead endf/b-iv mat 1288                              updated 08/12/94
90232          th-232  infinite dilution     hansen roach          updated 08/12/94
91233          protactinium-233 endf/b-iv mat 1297                  updated 08/12/94
92233          u-233                           hansen roach         updated 08/12/94
92234          u-234 endf/b-iv mat 1043                             updated 08/12/94
92235          u-235 yr                        hansen roach         updated 08/12/94
92236          u-236 endf/b-iv mat 1163                             updated 08/12/94
92238          u-238 y                         hansen roach         updated 08/12/94
93237          neptunium-237  endf/b-iv mat 1263                    updated 08/12/94
94238          pu-238                          hansen roach         updated 08/12/94
94338          pu-238 y                        persimmon
94239          pu-239                          hansen roach         updated 08/12/94
94240          pu-240                          hansen roach         updated 08/12/94
94241          pu-241 endf/b-iv mat 1266                            updated 08/12/94
94242          plutonium-242  endf/b-iv mat 1161                    updated 08/12/94
95241          am-241 endf/b-iv mat 1056                            updated 08/12/94
95243          am-243 endf/b-iv mat 1057                            updated 08/12/94
96244          cm-244 endf/b-iv mat 1162                            updated 08/12/94
```

M4.A.7 THE 18-GROUP GAMMA LIBRARY

```
table of contents for /scale4.4/data/scale.rev05.xg18          on logical unit  1
tape id                          18000
number of nuclides                 180
number of neutron groups             0
first thermal group                 22
number of gamma groups              18
       scale 4 - 18 gamma group shielding library
         based on ogre library data
           compiled for nrc       1/27/89
             last updated                                          02/24/97
               l.m.petrie       ornl
  900          dose factors                                       updated 02/24/97
 1001          hydrogen                                           updated 08/12/94
 1002          deuterium                                          updated 08/12/94
 1003          tritium                                            updated 08/12/94
 1901          hydrogen in polyethylene                           updated 08/12/94
 2003          helium-3                                           updated 08/12/94
 2004          helium-4                                           updated 08/12/94
 3006          lithium-6                                          updated 08/12/94
 3007          lithium-7                                          updated 08/12/94
 4009          beryllium                                          updated 08/12/94
 5000          boron                                              updated 08/12/94
 5010          boron-10                                           updated 08/12/94
```

5011	boron-11	updated 08/12/94
6012	carbon	updated 08/12/94
6312	graphite	updated 08/12/94
7014	nitrogen	updated 08/12/94
8016	oxygen	updated 08/12/94
9019	fluorine	updated 08/12/94
10000	neon	updated 10/13/89
11023	sodium	updated 08/12/94
12000	magnesium	updated 08/12/94
13027	aluminum	updated 08/12/94
14000	silicon	updated 08/12/94
14028	silicon-28	updated 08/12/94
15031	phosphorus-31	updated 08/12/94
16000	sulfur	updated 08/12/94
16032	sulfur-32	updated 08/12/94
17000	chlorine	updated 08/12/94
18040	argon	updated 10/13/89
19000	potassium	updated 08/12/94
19039	potassium-39	updated 08/12/94
20000	calcium	updated 08/12/94
20040	calcium-40	updated 08/12/94
21045	scandium	updated 08/12/94
22000	titanium	updated 08/12/94
23000	vanadium	updated 08/12/94
23051	vanadium-51	updated 08/12/94
24000	chromium	updated 08/12/94
24304	chromium in ss304	updated 08/12/94
24404	chromium in inconel	updated 08/12/94
25055	manganese-55	updated 08/12/94
26000	iron	updated 08/12/94
26304	iron in ss304	updated 08/12/94
26404	iron in inconel	updated 08/12/94
27059	cobalt-59	updated 08/12/94
28000	nickel	updated 08/12/94
28304	nickel in ss304	updated 08/12/94
28404	nickel in inconel	updated 08/12/94
30000	zinc	updated 08/12/94
31000	gallium	updated 08/12/94
32072	germanium-72	updated 08/12/94
32073	germanium-73	updated 08/12/94
32074	germanium-74	updated 08/12/94
32076	germanium-76	updated 08/12/94
33075	arsenic-75	updated 08/12/94
34076	selenium-76	updated 08/12/94
34077	selenium-77	updated 08/12/94
34078	selenium-78	updated 08/12/94
34080	selenium-80	updated 08/12/94
34082	selenium-82	updated 08/12/94
35079	bromine-79	updated 08/12/94
35081	bromine-81	updated 08/12/94
36080	krypton-80	updated 08/12/94
36082	krypton-82	updated 08/12/94
36083	krypton-83	updated 08/12/94
36084	krypton-84	updated 08/12/94
36086	krypton-86	updated 08/12/94
37085	rubidium-85	updated 08/12/94
37086	rubidium-86	updated 08/12/94
37087	rubidium-87	updated 08/12/94
38086	strontium-86	updated 08/12/94
38087	strontium-87	updated 08/12/94
38088	strontium-88	updated 08/12/94
38089	strontium-89	updated 08/12/94
38090	strontium-90	updated 08/12/94
39089	yttrium-89	updated 08/12/94
39090	yttrium-90	updated 08/12/94
39091	yttrium-91	updated 08/12/94
40000	zirconium	updated 08/12/94
40302	zircalloy	updated 08/12/94
41093	niobium-93	updated 08/12/94
42000	molybdnum	updated 08/12/94

43099	technetium-99	updated 08/12/94
44100	ruthenium-100	updated 08/12/94
44101	ruthenium-101	updated 08/12/94
44102	ruthenium-102	updated 08/12/94
44106	ruthenium-106	updated 08/12/94
45103	rhodium-103	updated 08/12/94
45105	rhodium-105	updated 08/12/94
46104	palladium-104	updated 08/12/94
46105	palladium-105	updated 08/12/94
46106	palladium-106	updated 08/12/94
46108	palladium-108	updated 08/12/94
47107	silver-107	updated 08/12/94
47109	silver-109	updated 08/12/94
48000	cadmium	updated 08/12/94
48113	cadmium-113	updated 08/12/94
49113	indium-113	updated 08/12/94
49115	indium-115	updated 08/12/94
50118	tin-118	updated 08/12/94
51124	antimony-124	updated 08/12/94
52126	tellurium-126	updated 08/12/94
53129	iodine-129	updated 08/12/94
53131	iodine-131	updated 08/12/94
54124	xenon-124	updated 08/12/94
54126	xenon-126	updated 08/12/94
54128	xenon-128	updated 08/12/94
54129	xenon-129	updated 08/12/94
54130	xenon-130	updated 08/12/94
54131	xenon-131	updated 08/12/94
54132	xenon-132	updated 08/12/94
54134	xenon-134	updated 08/12/94
54135	xenon-135	updated 08/12/94
54136	xenon-136	updated 08/12/94
55133	cesium-133	updated 08/12/94
55134	cesium-134	updated 08/12/94
55135	cesium-135	updated 08/12/94
56138	barium-138	updated 08/12/94
57139	lanthanium-139	updated 08/12/94
58000	cerium	updated 10/13/89
59141	praseodynium-141	updated 08/12/94
59143	praseodynium-143	updated 08/12/94
60143	neodynium-143	updated 08/12/94
60144	neodynium-144	updated 08/12/94
60148	neodynium-148	updated 08/12/94
61147	promethium-147	updated 08/12/94
61148	promethium-148	updated 08/12/94
61548	promethium-148m	updated 10/13/89
62147	samarium-147	updated 08/12/94
62148	samarium-148	updated 08/12/94
62149	samarium-149	updated 08/12/94
62150	samarium-150	updated 08/12/94
62151	samarium-151	updated 08/12/94
62152	samarium-152	updated 08/12/94
62154	samarium-154	updated 08/12/94
63151	europium-151	updated 08/12/94
63152	europium-152	updated 08/12/94
63153	europium-153	updated 08/12/94
63154	europium-154	updated 08/12/94
64000	gadolium	updated 08/12/94
65159	terbium-159	updated 08/12/94
66164	dysprosium-164	updated 08/12/94
67165	holmium-165	updated 08/12/94
68166	erbium-166	updated 08/12/94
68167	erbium-167	updated 08/12/94
69000	thulium	updated 10/13/89
70000	ytterbium	updated 10/13/89
71175	lutetium-175	updated 08/12/94
71176	lutetium-176	updated 08/12/94
72000	hafnium	updated 08/12/94
73181	tantalum-181	updated 08/12/94
73182	tantalum-182	updated 08/12/94

```
74000          tungsten                                          updated 08/12/94
74182          tungsten-182                                      updated 08/12/94
74183          tungsten-183                                      updated 08/12/94
74184          tungsten-184                                      updated 08/12/94
74186          tungsten-186                                      updated 08/12/94
75185          rhenium-185                                       updated 08/12/94
75187          rhenium-187                                       updated 08/12/94
76000          osmium                                  updated 10/13/89
77191          iridium-191                                       updated 08/12/94
77193          iridium-193                                       updated 08/12/94
78000          platinum                                updated 10/13/89
79197          gold-197                                          updated 08/12/94
80000          mercury                                 updated 10/13/89
81000          thallium                                updated 10/13/89
82000          lead                                              updated 08/12/94
83000          bismuth                                 updated 10/13/89
86000          radon                                   updated 10/13/89
90232          thorium-232                                       updated 08/12/94
92233          uranium-233                                       updated 08/12/94
92234          uranium-234                                       updated 08/12/94
92235          uranium-235                                       updated 08/12/94
92236          uranium-236                                       updated 08/12/94
92238          uranium-238                                       updated 08/12/94
94238          plutonium-238                                     updated 08/12/94
94239          plutonium-239                                     updated 08/12/94
94240          plutonium-240                                     updated 08/12/94
94241          plutonium-241                                     updated 08/12/94
94242          plutonium-242                                     updated 08/12/94
```

M4.A.8 THE 22n/18g STRAKER-MORRISON LIBRARY

```
table of contents for /scale4.4/data/scale.rev03.xn22g18          on logical unit  1
tape id                        4022018
number of nuclides                  36
number of neutron groups            22
first thermal group                 22
number of gamma groups              18
       scale 4 - 22 neutron 18 gamma group shielding library
         based on straker-morrison data with regenerated gamma cross sections
           compiled for nrc       1/27/89
             last updated                                                  08/12/94
               l.m.petrie       ornl
     900          dose factors                                  updated 9/07/89
    1001              hydrogen                                          updated 08/12/94
    2004              helium                                            updated 08/12/94
    3006              lithium-6                                         updated 08/12/94
    3007              lithium-7                                         updated 08/12/94
    4009              beryllium                                         updated 08/12/94
    5010              boron-10                                          updated 08/12/94
    5011              boron-11                                          updated 08/12/94
    6012              carbon                                            updated 08/12/94
    7014              nitrogen                                          updated 08/12/94
    8016              oxygen                                            updated 08/12/94
    9019              fluorine                                          updated 08/12/94
   11023              sodium                                            updated 08/12/94
   12000              magnesium                                         updated 08/12/94
   13027              aluminum                                          updated 08/12/94
   14000              silicon                                           updated 08/12/94
   17000              chlorine                                          updated 08/12/94
   19000              potassium                                         updated 08/12/94
   20000              calcium                                           updated 08/12/94
   22000              titanium                                          updated 08/12/94
   24000              chromium                                          updated 08/12/94
   25055              manganese                                         updated 08/12/94
   26000              iron                                              updated 08/12/94
   28000              nickel                                            updated 08/12/94
   29000              copper                                            updated 08/12/94
   40000              zirconium                                         updated 08/12/94
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 42000          molybdenum                                          updated 08/12/94
 50000          tin                                                 updated 08/12/94
 73181          tantalum                                            updated 08/12/94
 74000          tungsten                                            updated 08/12/94
 82000          lead                                                updated 08/12/94
 92235          uranium-235                                         updated 08/12/94
 92238          uranium-238                                         updated 08/12/94
 94239          plutonium-239                                       updated 08/12/94
 94240          plutonium-240                                       updated 08/12/94
500000      fake data set w/dose factors 10-17-77(1)
```

M4.A.9 THE 27n/18g COUPLED ENDF/B-IV LIBRARY

```
table of contents for /scale4.4/data/scale.rev04.xn27g18          on logical unit  1
tape id                    4027018
number of nuclides           83
number of neutron groups     27
first thermal group          15
number of gamma groups       18
       scale4 - 27 neutron 18 gamma group shielding library
         based on endf-b version 4 data
           compiled for nrc       1/27/89
             last updated                                                 08/12/94
               l.m.petrie        ornl
   900         dose factors                                    updated 9/07/89
   999         1/v cross sections normalized to 1.0 at 0.0253 ev       updated 08/12/94
  1001          hydrogen       endf/b-iv mat 1269/thrm1002             updated 08/12/94
  1002          deuterium      endf/b-iv mat 1120                      updated 08/12/94
  2004          helium-4       endf/b-iv mat 1270                      updated 08/12/94
  3006          lithium-6      endf/b-iv mat 1271                      updated 08/12/94
  3007          lithium-7      endf/b-iv mat 1272                      updated 08/12/94
  4009          beryllium-9    endf/b-iv mat 1289/thrm1064             updated 08/12/94
  5010          boron-10       endf/b-iv mat 1273                      updated 08/12/94
  5011          boron-11       endf/b-iv mat 1160                      updated 08/12/94
  6012          carbon-12      endf/b-iv mat 1274/thrm1065             updated 08/12/94
  7014          nitrogen-14    endf/b-iv mat 1275                      updated 08/12/94
  8016          oxygen-16      endf/b-iv mat 1276                      updated 08/12/94
  9019          fluorine       endf/b-iv mat 1277                      updated 08/12/94
 11023          sodium-23      endf/b-iv mat 1156                      updated 08/12/94
 12000          magnesium      endf/b-iv mat 1280                      updated 08/12/94
 13027          aluminum       endf/b-iv mat 1193                      updated 08/12/94
 14000          silicon        endf/b-iv mat 1194                      updated 08/12/94
 15031          phosphorus-31  lendl     mat 7019                      updated 08/12/94
 16000          sulfur         lendl     mat 7020                      updated 08/12/94
 17000          chlorine       endf/b-iv mat 1149                      updated 08/12/94
 19000          potassium      endf/b-iv mat 1150                      updated 08/12/94
 20000          calcium        endf/b-iv mat 4152                      updated 08/12/94
 22000          titanium       endf/b-iv mat 1286                      updated 08/12/94
 23051          vanadium       endf/b-iv mat 1196                      updated 08/12/94
 24000          chromium       endf/b-iv mat 1191                      updated 08/12/94
 24304          chromium(ss304)endf/b-iv mat 1191                      updated 08/12/94
 24404          chromium(inconlendf/b-iv mat 1191                      updated 08/12/94
 25055          manganese      endf/b-iv mat 1197                      updated 08/12/94
 26000          iron           endf/b-iv mat 1192                      updated 08/12/94
 26304          iron(ss304)    endf/b-iv mat 1192                      updated 08/12/94
 26404          iron(inconel)  endf/b-iv mat 1192                      updated 08/12/94
 27059          cobalt-59      endf/b-iv mat 1199                      updated 08/12/94
 28000          nickel         endf/b-iv mat 1190                      updated 08/12/94
 28304          nickel(ss304)  endf/b-iv mat 1190                      updated 08/12/94
 28404          nickel(inconel)endf/b-iv mat 1190                      updated 08/12/94
 29000          copper         endf/b-iv mat 1295                      updated 08/12/94
 35079          bromine-79     endf/b-iv mat 108                       updated 08/12/94
 35081          bromine-81     endf/b-iv mat 112                       updated 08/12/94
 40000          zirconium      endf/b-iv mat 7141                      updated 08/12/94
 40302          zircalloy      endf/b-iv mat 1284                      updated 08/12/94
 41093          niobium-93     endf/b-iv mat 1189                      updated 08/12/94
 42000          molybdenum     endf/b-iv mat 1287                      updated 08/12/94
 47107          silver-107     endf/b-iv mat 1138                      updated 08/12/94
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 47109          silver-109     endf/b-iv mat 1139                    updated 08/12/94
 48000          cadmium        endf/b-iv mat 1281                    updated 08/12/94
 49113          indium-113     endf/b-iv mat 445                     updated 08/12/94
 49115          indium-115     endf/b-iv mat 449                     updated 08/12/94
 50000          tin            endf/b-iv mat 7039                    updated 08/12/94
 54135          xenon-135      endf/b-iv mat 1294                    updated 08/12/94
 55133          cesium-133     endf/b-iv mat 1141                    updated 08/12/94
 56138          barium-138     endf/b-iv mat 7040                    updated 08/12/94
 64000          gadolinium     endf/b-iv mat 1030                    updated 08/12/94
 66164          dyprosium-164  endf/b-iv mat 1031                    updated 08/12/94
 71175          lutetium-175   endf/b-iv mat 1032                    updated 08/12/94
 71176          lutetium-176   endf/b-iv mat 1033                    updated 08/12/94
 72000          hafnium        endf/b-iv mat 1034                    updated 08/12/94
 73181          tantalum-181   endf/b-iv mat 1285                    updated 08/12/94
 74182          tungsten-182   endf/b-iv mat 1128                    updated 08/12/94
 74183          tungsten-183   endf/b-iv mat 1129                    updated 08/12/94
 74184          tungsten-184   endf/b-iv mat 1130                    updated 08/12/94
 74186          tungsten-186   endf/b-iv mat 1131                    updated 08/12/94
 75185          rhenium-185    endf/b-iv mat 1083                    updated 08/12/94
 75187          rhenium-187    endf/b-iv mat 1084                    updated 08/12/94
 79197          gold-197       endf/b-iv mat 1283                    updated 08/12/94
 82000          lead           endf/b-iv mat 1288                    updated 08/12/94
 90232          thorium-232    endf/b-iv mat 1296                    updated 08/12/94
 91233         pa-233 1297 218 gp wt f-1/e-m 090376 p3 293k          updated 08/12/94
 92233          uranium-233    endf/b-iv mat 1269                    updated 08/12/94
 92234          uranium-234    endf/b-iv mat 1043                    updated 08/12/94
 92235          uranium-235    endf/b-iv mat 1261                    updated 08/12/94
 92236          uranium-235    endf/b-iv mat 1163                    updated 08/12/94
 92238          uranium-238    endf/b-iv mat 1262                    updated 08/12/94
 93237          neptunium-237  endf/b-iv mat 1263                    updated 08/12/94
 94238          plutonium-238  endf/b-iv mat 1050                    updated 08/12/94
 94239          plutonium-239  endf/b-iv mat 1264                    updated 08/12/94
 94240          plutonium-240  endf/b-iv mat 1265                    updated 08/12/94
 94241          plutonium-241  endf/b-iv mat 1266                    updated 08/12/94
 94242          plutonium-242  endf/b-iv mat 1161                    updated 08/12/94
 95241         am-241 1056 sigp=5+4 newxlacs 218ngp p-3 293k         updated 08/12/94
 95243         am-243 1057 218 gp wt f-1/e-m 090376 p3 293k          updated 08/12/94
 96244          curium-244     endf/b-iv mat 1162                    updated 08/12/94
500000         fake data set of dose factors
```

M4.B LOCAL EXPERIENCE WITH THE 218- AND 27-GROUP ENDF/B-IV LIBRARIES

Continuous efforts are made at ORNL to identify the cause of any calculational bias observed when using the SCALE system. Bias exists when a calculated value differs from an experimental value or a value calculated by another code or cross-section library for the same system. Cross-section bias is routinely studied when two calculations of the same system or a calculation of an experiment disagree by more than about 0.5%. (Agreement between calculation and experiment to about 0.5% appears to be an acceptable limit considering that the SCALE codes and cross sections are intended for very general applications.) One way to study cross-section bias is to change suspected cross sections and then demonstrate that the bias diminishes or disappears. This process has led to discovery of some deficiencies in the 218- and 27-group ENDF/B-IV libraries currently in SCALE. These deficiencies are discussed in this section.

M4.B.1 CHARACTERISTICS OF THE ENDF/B-IV LIBRARIES

The ENDF/B-IV libraries have generally displayed a negative bias of approximately 1%, and in some cases as much as 2%, for low-enriched, water-moderated UO_2 rods. The bias appears to be greatest for epithermal systems (e.g., borated water and/or closely spaced rods) and less significant for more thermalized systems. The bias has been traced to the lack of data in the unresolved resonance region for ^{238}U in ENDF/B-IV. The unresolved resonance region in the SCALE ENDF/B-IV libraries was processed at s_p = 50,000 barns, compared to s_p values of 3500 barns for ^{235}U and 65 barns for ^{238}U in a typical LWR lattice. Improved data in ENDF/B-V eliminated this bias in the 44-group library.

A positive bias has been routinely observed in the 27-group library for thermal ^{239}Pu systems (up to 2%) and mixed oxide (MOX) fuel rods (up to 1%). The bias increases with increasing thermalization. One problem identified in the 27-group library was inadequate group structure to account for flux changes across the 0.3-eV resonance of ^{239}Pu. This problem has been rectified in the 44-group library by the addition of more energy groups in this energy range. However, the positive bias still exists in the 44-group library as well.

Carbon system numerical benchmarks have shown a negative bias of as much as 2.5% with the ENDF/B-IV libraries when compared to the Hansen-Roach and ENDF/B-V libraries. Analysis of the 218-group cross-section data has revealed an incorrect scatter matrix for carbon in energy group 10.

M4.B.2 KNOWN CROSS-SECTION IRREGULARITIES

The hafnium cross-section data available in the 218- and 27-group ENDF/B-IV libraries are not ENDF/B-IV data (ENDF/B-IV did not include hafnium). Known irregularities are present in the cross section, and no resonance data are available with the nuclide. The cross sections are infinite dilution (1/E weighting) across the resonance range. Use of the above sets of hafnium data should be done with caution.

Systems containing gadolinium have not calculated well with the 27-group library. The problem stems from the characteristic of the gadolinium data in the thermal range. Gadolinium has low-energy resonance data down to 10^{-5} eV. The resonances are so broad that the implementation of the Nordheim treatment in NITAWL-II fails to have a mesh point in group 27 of the 27-group structure. This has been addressed by setting the bottom energy of the resonance data to that of group 26 and carrying infinite dilution cross sections in group 27 of the master library. Use of the gadolinium data in the 27-group library, especially for very dilute systems, should be done with caution.

M4.B.3 THERMAL-SCATTERING DATA LIMITATION

A discrepancy was discovered in comparing KENO V.a calculations using the 27-group library and CASMO-3[1] calculations for LWR fuel assemblies in a storage configuration as a function of temperature. The two codes were in relative agreement at low temperatures (20°C) and small water gaps between assemblies. However, as the temperature of the system was increased to 120°C, the CASMO calculations gave increasingly larger values of k_{eff} relative to KENO. Larger water gaps (between assemblies) enhanced the temperature effects on calculated k_{eff}. The KENO results were as much as 3% lower than CASMO at 120°C.

The cause of this discrepancy has been identified as a limitation in processing the thermal-scattering data when NITAWL makes a working library in versions of SCALE prior to 4.3. The SCALE 27-group ENDF/B-IV hydrogen has scattering matrices at 293 K and 550 K (20°C and 277°C). When NITAWL processes hydrogen, the scattering matrix with a temperature closest to that specified is used. It was determined that the temperature dependence of the scattering can increase the multiplication factor by as much as 2.5%. Users of earlier versions of SCALE should be aware of this problem and ensure that the hydrogen-scattering matrices used in their analyses are either appropriate or conservative with respect to k_{eff}.

With regard to other nuclides or the other criticality libraries in SCALE, information on the thermal kernels may be found in Tables M4.2.5, M4.2.7, and M4.2.9.

REFERENCE OF APPENDIX B

1. M. Edenius, A. Ahlin, and B. Forssen, "CASMO-3G, A Fuel Assembly Burnup Program," *User's Manual*, STUDSVIK/NFA-86/7, November 1986.

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Computational Physics and Engineering Division

THERMAL MATERIAL PROPERTIES LIBRARY

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ABSTRACT

The thermal property data compiled and prepared at Lawrence Livermore National Laboratory by Dr. A. L. Edwards have long been used in conjunction with the HEATING series of codes. The thermal property data including density, specific heat, and thermal conductivity were tabulated against temperature, transition temperatures, and latent heats of transition for more than 1000 materials. These data were collected from over 50 references, most of which contain extensive data tabulations and bibliographies. In addition to the data obtained from the sources listed, estimates were also made for many materials for which data could not be found. These estimates were done wherever the estimates appeared to be as accurate as measured values for similar materials. The data library is arranged such that materials are identified numerically according to a general and flexible classification system. An accompanying alphabetical index describes each material, assigns it an identification number, references the sources of the data by code number, and codes the quality or reliability of the data.

This collection of thermal data makes up the thermal material properties library distributed with the SCALE system for use by the HEATING and HTAS1 modules. This section of the SCALE Manual relies heavily on the text of UCRL-50589 to provide SCALE users with a thorough description of the available thermal material properties library.

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LIST OF TABLES

ACKNOWLEDGMENT

The developers of HEATING and the SCALE system gratefully acknowledge A. L. Edwards' consent to use an edited version of his earlier published document, *A Compilation of Thermal Property Data for Computer Heat-Conduction Calculations*, UCRL-50589 (1969), as the basis for this section of the SCALE Manual.

M5.1 INTRODUCTION

The availability of computer programs for solving problems in transient and steady-state heat conduction makes it possible to rapidly and accurately solve large numbers of problems involving a wide variety of materials, provided that accurate input data are used. In particular, the thermal properties of the materials, including density, specific heat, and thermal conductivity and the dependence of these properties on temperature, temperatures, latent heats of transition, and the temperature ranges for specific applications, should be known as accurately as possible. Some of these properties are difficult to measure and may vary from sample to sample, depending on the method of fabrication and previous history. Therefore, when used in calculations, the possible inaccuracy or variability of thermal data should be accounted for in interpreting the results. For this reason, Dr. A. L. Edwards of the Lawrence Livermore National Laboratory (LLNL) compiled a library of thermal property data (see Ref. 1) in the late 1960s that is still being widely used in heat transfer calculations.

For many years, this LLNL library of thermal material properties has been used by the HEATING series of codes developed at Oak Ridge National Laboratory (ORNL). Therefore, this library was selected for inclusion in, and subsequent distribution with, the SCALE computational system that contains HEATING as one of its functional modules (see Sect. F10). The HTAS1 control module (see Sect. H1), which accesses HEATING, also uses the material properties library. The HEATING and HTAS1 programs give the user the option of inputting thermal data for a problem on the material input cards or of allowing the program to extract the properties from the LLNL material properties library. The material properties available in the library are density, thermal conductivity, specific heat, transition temperature, and latent heat. The density of the material is typically either the value at or near room temperature or the lowest temperature for which specific heat or conductivity is tabulated, whichever is highest. The thermal conductivity and specific heat of the material are given if they are constant or if the temperature dependence is unknown. When a table of thermal conductivity or specific heat vs temperature is listed in the library, the table will be stored and used as a tabular function by HEATING. The transition temperature is the temperature at which either a phase change or a solid-state transition occurs. The latent heat is the amount of heat absorbed by the material when the temperature is increased past the transition temperature.

The material properties library is available in SCALE with the centimeter gram second-calorie-degrees Celsius (cgs-cal-°C) system. Conversion to any other unit system can be controlled through HEATING (see Sect. F10) input data. HEATING accesses logical unit IMATLB (currently equal to 78) whenever the input specifies that data be extracted from the material properties library. Conversion to the English units employed in HTAS1 is handled automatically.

This section of the SCALE Manual provides documentation on the format and contents of the LLNL thermal material properties library provided with the SCALE system. Information and tables describing the format and contents are taken directly from Ref. 1 with the permission of the author, Dr. A. L. Edwards.

M5.2 DESCRIPTION OF THE LIBRARY

Thermal property data for over 1000 materials have been compiled in the material properties library. The compilation includes (1) a numbered list of data sources, primarily those containing extensive data tabulations and bibliographies; (2) a numerical classification system used as a guide in assigning a permanent identification number to each material included in the system; (3) a system of quality indicators used to show the general reliability or accuracy of data included in the compilation; (4) thermal property data sheets for each material, including all tabular and graphical data collected or estimated by A. L. Edwards and converted to a standard system of units; (5) an alphabetical index of materials that includes the identification number assigned to each material, an alphanumeric designator for auxiliary identification, a list of data sources by number, and a quality indicator for each type of data given for the material; and (6) a list of material property data arranged according to the material identification numbers. These material properties data include the material identification number and alphanumeric designator, density, specific heat, thermal conductivity, phase-change or transition temperature, latent heat effect, and tables of specific heat and thermal conductivity vs temperature.

The data compilation described herein was completed about 1969 and, even at that time, no claim of completeness or comprehensiveness was made. However, developers of the HEATING codes never updated the library. Analysts should check subsequent tables in this document for the source of the data for a given material to be used. Also, the analysts can disregard the material properties library and input original or updated data into HEATING. Thermal data for new or special materials not in the library should also be obtained by the analyst.

M5.3 LIBRARY DATA SOURCES

The sources for most of the data included in the compilation and several other general sources are listed in abbreviated form in Table M5.3.1. The numbers of the first column are used in the alphabetical material index to cross-reference the sources. Asterisks indicate the data sources actually used for the compilation. Classified data sources were omitted from Ref. 1 and this report. The source used most extensively for the compilation is that edited by Touloukian (No. 20) of Table M5.3.1.

Reference 1 provides an estimate of the thermal properties for a large number of materials for which no reliable data could be found. These estimates have been included whenever the estimates appeared to be as accurate as available data for similar materials.

Many errors were found in the literature and corrected before including the data in the original compilation (Ref. 1). Most of these errors were introduced by incorrect conversion from one unit system to another, incorrect labelling or interpretation of axes labels or scales on graphs, and confusion between units of mass or gram-molecular weight used for specific heats.

Table M5.3.1 Data sources

		MATERIAL PROPERTIES REFERENCES.		
1	*	PERRY J H	CHEMICAL ENGINEERS HANDBOOK 4TH ED	1963
2	*	MCADAMS W H	HEAT TRANSMISSION 3RD ED	1954
3	*		LIQUID METALS HANDBOOK 2ND ED	1952
4	*	MARKS L S	MECHANICAL ENGINEERS HANDBOOK 5TH ED	1951
5	*	FLEMING P	PRIVATE COLLECTION OF PLASTICS DATA	1968
6	*		MATERIALS ENGR MATL SELECTOR ISSUE	1967
7		PFEIFER H	PRIVATE COLLECTION OF MATERIALS DATA	1968
8	*	JAMES E	PROPERTIES OF CHEMICAL EXPLOSIVES UCRL 14592	1965
9			ASRE DATA BOOK	
10			AIRPLANE AIR CONDITIONING ENGR DATA	1952
11			INTERNATIONAL CRITICAL TABLES	1926
12		JOHNSON A I	THERMAL CONDUCTIVITY CHART FOR GASES	1954
13		HILSENRATH J	TABLES OF THERMAL PROPERTIES OF GASES NBS 564	1955
14	*	TIPTON C R JR	THE REACTOR HANDBOOK 2ND ED VOL 1	1960
15		KUONG J F	THERMAL PROPERTIES OF LIQUIDS	1963
16			THE REACTOR HANDBOOK VOL 3 ENGINEERING	1963
17			ENGLISH TRANSL OF HANDBUCH DER PHYSIC	1962
18		HOYT S L	METAL DATA	1952
19		AVDUYEVSKIY V S	FUNDLS OF HEAT TRANSFER IN AV AND RKT ENGR	1962
20	*	TOULOUKIAN Y S	THERMOPHYSICAL PROP OF HIGH TEMP SOLID MATLS	1967
21			PRELIM REPT ON THE PROP OF LI BE MG AL NBS6297	1959
22			TH PROP OF SELD LIGHT ELEMENT CPDS NBS7437	1962
23		KOWALCZYK L S	THERMAL COND AND ITS VARN WITH T AND P	1955
24		JOHNSON V J	A COMPDM OF PROP OF MATL AT LOW TEMP NBS	1960
25			JANAF THERMOCHEMICAL TABLES	
26		KELLEY K K	ENTROPIES OE ELEMENTS AND INORG CPDS BM592	1961
27	*	WEAST R C	HANDBOOK OF CHEMISTRY AND PHYSICS 47TH ED	1966
28	*	JESTER M	PRIVATE COLLECTION OF LIQUID METAL PROPERTIES	1968
29	*	WICKS C E	THERMODYN PROP OF 65 ELEMENTS BU MINES 605	1963
30	*	PETERS R L	MATERIALS DATA NOMOGRAPHS	1965
31	*	THOMPSON B	ENERGY CONTENT VS TEMP FOR D-PU A-PU AND U	
32	*	KELLEY K K	ENTHALPY PLOTS DWG K38745 BU MINES 584	1960
33	*	KELLEY K K	BU MINES 371	1939
34	*	LABER D	BMI FINAL REPT ON SANL TASKS 309/032A 401/027	1967
35	*		Y-12 DATA SHEETS	
36	*	SCHAUER D	WEAPONS MATL DATA BOOK	
37	*	SCHORSCH R H	ENGINEERING PROPERTIES OF SELECTED MATLS	1966
38	*		MODERN PLASTICS ENCYCLOPEDIA	1968
39	*		HANDBOOK OF MOLDED AND EXTR RUBBER GOODYEAR	
40	*		MACHINE DESIGN REFERENCE ISSUE PLASTICS	1964
41	*		METALS HANDBOOK 8TH ED	1961
42	*	STULL D R	THERMODYNAMIC PROPERTIES OF THE ELEMENTS ACS	1956
43	*	HAMPEL C A	RARE METALS HANDBOOK 2ND ED	1961
44	*	MOYER J	PRIVATE COLLECTION OF THERMAL DATA	1968
45	*	HODGE A W	PROP OF HIGH TEMP TI ALLOYS DMIC MEMO 230	1968
46	*	CARSLAW H JAEGER J	CONDUCTION OF HEAT IN SOLIDS 2ND ED OXFORD	1959
47	*	SMITHELLS C J	METALS REFERENCE BOOK 4TH ED VOL 3	1967
48	*	LYNCH J F RUDERER	ENGR PROP OF SEL CERAM KATLS BMI AM CER SOC	1966
49	*		PROP OF KENNAMETAL HARD CARBIDE ALLOYS	1963
50	*		PROP HANDBOOK CARBOLOY ETC GE MET PROD	1958
51	*	CLARK S P JR	HANDBOOK OF PHYSICAL CONSTANTS GEOL SOC AMER	1966
52	*	STEPHENS D R MAIMO	THE THERMAL COND OF ROCK SALT UCRL 6894-II	1964
53	*	SEDDON B J	PHYS PROP OF PU CERAMIC CPDS TRG1601	1968
54	*	STORMS E K	THE REFRACTORY CARBIDES	1967

M5.4 MATERIAL CLASSIFICATION SYSTEM

The material classification system tabulated in Table M5.4.1 was used to assign identification numbers to the materials included in this report. The classification of many materials was arbitrary. The range of numbers in each category of materials is sufficient to include most materials of interest and importance. Many unused numbers remain within each category for new materials that can be included in the compilation.

The alphanumeric identifiers assigned to each material aid in identifying the materials on the material data list. In the cases of the elements and most simple compounds, the atomic or molecular formulae are used. In most other cases, acronyms or mnemonics are used.

Table M5.4.1 Material classification system

1000	ELEMENTS	
	1001-1499	SOLIDS, LIQUIDS
	1501-1599	GASES
	1601-1999	NOT USED
2000	ALLOYS	
	2001-2099	ALUMINUM ALLOYS
	2101-2399	COPPER ALLOYS
	2401-2499	MAGNESIUM ALLOYS
	2501-2599	NICKEL ALLOYS
	2601-2699	COBALT ALLOYS
	2701-2799	TITANIUM ALLOYS
	2801-2999	NOT USED
3000	ALLOYS (CONTINUED)	
	3001-3099	IRON ALLOYS
	3101-3299	STEELS
	3301-3499	SUPER ALLOYS (CR-NI-FE)
	3501-3599	BERYLLIUM ALLOYS
	3601-3649	LEAD, TIN, AND INDIUM ALLOYS
	3651-3679	NOLYBDENUM ALLOYS
	3681-3699	NIOBIUM (COLUMBIUM) ALLOYS
	3701-3749	PLUTONIUM ALLOYS
	3751-3779	SILVER ALLOYS
	3781-3799	TANTALUM ALLOYS
	3801-3829	TUNGSTEN ALLOYS
	3831-3859	URANIUM ALLOYS
	3861-3879	ZINC ALLOYS
	3881-3899	ZIRCONIUM ALLOYS
	3901-3999	MISCELLANEOUS ALLOYS
4000	INORGANIC COMPOUNDS	
	4001-4199	OXIDES (SINGLE)
	4201-4299	OXIDES (MIXED)
	4301-4399	SILICATES
	4401-4499	NITRIDES
	4501-4599	CARBIDES
	4601-4699	BORIDES
	4701-4739	BERYLLIDES
	4741-4759	SULFIDES
	4761-4769	PHOSPHIDES
	4771-4799	SILICIDES
	4801-4899	HALIDES
	4901-4949	INTERMETALLICS, METALLOIDS
	4951-4999	MISCELLANEOUS COMPOUNDS
5000	INORGANIC MIXTURES	
	5001-5199	GLASSES
	5201-5299	CERAMICS, BRICKS
	5301-5399	NOT USED
	5401-5499	CERMETS
	5501-5799	GAS MIXTURES
	5801-5999	NOT USED
6000	INORGANIC COMPOSITES	
	6001-6099	ROCKS, MINERALS, SANDS, SOILS
	6101-6999	NOT USED
7000	ORGANIC COMPOUNDS AND MIXTURES	
	7001-7499	POLYMERS (INCLUDING FOAMS)
	7501-7599	HIGH EXPLOSIVES (INCLUDING MOCK H. E.)
	7601-7699	NOT USED
8000	ORGANIC COMPOSITES AND NATURAL MATERIALS	
	8001-8499	MISCELLANEOUS
	8501-8599	WOODS
	8601-8999	NOT USED
9000	MISCELLANEOUS	
	9001-9099	IDEALIZED MATERIALS
	9101-9999	NOT USED

M5.5 QUALITY INDICATOR SYSTEM

The data for each material were chosen as the best values. For cases in which conflicting or inaccurate data were found in the literature, Ref. 1 provided the best values available for each material. The numerical quality indicators are necessarily crude and general but may be interpreted approximately as follows:

Quality Type 0 (or Blank)

Data were good, or no statement was made in data source restricting their accuracy. No conflicting data were found in any other data sources. Most data in this category are probably accurate to within 1–2% for density, 5–10% for specific heat, and 10–20% for thermal conductivity. When tables or specific heat vs temperature or thermal conductivity vs temperature are included, the constant values are included only for information and generally apply only to temperatures ranging from 0–100°C or at the lower end of the indicated temperature range of the table, whichever is higher.

Quality Type 1

Good data but specific heat or thermal conductivity were reported only for a limited temperature range. The temperature range has been extended by extrapolation, and the resulting values are probably as accurate as reported values.

Quality Type 2

Either the accuracy of the data was poor, or values reported by different sources disagreed. The best values were used whenever a judgment could be made, or average values were used with consideration given to data for similar materials.

Quality Type 3

No data could be found in the literature; however, the author made an estimate based on theoretical or empirical grounds or on data for similar materials. These estimates were included whenever they appeared to be about as accurate as reported data for similar materials.

Quality Type 4

No data could be found in the literature, and no accurate estimate could be made. The data, therefore, are considered to be a rough estimate based, in most cases, on data for similar materials.

Quality Type 5

No data could be found in the literature, and no estimate was made. A minimum requirement for inclusion of a material in the alphabetical index and material data list is the availability of at least estimated constant values of density, specific heat, and thermal conductivity.

M5.6 MATERIAL INDEX

Table M5.6.1 is an alphabetical index of material descriptions that are available in the library. The format used for the information on each card-image record is as follows:

Columns 1-5

Alphanumeric identifier that always starts in column 1 and begins with a letter. This identifier is provided as an aid in identifying the material on the material data list. The atomic or molecular formulae are used for all elements and most simple compounds; short names, abbreviations, acronyms, or mnemonics are used in other cases.

Column 6

Always left blank.

Columns 7-10

Material identification number, in the range from 1001-9999, and never exactly divisible by 1000. Each material is assigned its own identification number.

Column 11

Always left blank.

Columns 12-50

Material description, including as much information as necessary to identify the specific material. Many abbreviations are used, such as these examples: HP (hot pressed), SINT (sintered), 89 D (89% of theoretical density), 22 P (22% porosity), PRSD (pressed), FRD (fired), and HT (hot treated). A number of other standard abbreviations also are used for special alloys. Mass percentages follow component names. Atomic percentages precede the name of the molecular species.

Column 51

Normally left blank except when more than one card is used to list the data source numbers. In these cases, the additional cards have a + in column 51.

Columns 52-72

Data source numbers, specified in the list of data sources or other information identifying the sources of the compiled data. No classified data sources are listed. For all data estimated by the author or obtained from unknown data sources, a data source number is not indicated.

Columns 73–79

The numerical quality indicators for the data. One column is provided for each of the following properties: density (b), constant specific heat (c), constant thermal conductivity (k), temperature of transition or maximum service temperature (t), latent heat of transition (h), table of specific heat vs temperature (c), and table of thermal conductivity vs temperature (k). The one-letter abbreviation for each property is listed in Table M5.6.1 over the column containing the corresponding quality indicator.

Column 80

Always left blank.

Many materials appear more than once in the index. The reason for this duplication is that several common names exist for the same material or additional identifying information is included under separate entries.

Table M5.6.1 Material index

ID	No.	Material	References	Quality Index DCKTHCK[a]
ALOXD	4012	ALUMINUM OXIDE (AL203) (POLYXTAL 100 D)	1,20,27,32,47,48,51	200
ALOXP	4014	ALUMINUM OXIDE (AL203) (POLYXTAL, 55 D)	1,20,27,32,47,48,51	200
ALOXS	4016	ALUMINUM OXIDE (AL203) (SINGLE XTAL)	1,20,27,32,47,48,51	202
ALCR1	5412	ALUMINUM OXIDE + CR (AL203 23, CR 77)	20,48	302530
ALCR2	5413	ALUMINUM OXIDE + CR (AL203 70, CR 30)	20,48	302535
ANDAL	4312	ALUMINUM SILICATE (AL203.SIO2) (ORTHO)	20,27,47,51	20505
KYAN	4314	ALUMINUM SILICATE (AL203.SIO2) (TRICL)	20,27,47,51	500
MULL	4316	ALUMINUM SILICATE (3AL203.2SIO2) (100 D)	20,27,47,48,51	500
AM	1430	AMERICIUM	20,27	342555
NH3	4881	AMMONIA (NH3) (GAS)	1,27,47	0
NH3LQ	4880	AMMONIA (NH3) (LIQUID UNDER PRESSURE)	1,27,47	500
NH4BR	4812	AMMONIUM BROMIDE (NH4BR) (PRSD 8 KB)	27,47	300530
NH4CL	4814	AMMONIUM CHLORIDE (NH4CL) (PRSD 8 KB)	27,47	10
ANALC	4329	ANALCITE (NA20.AL203.4SIO2.4H2O) (XTAL)	27,51	305555
ANDAL	4312	ANDALUSITE (AL203.SIO2) (ORTHO XTAL)	20,27,51	20505
SB	1006	ANTIMONY	20,1,32,42,27	0
SBLIQ	1007	ANTIMONY (LIQUID)	1,47,42,27,20,14	0
SBTEC	4913	ANTIMONY TELLURIDE (SB2TE3) (CPR, N DR)	20,27	300555
SBTEP	4912	ANTIMONY TELLURIDE (SB2TE3) (POLYXTAL)	20,27	300555
ARGAS	1501	ARGON (GAS)	27,2,42,41	0
AS	1008	ARSENIC, GREY	1,27,41,42	40005
ASTEX	4914	ARSENIC TELLURIDE (AS2TE3) (V ZONE MLT)	20	3305555
ART1	9001	ARTIFICAL MATERIAL 1 (D=C=K=0)	0	
ART2	9002	ARTIFICAL MATERIAL 2 (D=C=0, K=10**9)		0
ART3	9003	ARTIFICAL MATERIAL 3 (D=C=K=1)		0
ART4	9004	ARTIFICAL MATERIAL 4 (D=C=1, K=10**9)		0
ART5	9005	ARTIFICAL MATERIAL 5 (D=1, C=K=10**9)		0
ART6	9006	ARTIFICAL MATERIAL 6 (D=C=K=TM=HM=1)		0
ART7	9007	ARTIFICAL MATERIAL 7 (DCKTM=1,HM=10**91		0
AT	1437	ASTITINE	42	3343335
BRTOL	7501	BARATOL H.E. (TNT 26, BA NITRATE 76)	8	555
BA	1241	BARIUM	20,27,29,42,43	40005
BAB6	4612	BARIUM BORIDE (BAB6)	27,48	300555
BAF2	4816	BARIUM FLUORIDE (BAF2) (SINGLE CRYSTAL)	20,27,51	300230
BANO3	4952	BARIUM NITRATE (BA(NO3)2) (PRSD 8 K8)	1,27	300050
BASO4	4954	BARIUM SULFATE (BASO4) (CRYSTAL)	27,51	300550
BATIS	4213	BARIUM TITANATE (BAO.TIO2) (SINTERED)	20,27,48	500
BATIT	4212	BARIUM TITANATE (BAO.TIO2) (100 D)	20,27,48	500
BATIM	4214	BARIUM TITANATE (BAO.TIO2) (+MN,NB OX)	20,27,48	500
BK	1440	BERKELIUM	27	4445555
BERYL	4318	BERYL (3BEO.AL203.6SIO2)	20,27,51	320502
BE	1011	BERYLLIUM	20,6,1,32,34,27,36,42	22
BEBEO	5420	BERYLLIUM + BEO (BE, BEO 0.6-1.7)	20	3300
BE96A	3501	BERYLLIUM ALLOY (BE96.5) (AS RECEIVED)	20	303331
BE96H	3502	BERYLLIUM ALLOY (BE96.5) (ANNEALED)	20	303331
BE98A	3503	BERYLLIUM ALLOY (BE98.5) (AS RECEIVED)	20	303331
BE98H	3504	BERYLLIUM ALLOY (BE98.5) (ANNEALED)	20	303331
BE995	3505	BERYLLIUM ALLOY (BE99.5)	20	3033313
BERYL	4318	BERYLLIUM ALUMINOSILICATE (BERYL)	20,27,51	320502
BE2C	4512	BERYLLIUM CARBIDE (BE2C) (HP OR SNT)	14,20,28,47	2220022
CUBER	2181	BERYLLIUM COPPER (CU BAL, BE 0.38-0.55)	1	331
CUBEH	2182	BERYLLIUM COPPER (CU BAL, BE1.7-1.9)	1,6,41	2335
BE3N2	4414	BERYLLIUM NITRIDE (BE3N2) (PRSD 3.4 KB)	20,47	5
BEOXP	4024	BERYLLIUM OXIDE (BEO) (76 PC DENS)	14,20,27,36,43,44,	0
BEOXP	4024	BERYLLIUM OXIDE (BEO) (76 PC DENS)	+47,48,51	0

Table M5.6.1 (continued)

ID	No.	Material	References	Quality Index DCKTHCK[a]
BEO	4022	BERYLLIUM OXIDE (BEO) (96 PC DENS)	14,20,27,36,43,44,	0
BEO	4022	BERYLLIUM OXIDE (BEO) (96 PC DENS)	+47,48,51	0
BEOBE	5414	BERYLLIUM OXIDE + BE (BEO, BE 3-12)	20	5500
BEOMO	5416	BERYLLIUM OXIDE + BE + MO (BE 7, MO 7)	20	5501
BEOSI	5418	BERYLLIUM OXIDE + BE + SI	20	305530
PORBE	5280	BERYLLIUM OXIDE PORCELAIN 4811	20	305530
BSPOD	4320	BETA-SPODUMENE (LI20.AL203.4SIO2) (TET)	20,27,51	305550
BI	1016	BISMUTH	2,1,27,43,41,42,47	0
BILIQ	1017	BISMUTH (LIQUID)	1,14,27,43,47	0
BITEP	4916	BISMUTH TELLURIDE (BI2TE3-P) (PLANE DR)	20,47	220522
BITES	4918	BISMUTH TELLURIDE SULFIDE (BI2TE2S)	20	3305550
ZRB2Z	5498	BORIDE Z CERMET (ZRB2 81-87, MOSI2 13)	47,48	2000500
ZRB2B	5496	BOROLITE 101 CERMET (ZRB2 93-96, B 4-7)	47,48	505
BORON	1266	BORON	20,27,30,42,43,48	20205
B4C-D	4514	BORON CARBIDE (B4C) (DENSE)	20,27,48	2002500
B4C-P	4515	BORON CARBIDE (B4C) (POROUS)	20,27,48	2002500
BN	4416	BORON NITRIDE (BN) (PERP PR AXIS, 95 D)	20,27,36,47,48	500
BNPPA	4418	BORON NITRIDE (BN) (PRS AXIS, 94 D)	20,27,36,47,48	500
BNAC	4424	BORON NITRIDE (BN 80, C 20) (PRS AXIS)	20	5500
BNOX2	4420	BORON NITRIDE (BN 97, BN2O3 2) (PERP P)	20	5500
BNOXP	4422	BORON NITRIDE (BN 97, BN2O3 2) (PRS AX)	20	5500
SIB4	4614	BORON SILICIDE (B4SI)	27,48	300530
BRALM	2101	BRASS, ALUMINUM (CU76, ZN22, AL2)	1	555
BRCAR	2105	BRASS, CARTRIDGE (CU70, ZN30)	1,2,20,41,46	500
BRPBL	2111	BRASS, LEADED	6,41	3555
BRMUM	2116	BRASS, MUNTZ METAL	1,41	5555
BRRDC	2121	BRASS, RED, CAST (CU85, ZN5, PB5, SN3)	1,41	3555
BRRDW	2122	BRASS, RED, WROUGHT (CU85, ZN15)	1,41	20555
BRTIN	2126	BRASS, TIN (NAVAL AND ADMIRALTY)	1,2,41	2555
BRYEL	2131	BRASS, YELLOW (CU65, ZN35)	1,6,41	555
BRICR	5232	BRICK, CHROME (CR203 32)	1,27,41	5530
BRCRM	5234	BRICK, CHROME MAGNESITE (SEE REF 47)	20,47	330
DIATA	5246	BRICK, DIATOMACEOUS EARTH (ACCR STRATA)	4	305530
DIATH	5249	BRICK, DIATOMACEOUS EARTH (HIGH BURN)	4	305530
DIATM	5248	BRICK, DIATOMACEOUS EARTH (MOLDED, FRD)	4	305530
DIATP	5247	BRICK, DIATOMACEOUS EARTH (PRLL STRATA)	4	305530
DIATT	5251	BRICK, DIATOMACEOUS EARTH (USE TO 1100)	4	305530
DIATL	5250	BRICK, DIATOMACEOUS EARTH (USE TO 850C)	4	305530
BRIEF	5256	BRICK, EGYPTIAN FIRE (SIO2 64-71)	20	2323532
BRICF	5224	BRICK, FIRED CARBON	1,20,27,42,47	5505
BRIFR	5262	BRICK, FORSTERITE (MGO 58 SIO2 38)(20P)	20,47	335
BRALF	5212	BRICK, FUSED ALUMINA (AL203 96)(22 P)	1,20,47	2330
BRISI	5294	BRICK, HARD FIRED SILICA (SIO2 94-95)	20	330
BRAL1	5214	BRICK, HIGH ALUMINA (AL203 53) (20 P)	47	322335
BRAL2	5215	BRICK, HIGH ALUMINA (AL203 83) (28 P)	47	322335
BRAL3	5216	BRICK, HIGH ALUMINA (AL203 87) (22 P)	20	303330
BRIKB	5265	BRICK, KAOLIN INSULATING (D = 0.30)	1,20	5510
BRIKA	5264	BRICK, KAOLIN INSULATING (D = 0.43)	1,20	5510
MAGNP	5267	BRICK, MAGNESITE (MGO 87)	1,20,27,47,48	330
MAGNA	5268	BRICK, MAGNESITE A (MGO 90) (14.5 P)	1,20,27,47,48	330
MAGNB	5269	BRICK, MAGNESITE B (MGO 93) (22.6 P)	1,20,27,47,48	330
MAGNC	5270	BRICK, MAGNESITE C (MGO 86) (17.8 P)	1,20,27,47,48	330
MAGNS	5266	BRICK, MAGNESITE SPALL RES (MGO 89)	1,20,27,47,48	335
BRIMM	5218	BRICK, MASONRY, MEDIUM	1,2,27,46	2025535
BRIFM	5259	BRICK, MISSOURI FIRECLAY	1,47	3300530

Table M5.6.1 (continued)

ID	No.	Material	References	Quality Index DCKTHCK[a]
BRIFN	5258	BRICK, NORMAL FIRECLAY (22 P)	47	535
BRISL	5296	BRICK, SILICEOUS (SIO2 89 AL203 9)(25P)	47	335
BRIFS	5260	BRICK, SILICEOUS FIRECLAY (23 P)	47	535
BRISK	5298	BRICK, SILLIMANITE (22 PC POROSITY)	20	300530
BRIDS	5254	BRICK, STABILIZED DOLOMITE (22 P)	1,47	530
VERMI	4986	BRICK, VERMICULITE	20	305550
BRGAS	1546	BROMINE (GAS)	27,1,42	0
BRONZ	2141	BRONZE (CU75, SN25)	1,2	305555
BROAL	2146	BRONZE, ALUMINUM (CU92, AL8)	1,6,41	2000555
BROAR	2151	BRONZE, ARCHITECTURAL	1,41	2300555
BROCM	2156	BRONZE, COMMERCIAL	1,2,38,41	555
BROMN	2161	BRONZE, MANGANESE	1,41	555
BROPH	2166	BRONZE, PHOSPHER 10 PERCENT	1,41	5555
BROPL	2168	BRONZE, PHOSPHER 1.25 PERCENT	6,41	555
BROPM	2167	BRONZE, PHOSPHER 5 PERCENT	6,41	555
BRSIH	2171	BRONZE, SILICON, HIGH	1,6,41	550
BRSIL	2172	BRONZE, SILICON, LOW	1,6,41	555
BRSNH	2176	BRONZE, TIN (CAST), HIGH LEADED	6,41	23555
BRSNL	2177	BRONZE, TIN (CAST), LEADED	6	3555
BUACR	7026	BUTADIENE-ACRYLONITRILE RUBBER + C	20	5555
BUTYR	7031	BUTYL RUBBER	6,39	555
CD	1041	CADMIUM	2,1,32,42,43,27,41,47	0
CDLIQ	1042	CADMIUM (LIQUID)	2,1,32,42,43,27,41,47	0
CACCP	4957	CALCITE (CACO3) (CRYSTAL) (C AXIS)	1,27,51	0
CACCS	4958	CALCITE (CACO3) (CRYSTAL) (A AXIS)	1,27,51	0
CA	1306	CALCIUM	27,1,42,43,41	5
CAB6	4616	CALCIUM BORIDE (CAB6)	27,48	300555
CACCP	4957	CALCIUM CARBONATE (CACO3) (CALCITE) (C)	1,27,51	0
CACCS	4958	CALCIUM CARBONATE (CACO3) (CALCITE) (A)	1,27,51	0
CACON	4956	CALCIUM CARBONATE (CACO3) (NATURAL)	1,27,51	5
CAF2A	4820	CALCIUM FLUORIDE (CAF2) (MINERAL AGGR)	1,20,27,47,51	205
CAF2	4818	CALCIUM FLUORIDE (CAF2) (SINGLE XTAL)	1,20,27,47,51	200
DOLOM	4960	CALCIUM MAGNESIUM CARBONATE (CAMGC206)	1,27,51	20515
CAO	4026	CALCIUM OXIDE (CAO) (PRESSED, 91 DENS)	1,20,27,47,48,51	200
CAOPP	4028	CALCIUM OXIDE (CAO) (PACKED PWD, 50 D)	1,20,27,47,48	200
GYPSM	4962	CALCIUM SULFATE DIHYDRATE (CASO4.4H2O)	1,27,51	555
CATIT	4216	CALCIUM TITANATE (CAO.TIO2)	20,27,48,51	500
CF	1443	CALIFORNIUM		4445555
CAMOR	1071	CARBON, AMORPHOUS (CARBON STOCK)	27,1	22
CGEM1	1061	CARBON, DIAMOND GEM QUALITY TYPE 1	1,20,27	500
CGRAF	1066	CARBON, GRAPHITE (TYPICAL K)	1,2,20,27,32,42,51	2000002
BRICF	5224	CARBON BRICK, FIRED	1,20,27,42,47	5505
CO2	4027	CARBON DIOXIDE	1,2,27	0
COGAS	4029	CARBON MONOXIDE	1,27	300030
CELA2	7037	CELLULOSE ACETATE (HIGH K)	6,38	20555
CELA1	7036	CELLULOSE ACETATE (LOW K)	6,38	20555
CEAB2	7042	CELLULOSE ACETATE BUTYRATE (HIGH K)	6,38	225555
CEAB1	7041	CELLULOSE ACETATE BUTYRATE (LOW K)	6,38	225555
CENIP	7046	CELLULOSE NITRATE (PYROXYLIN)	6,38	200555
CEPR1	7051	CELLULOSE PROPRIONATE (LOW K)	6,38	225555
CEPR2	7052	CELLULOSE PROPRIONATE (HIGH K)	6,38	225555
CETRA	7056	CELLULOSE TRIACETATE	38	5555
CE	1356	CERIUM	41,27,20,42	20205
CEB6	4626	CERIUM BORIDE (CEB6) (99.0 PC DENSE)	48	300555
CEO2	4030	CERIUM OXIDE (CEO2) (PRSD, SNTRD, 86 D)	1,20,47	201

Table M5.6.1 (continued)

ID	No.	Material	References	Quality Index DCKTHCK[a]
CES	4742	CERIUM SULFIDE (CES)	20,48	22505
CE2S3	4744	CERIUM SULFIDE (CE2S3)	20,48	20512
CS	1231	CESIUM	1,14,27,28,32,43,47	40005
CSLIQ	1232	CESIUM (LIQUID)	14,27,28,32,43,47	22
CHALK	6018	CHALK (AV PROP)	1,46	25555
CLGAS	1506	CHLORINE (GAS)	27,1,42,2	0
CRALM	4973	CHROME ALUM (CR2(SO4)3.K2SO4.24H2O)	1,27	550
BRICR	5232	CHROME BRICK (CR2O3 32)	1,27,41	5530
BRCRM	5234	CHROME MAGNESITE BRICK (SEE REF 47)	20,47	330
CNISA	3312	CHROME-NICKEL-IRON SUPERALLOYS	6	555
CR	1201	CHROMIUM	20,1,27,32,43,42	0
CHCNI	5422	CHROMIUM CARBIDE + NI (CR(X)C(Y), NI)	48	2000555
CUCHR	2183	CHROMIUM COPPER (CU BAL, CRO.5)	6,20,47	2330
CRN	4426	CHROMIUM NITRIDE (CRN) (PRSD, 100 PC D)	27,47,48	505
CR2N	4428	CHROMIUM NITRIDE (CR2N) (PRSD, 100 D)	27,47,48	200505
CRSI2	4772	CHROMIUM SILICIDE (CRSI2)	20,27,48	500
CO	1046	COBALT	20,27,1,32,43,30,41,	0
CO	1046	COBALT	+42	0
COCRW	2646	COBALT ALLOY (CO64,CR30,W6)	20	330333
CO			20	3300
COH21	2614	COBALT ALLOY HS-21 (AS CAST)	1,14,20,41	310
COH2A	2615	COBALT ALLOY HS-21 (AGED)	1,14,20,41	310
COH23	2616	COBALT ALLOY HS-23	14,20	303330
COH25	2618	COBALT ALLOY HS-25 (L-605) (WROUGHT)	1,14,41	330
COH27	2620	COBALT ALLOY HS-27 (AS CAST)	14,20	303330
COH30	2622	COBALT ALLOY HS-30 (422-19) (AS CAST)	14,20	333333
COH31	2624	COBALT ALLOY HS-31 (X-40) (AS CAST)	1,14,20,41	300330
COH36	2626	COBALT ALLOY HS-36 (CAST)	1,14,20	333
COJG3	2628	COBALT ALLOY JESSOP G-32	20	303330
COJ15	2630	COBALT ALLOY J-1570	20	3333330
COK42	2632	COBALT ALLOY K-42B	14	3323332
COMTL	2636	COBALT ALLOY MULTIMET (N-155) (LOW C)	1,14,20,41	330
COMTM	2634	COBALT ALLOY MULTIMET (N-155) (WROUGHT)	1,14,20,41	330
COS59	2638	COBALT ALLOY S-590 (WROUGHT)	14,41	330
COS81	2640	COBALT ALLOY S-816 (WROUGHT)	1,14,20,41	330
COV36	2642	COBALT ALLOY V-36 (WROUGHT)	41	333333
COW52	2644	COBALT ALLOY WI-52	20	3333330
COW5G	2645	COBALT ALLOY WI-52 (CR COATED SAMPLE)	20	3333330
CNLOX	4218	COBALT NICKEL OXIDE (46COO.46NIO.8LIO)	20,27	3305555
COBOX	4034	COBALT OXIDE (COO)	20,27,47,48	2005
COS	4774	COBALT SILICIDE (COS)	20,48	305555
NBTAW	3681	COLOMBIUM ALLOY (CB61,TA28,W10,ZR0.5)	20	3300
NBWMO	3684	COLOMBIUM ALLOY (CB80, W15, MO5)	20	3300
NBTIZ	3682	COLOMBIUM ALLOY (CBS5, TI10, ZR5)	20	3300
NBTA5	3683	COLOMBIUM ALLOY (CB95, TA5)	20	3303330
CMB-3	7502	COMPOSITION B-3 H.E. (RDX 60, TNT 40)	8	555
CMC-4	7503	COMPOSITION C-4 H.E. (RDX 90, BINDERS)	8	5555
CONCN	5240	CONCRETE, CINDER	1,2,20,27,46	25535
CONLW	5243	CONCRETE, LIGHTWEIGHT	1,2,20,27,46	5530
CONCS	5241	CONCRETE, STONE (1-2-4 MIX)	1,2,20,27,46	25535
CON14	5242	CONCRETE, 1-4 DRY	1,2,20,27,46	25535
CU	1051	COPPER	20,1,27,32,34,37,42,	0
CU	1051	COPPER	+47	0
CUWGT	2191	COPPER, WROUGHT (ETP, DHP, TE0.5, PB1)	41	3535
CUBER	2181	COPPER ALLOY (CU BAL, BE 0.38-0.55)	1	331

Table M5.6.1 (continued)

ID	No.	Material	References	Quality Index DCKTHCK[a]
CUBEH	2182	COPPER ALLOY (CU BAL, BE 1.7-1.9)	1,6,41	2335
CUCHR	2183	COPPER ALLOY (CU BAL, CR0.5)	6,20,47	2330
CUPR3	2203	COPPER ALLOY (CU70, NI30)	1,6,41	2555
CUPR1	2202	COPPER ALLOY (CU90, NI10)	1,6,41	2555
CUAL1	2201	COPPER ALLOY (CU99.4, AL0.3, ZR0.27)	20	3303331
NICON	2506	COPPER ALLOY CONSTANTAN (CUS5, NI45)	1,2,14,41,47	331
CUMAN	2195	COPPER ALLOY MANGANIN	2	3305550
CUNIS	2185	COPPER ALLOY NICKEL SILVER (NI 10-20)	1,2,6,41,47	2222555
CUGZN	2186	COPPER GILDING METAL (CU95, ZN5)	1,41	555
CUOLI	4220	COPPER LITHIUM OXIDE (96CUO.4LIO)	20,27	3305550
CUO	4036	COPPER OXIDE (CUO) (TENORITE)	1,20,27,47,51	2002220
CUSO4	4966	COPPER SULFATE (CUS04) (CRYSTAL)	27	550
BLUEV	4967	COPPER SULFATE HYDRATE (CUS04.5H2O)	1,27,51	555
CORDR	4322	CORDIERITE (2MGO.2AL203.5SIO2)	20,51	5510
CORKG	8514	CORK, GROUND	2,46	5555
CORKR	8515	CORK, GROUND, REGRANULATED	2,46	5555
CUPR3	2203	CUPRONICKEL (CU70, NI30)	1,6,41	2555
CUPR1	2202	CUPRONICKEL (CU90, NI10)	1,6,41	2555
CM	1446	CURIUM	20,27	4445555
DAN35	3901	DANDELION 35	34,36	5500
DATB	7504	DATB H.E. (DIANINO TRINITROBENZENE)	8	300555
D-GAS	1551	DEUTERIUM	27	3305530
D2O	4118	DEUTERIUM OXIDE (D2O) (LIQUID)	14,27	300
DIABG	5020	DIABASIC GLASS (ARTIFICIAL)	27,51	3305530
DAPON	7061	DIALLYL PHTHALATE (DAPON)	35	2025555
DIATA	5246	DIATOMACEOUS EARTH BRICK (ACCR STRATA)	4	305530
DIATH	5249	DIATOMACEOUS EARTH BRICK (HIGH BURN)	4	305530
DIATM	5248	DIATOMACEOUS EARTH BRICK (MOLDED, FRD)	4	305530
DIATP	5247	DIATOMACEOUS EARTH BRICK (PRLL STRATA)	4	305530
DIATT	5251	DIATOMACEOUS EARTH BRICK (USE TO 1100C)	4	305530
DIATL	5250	DIATOMACEOUS EARTH BRICK (USE TO 850C)	4	305530
DOLOM	4960	DOLOMITE (CAMG(CO3)2) (AVG PROP)	1,27,51	20555
BRIDS	5254	DOLOMITE BRICK, STABILIZED (22 P)	1,47	530
DY	1391	DYSPROSIUM	41,27,20,42	35
BRIEF	5256	EGYPTIAN FIRE BRICK (SIO2 64-71)	20	2323532
ES	1449	EINSTEINIUM		4445555
EPCR1	7066	EPOXY, DER 332 (C), HYSOL 6000-OP (K)	6,20,38	2220505
EPGFM	7071	EPOXY, GLASS FIBER FILLED (MOLDED)	20,38	25552
EPSFC	7076	EPOXY, SILICA FILLED, CAST	38	2225555
EPUNC	7081	EPOXY, UNFILLED, CAST	38	2025555
EPSOM	4971	EPSOMITE (MGSO4.7H2O) (CRYSTAL)	1,27,51	555
ER	1401	ERBIUM	41,27,20,42	5
ETHCE	7086	ETHYL CELLULOSE (WIDE RANGE OF C, K)	6,38	225555
ETHVA	7091	ETHYL VINYL ACETATE	38	25555
EU	1376	EUROPIUM	20,27,41,43	30005
EUB6	4634	EUROPIUM BORIDE (EUB6) (93.0 PC DENSE)	48	305555
FM	1452	FERMIUM		4445555
FBRFX	8201	FIBERFAX PAPER (CARBORUNDUM CO.)	44	5500
BRIFM	5259	FIRECLAY BRICK, MISSOURI	1,47	3300530
BRIFN	5258	FIRECLAY BRICK, NORMAL (22 P)	47	535
BRIFS	5260	FIRECLAY BRICK, SILICEOUS (23 P)	47	535
FLINT	5022	FLINT GLASS	1,27,46	25532
ART5	9005	FLUID, HEAT SINK (D=1, C=K=10**9)		0
ART4	9004	FLUID, WELL STIRRED (D=C=1, K=10**9)		0
F-GAS	1511	FLUORINE (GAS)	27,42	0

Table M5.6.1 (continued)

ID	No.	Material	References	Quality Index DCKTHCK[a]
FCCTF	7101	FLUOROCARBONS, CFE AND CTFE	6,38	555
FCFEP	7106	FLUOROCARBONS, FEP	6,38	555
FCTFE	7111	FLUOROCARBONS, TFE (TEFLON)	1,6,20,38	2500
GLASF	5024	FOAMED GLASS (D = 0.144)	1	305532
FORST	4324	FORSTERITE (2MGO.SIO2) (100 PC DENSE)	1,20,27,51	0
BRIFR	5262	FORSTERITE BRICK (MGO 58 SIO2 38)(20 P)	20,47	335
FR	1455	FRANCIUM	42	4343335
SIO2	4062	FUSED SILICA GLASS	1,20,27,47,51	2200
SIO2	4062	FUSED QUARTZ GLASS (SIO2)	1,20,27,47,51	2200
GD	1381	GADOLINIUM	41,27,20,42	5
GDB6	4636	GADOLINIUM BORIDE (GDB6) (95.6 PC DENS)	48	300555
GD203	4038	GADOLINIUM OXIDE (GD203) (MONOC) (98 D)	20,47,48	2000505
GA	1311	GALLIUM	27,42,43,1	20005
GALIQ	1312	GALLIUM (LIQUID)	1,14,27,43,47	20005
GE-IP	1261	GERMANIUM (INTRINSIC, P-TYPE)	20,27,42,43,1,48	2
GE-N	1262	GERMANIUM (N-TYPE)	20,27,42,43,1,48	0
GLASS	5012	GLASS (SEE REP 27, PP E5-E8) (AVG PROP)	27	2225555
GLABC	5014	GLASS, BOROSILICATE CROWN	27,51	25502
PYRC6	5018	GLASS, CERAMIC, PYROCERAM 9606	20	5500
PYRC8	5019	GLASS, CERAMIC, PYROCERAM 9608	20	5500
DIABG	5020	GLASS, DIABASE (ARTIFICIAL)	27,51	3305530
FLINT	5022	GLASS, FLINT	1,27,46	25532
GLASF	5024	GLASS, FOAMED (D = 0.144)	1	305532
SIO2	4062	GLASS, FUSED QUARTZ (SIO2)	1,20,27,47,51	2200
SIO2	4062	GLASS, FUSED SILICA OR VITROUS SILICA	1,20,27,47,51	2200
GLASL	5026	GLASS, LEAD	20	305530
GLASW	5028	GLASS, LIME WINDOW	20	305530
OBSID	5030	GLASS, OBSIDIAN	27,51	305530
PYREX	5016	GLASS, PYREX	2,20,27,51	500
GLASP	5034	GLASS, SODA PLATE	20,51	305532
GLASC	5032	GLASS, SODA-LIME	20,27	3325532
VYCOR	5036	GLASS, VYCOR	20,27	500
AU	1056	GOLD	20,6,1,32,27,42,41,2	0
AULIQ	1057	GOLD (LIQUID)	14,20,27,42,43	40005
GRNTM	6014	GRANITE (AV PROP) (SEE REF 51)	1,2,27,46,51	25555
GRNTH	6013	GRANITE (HIGH K)	1,2,27,46,51	25555
GRNTL	6012	GRANITE (LOW K)	1,2,27,46,51	25555
GYPSM	4962	GYPSUM (CASO4.4H2O) (MINERAL) (HIGH D)	1,27,51	555
GYPSA	4964	GYPSUM (CASO4.4H2O) (ARTIFICIAL)	1,27	555
HF	1271	HAFNIUM	20,32,27,42,43,41	0
HFB2	4618	HAFNIUM BORIDE (HFB2)	20,27,48	20502
HFC	4518	HAFNIUM CARBIDE (HFC)	20,27,48,54	22502
HFN	4430	HAFNIUM NITRIDE (HFN) (HP STRD 78-92 D)	20,27,48	2020502
HFO2	4040	HAFNIUM OXIDE (HFO2) (MONOC) (94 D)	20,27,48	21
D2O	4118	HEAVY WATER (D2O) (LIQUID)	14,27	300
HEGAS	1516	HELIUM (GAS)	27,1,2,42	0
FE203	4042	HEMATITE (FE203)	1,27,32,47,48,51	20505
HO	1396	HOLMIUM	20,27,41,42,43	30005
H-GAS	1521	HYDROGEN (GAS)	27,2,42,1	0
ICE	4116	ICE (H2O) (SOLID)	27,46,51	0
IN	1211	INDIUM	1,27,43,30,42,41	20005
INLIQ	1212	INDIUM (LIQUID)	1,42,43,47	5
SOLD1	3611	INDIUM ALLOY (IN25, SN37.5, PB37.5)	36	3355
INSBP	4920	INDIUM ANTIMONIDE (INSB) (IMP 0.16)	20,27	3000000
INSBS	4921	INDIUM ANTIMONIDE (INSB) (IMP 0.33-1.2)	20,27	3000000

Table M5.6.1 (continued)

ID	No.	Material	References	Quality Index DCKTHCK[a]
INASP	4922	INDIUM ARSENIDE (INAS) (POLYX, IMP 3.0)	20,27	3000500
INASS	4923	INDIUM ARSENIDE (INAS) (PURE, S-DOPED)	20,27	3000500
INTE	4924	INDIUM TELLURIDE (IN2TE3)	20,27	300550
I-SOL	1316	IODINE (SOLID)	27,42,41,1	5
IR	1276	IRIDIUM	27,41,20,42,43	20002
FEFUR	1083	IRON (0 TO 3000 DEG C)	20,1,32,27,42,44,51	0
FECRY	1082	IRON (-273 TO 763 DEG C)	20,1,32,27,42,44,51	0
FE	1081	IRON (-51 TO 1537 DEG C)	20,1,32,27,42,44,51	0
INDO2	3022	IRON, DUCTILE (MG CONTAINING)	1	300355
INDO3	3023	IRON, DUCTILE (MG CONTAINING, HEAT RES)	1	300355
INDO1	3021	IRON, DUCTILE (0.06 MG)	1,6	323333
GCIO1	3001	IRON, GREY CAST, FERRITIC (2.3-3.0 C)	1,2,6,20,27,33,46	3300
GCIO2	3002	IRON, GREY CAST, FERRITIC (3.2-3.8 C	1,2,6,20,27,33,46	303330
GCIO3	3003	GREY CAST, PEARLITIC (2.3-3.0 C)	1,2,6,20,27,33,46	303330
GCIO4	3004	IRON, GREY CAST, PEARLITIC (3.0-3.2 C)	1,2,6,20,27,33,46	303330
GCIO5	3005	IRON, GREY CAST, PEARLITIC (3.4 C)	1,2,6,20,27,33,46	303330
GCIO6	3006	IRON, GREY CAST, PEARLITIC (3.7-3.8 C)	1,2,6,20,27,33,46	303330
GCIO7	3007	IRON, GREY CAST, PEARLITIC (4.12 C)	1,2,6,20,27,33,46	303330
FE	1081	IRON, INGOT (FE99.9+)	1,20,27,32,42,44	0
KOVAR	3031	IRON, NI-HARD TYPES 1 AND 2 (KOVAR)	1,20	200320
INNRD	3035	IRON, NI-RESIST, TYPE D2 (CAST)	1	300355
INNR3	3033	IRON, NI-RESIST, TYPE 3 (CAST)	1	355
INNR4	3034	IRON, NI-RESIST, TYPE 4 (CAST)	1	355
INNIR	3032	IRON, NI-RESIST, TYPES 1 AND 2 (CAST)	1,20	325
INNIT	3041	IRON, NI-TENSYLIRON (CAST, HEAT TREAT)	1	300355
INCFB	3026	IRON, NODULAR CAST, FERRITIC BASE	1,2,20	303330
INCPB	3027	IRON, NODULAR CAST, PEARLITIC BASE	1,2,20	303330
INKAL	3036	IRON, MALLEABLE (2.5 C)	1,6	5555
INWRT	3037	IRON, WROUGHT (VARIOUS)	1,2,6,27	2330
NINVR	2501	IRON ALLOY INVAR (FE64, NI36)	6,41,47	20355
FE2O3	4042	IRON OXIDE (FE2O3) (HEMATITE)	1,27,32,47,48,51	20505
FE3O4	4044	IRON OXIDE (FEO.FE2O3) (MAGNATITE)	20,27,47,51	2000005
FES2	4746	IRON SULFIDE (FES2) (SINGLE CRYSTAL)	27,47,51	505
BRIKB	5265	KAOLIN BRICK, INSULATING (D = 0.30)	1,20	5510
BRIKA	5264	KAOLIN BRICK, INSULATING (D = 0.43)	1,20	5510
KRGAS	1556	KRYPTON (GAS)	27,1,42	0
KYAN	4314	KYANITE (AL2O3.SIO2) (TRICL CRYSTAL)	20,27,51	500
LA	1351	LANTHANUM	41,27,1,20,42	5
LAB6	4624	LANTHANUM BORIDE (LAB6) (99.5 PC DENSE)	48	300555
LW	1491	LAWRENCIUM		4445555
PB	1091	LEAD	2,1,32,27,37,42	0
PBLIQ	1092	LEAD (LIQUID)	1,2,14,27,37,42,43,47	2
PB	1091	LEAD (0.07 CA)	36	0
PBANT	3601	LEAD, ANTIMONIAL (PB, SB 4-6) (HARD)	1,6,41	355
PBSBH	3602	LEAD, ANTIMONIAL (PB, SB 8-9)	1,6,41	355
PB	1091	LEAD, ANTIMONIAL (PB, SB1)	1,41	0
PB	1091	LEAD, TELLURIUM	1	0
SOLD1	3611	LEAD ALLOY (PB37.5, SN37.5, IN25)	36	3355
SOLD2	3612	LEAD ALLOY (PB39.2, SN60.8) (SOLDER)	34,41	5
SOLD4	3613	LEAD ALLOY (PB50, SN50) (SOLDER)	1,41	50
SOLD3	3614	LEAD ALLOY (PB60, SN40) (SOLDER)	1,41	55
GLASL	5026	LEAD GLASS	20	305530
PBO	4046	LEAD OXIDE (PBO) (YELLOW)	1,20,27,32,47	201
PBTEP	4927	LEAD TELLURIDE (PBTE) (POLYXTAL)	20,27	300550
PBTES	4926	LEAD TELLURIDE (PBTE) (SINGLE CRYSTAL)	20,27	300550

Table M5.6.1 (continued)

ID	No.	Material	References	Quality Index DCKTHCK[a]
LIMST	6016	LIMESTONE (DENSE, DRY)	1,2,27,46,51	5555
LIMSW	6017	LIMESTONE (H2O 15.3)	1,2,27,46,51	5555
LI	1216	LITHIUM	1,27,28,41,43,42,47	0
LILIQ	1217	LITHIUM (LIQUID)	1,27,28,41,42,43,47	202
BSPOD	4320	LITHIUM ALUMINUN SILICATE (B-SPODUMENE)	20,27,51	305550
CNLOX	4218	LITHIUM COBALT NICKEL OXIDE (8-46-46 M)	20,27	3305555
CUOLI	4220	LITHIUM COPPER OXIDE (4LIO.96CUO)	20,27	3305550
LIH	4882	LITHIUM HYDRIDE (LIH) (CAST, VAC VOIDS)	20	200
LIH	4882	LITHIUM HYDRIDE (LIH) (POWDER COMPACT)	20	200
LIHCG	4884	LITHIUM HYDRIDE (LIH) (CAST GAS VOIDS)	20	200
LIF	4822	LITHIUM FLUORIDE (LIF) (SINGLE CRYSTAL)	1,20,27,47,51	20202
LIFPB	4824	LITHIUM FLUORIDE (LIF 96) (PLASTIC BND)	1,20,27,47,51	200
MNSEL	4928	LITHIUM MANGANESE SELENIDE (97MN.3LI.-)	20,27	3305530
NIOLI	4222	LITHIUM NICKEL OXIDE (5LIO.95NIO)	20,27	3305550
LITBR	4968	LITHIUM TETRABORATE (LI2O.2B2O3) (EPOX)	27	555
LU	1416	LUTETIUM	20,27,41	230025
LX041	7505	LX-04-1 H.E. (HMX 85, VITON A 15)	8	200551
FE304	4044	MAGNATITE (FEO.FE203)	20,27,47,51	2000005
MAGNA	5268	MAGNESITE A BRICK (MGO 90) (14.5 P)	1,20,27,47,48	330
MAGNB	5269	MAGNESITE B BRICK (MGO 93) (22.6 P)	1,20,27,47,48	330
MAGNP	5267	MAGNESITE BRICK (MGO 87)	1,20,27,47,48	330
MAGNS	5266	MAGNESITE BRICK, SPALL RES (NGO 89)	1,20,27,47,48	335
MAGNC	5270	MAGNESITE C BRICK (MGO 86) (17.8 P)	1,20,27,47,48	330
MG	1096	MAGNESIUM	20,1,32,27,42	0
MGLIQ	1097	MAGNESIUM (LIQUID)	1,14,20,27,32,43	30005
MG042	2462	MAGNESIUM ALLOY (MG,AG2.5,CE2,ZR0.6)	47	333
MG001	2421	MAGNESIUM ALLOY AM100A (CASTING)	41	33
MG002	2422	MAGNESIUM ALLOY AZ31(X,S) (WROUGHT)	14,20,47	10
NG003	2423	MAGNESIUM ALLOY AZ31B(P,S) (WROUGHT)	1,20,41	0
MG004	2424	MAGNESIUM ALLOY AZ61A(X), AZM (WROUGHT)	14,41,47	33
MG005	2425	MAGNESIUM ALLOY AZ63A(AC,F) (CASTING)	14,41	33
MG006	2426	MAGNESIUM ALLOY AZSOA(X,FRGD) (WROUGHT)	1,20,37,41	303
MG007	2427	MAGNESIUM ALLOY AZ81A(T4) (CASTING)	41	300333
MG008	2428	MAGNESIUM ALLOY AZ855(X) (WROUGHT)	47	333
MG009	2429	MAGNESIUM ALLOY AZ91A,B (DC) (CASTING)	1,14,41,47	31
MG010	2430	MAGNESIUM ALLOY AZ91C(AC) (CASTING)	1,41	33
MG011	2431	MAGNESIUM ALLOY AZ92A(AC) (CASTING)	1,14,41	33
MG012	2432	MAGNESIUM ALLOY A3A (WROUGHT)	41	33333
MG013	2433	MAGNESIUM ALLOY A8(AC OR ST) (CASTING)	47	333
MG014	2434	MAGNESIUM ALLOY BZ33A(AC,AH) (CASTING)	1	333
MG015	2435	MAGNESIUM ALLOY EK30A, H812 (CASTING)	20,41	31
MG017	2437	MAGNESIUM ALLOY EK33A, H811 (CASTING)	20,41	32
MG016	2436	MAGNESIUM ALLOY EK41A(T5,T6) (CASTING)	41	333
MG018	2438	MAGNESIUM ALLOY HK31A(H24) (CASTING)	1,20,41	0
MG019	2439	MAGNESIUM ALLOY HK31A(O) (CASTING)	1,20,41	0
MG020	2440	MAGNESIUM ALLOY HK31A(T6) (CASTING)	1,20,41	0
MG021	2441	MAGNESIUM ALLOY HM21A(O,H24) (WROUGHT)	41	313
MG022	2442	MAGNESIUM ALLOY HM31A (WROUGHT)	20,41	3
MG023	2443	MAGNESIUM ALLOY HZ32A(AC),ZT1 (CASTING)	1,20,41,47	33
MG024	2444	MAGNESIUM ALLOY MAGNOX A12(X) (WROUGHT)	47	333
MG025	2445	MAGNESIUM ALLOY M1(AC) (CASTING)	14,47	333
MG026	2446	MAGNESIUM ALLOY M1(X,S) (WROUGHT)	14,47	333
MG027	2447	MAGNESIUM ALLOY M1A (WROUGHT)	41	33
MG028	2448	MAGNESIUM ALLOY PE (WROUGHT)	41	30033
MG029	2449	MAGNESIUM ALLOY ZA(AC) (CASTING)	47	3333

Table M5.6.1 (continued)

ID	No.	Material	References	Quality Index DCKTHCK[a]
MG030	2450	MAGNESIUM ALLOY ZE10A(O,H24) (WROUGHT)	41	33
MG031	2451	MAGNESIUM ALLOY ZE41A(T5,HT) (CASTING)	20,41,47	330
NG032	2452	MAGNESIUM ALLOY ZH42 (CASTING)	41	33
MG033	2453	MAGNESIUM ALLOY ZH62A(AC),TZ6 (CASTING)	20,41,47	31
MG034	2454	MAGNESIUM ALLOY ZK20A (WROUGHT)	20,41	3303333
MG035	2455	MAGNESIUM ALLOY ZK51A, H807 (CASTING)	20,41,47	0
MG036	2456	MAGNESIUM ALLOY ZK60A, B, ZW6 (CASTING)	1,14,20,41,47	1
MG037	2457	MAGNESIUM ALLOY ZRE0 (EZ30) (CASTING)	20	303331
NG038	2458	MAGNESIUM ALLOY ZRE1(AA) (CASTING)	47	333
MG039	2459	MAGNESIUM ALLOY ZTY(X) (HK11) (WROUGHT)	20,47	331
MG040	2460	MAGNESIUM ALLOY ZW1(X) (ZK11) (WROUGHT)	47	333
MG041	2461	MAGNESIUM ALLOY ZW3(X) (ZK31) (WROUGHT)	47	333
MG043	2463	MAGNESIUM ALLOY 1959 (MG,CE4.33)	20	3303335
MG044	2464	MAGNESIUM ALLOY 1960 (MG,CE6.7)	20	3303330
MG045	2465	MAGNESIUM ALLOY 1961 (MG,CE11.85)	20	3303330
MG046	2466	MAGNESIUM ALLOY 1964 (MG,CE5,CO2,MN0.8)	20	3303330
MG047	2467	MAGNESIUM ALLOY 1992 (MG,CE4.45,CO3)	20	3303330
SPINX	4224	MAGNESIUM ALUMINATE (MGO.AL2O3) (XTAL)	20,27,47,48,51	500
SPINL	4225	MAGNESIUM ALUMINATE (MGO.AL2O3) (100 D)	20,27,47,48,51	500
CORDR	4322	MAGNESIUM ALUMINUM SILICATE (CORDIERIT)	20,51	5510
MGOPX	4050	MAGNESIUM OXIDE (MGO) (POLYXTAL, 100 D)	1,20,27,47,48,51	2000
MGOX	4048	MAGNESIUM OXIDE (MGO) (SINGLE CRYSTAL)	1,20,27,47,48	0
FORST	4324	MAGNESIUM SILICATE (2MGO.SIO2) (100 D)	1,20,27,51	0
STEAT	4326	MAGNESIUM SILICATE (MGO.SIO2) (COMMERC)	1,20,27,51	505
MG2SI	4776	MAGNESIUM SILICIDE (MG2SI)	20,27,48	300530
MGSO4	4970	MAGNESIUM SULFATE (MGSO4) (CRYSTAL)	1,27	50
EPSOM	4971	MAGNESIUM SULFATE HYDRATE (MGSO4.7H2O)	1,27,51	555
PORMT	5283	MAGNESIUM TITANATE PORCELAIN	20,48	305530
MNCRY	1101	MANGANESE	20,1,32,27,43,42	0
MNO	4052	MANGANESE OXIDE (MNO) (SINGLE XTAL)	1,27,48	5
MN3O4	4054	MANGANESE OXIDE (MN3O4) (87 PC DENSE)	20,27,48,51	22005
MNSEL	4928	MANGANESE SELENIDE (97MNSE.3LISE)	20,27	3305530
MNSI2	4778	MANGANESE SILICIDE (MNSI2)	20,27,48	300530
MNTEA	4930	MANGANESE TELLURIDE (95MNTE.5MNAS)	20	3305530
MNTEN	4931	MANGANESE TELLURIDE (99MNTE.NATE)	20	3305530
CUMAN	2195	MANGANIN (CU84, NI4, MN12)	2	3305550
MARBL	6021	MARBLE (AV PROP) (SEE REF 51)	1,27,51	25555
MARBD	6020	MARBLE DIELECTRIC (XTAL) (CACO3-99.99)	1,27,51	5550
MELM2	7122	MELAMINE (HIGH DENS, HIGH K)	6,38	2022555
MELM1	7121	MELAMINE (LOW DE14S, LOW K)	6,38	2022555
MELAC	7123	MELAMINE, ALPHA CELLULOSE FILLED	38	22555
MELAS	7124	MELAMINE, ASBESTOS FILLED (MST 95-205)	38	2022555
MELAF	7125	MELAMINE, CELLULOSE FILLED (MST 95-205)	38	22555
MELFF	7127	MELAMINE, FABRIC OR FLOCK FILLED	6,38	555
MELGF	7126	MELAMINE, GLASS FIBER FILLED (MST 205)	6,38	555
MD	1461	MENDELEVIUM		4445555
HGLIQ	1207	MERCURY (LIQUID)	1,27,28,42,43,47,14	0
HGCL2	4826	MERCURY CHLORIDE (HGCL2) (PRSD 8 KB)	1,27,47	10
CH4	4890	METHANE (CH4) (GAS)	1,27	0
MEMAC	7131	METHYL METHACRYLATE	1,38	25550
MICAX	4982	MICA (SINGLE CRYSTAL) (A OR B AXES)	20,51	305555
MICAC	4983	MICA (SINGLE CRYSTAL) (C AXIS)	20,51	305555
MICAS	4984	MICA (SINGLE CRYSTAL) (SYNTHETIC) (98D)	20	305550
MICAB	4985	MICA BRICK (RED OR WHITE) (AVG PROP)	20	305552
MICAP	4987	MICA INSULATING POWDER	20	305550

Table M5.6.1 (continued)

ID	No.	Material	References	Quality Index DCKTHCK[a]
HEM01	7514	MOCK H.E. LM-04-0 H4-048-A294-3	5,8	5530
HEM02	7515	MOCK H.E. LM-04-0 H7-048-A522.1	5,8	5500
HEM03	7506	MOCK H.E. RM-04-BG (LX-04-1 MECH MOCK)	8	5555
HEM04	7507	MOCK H.E. 90010 (PBX-9404 MECH MOCK)	8	5555
MO	1106	MOLYBDENUM	20,6,1,32,41,43,42,	0
MO	1106	MOLYBDENUM	+47,14	0
MOAFE	3672	MOLYBDENUM ALLOY (MO BAL, FE 0.25)	20	333311
MOW30	3673	MOLYBDENUM ALLOY (MO70, W30)	20	3300
MOATI	3671	MOLYBDENUM ALLOY (MO99.5, TI0.5)	1,6,41	300
MOBED	4712	MOLYBDENUM BERYLLIDE (MOBE12)	20,48	500
MO2C	4520	MOLYBDENUM CARBIDE (MO2C)	20,27,48	2022502
MO2N	4432	MOLYBDENUM NITRIDE (MO2N) (PR SRD 100 D)	47,48	2000505
MOSE2	4932	MOLYBDENUM SELENIDE (MOSE2)	20	3303555
MOSI2	4780	MOLYBDENUM SILICIDE (MOSI2)	20,27,48	2500
MOTE2	4934	MOLYBDENUM TELLURIDE (MOTE2)	20	3305555
MULBY	3831	MULBERRY (U90, NB7.5, ZR2.5)	34,36,37	0
MULL	4316	MULLITE (3AL2O3.2SIO2) (100 PC DENSE)	20,27,48,51	500
ND	1366	NEODYMIUM	41,20,42	30225
NDB6	4630	NEODYMIUM BORIDE (NDB6) (97.3 PC DENSE)	48	300555
NEGAS	1526	NEON (GAS)	27,2,1,42	20000
NEOPR	7136	NEOPRENE RUBBER	6,38,39	555
NP	1464	NEPTUNIUM	20,27	2440555
NI	1111	NICKEL	20,2,1,32,37,41,42,51	2
NIAL3	2588	NICKEL ALLOY (NI35,CR20,FE45)	41	5533
NIAL2	2586	NICKEL ALLOY (NI60,CR16,FE24)	41	5533
NIAL1	2584	NICKEL ALLOY (NI62,CR12,FE26)	2,41	3305533
NI995	2590	NICKEL ALLOY (NI99.5) LOW C, 220, 225	1,14	320
NICKA	2503	NICKEL ALLOY A (NI99.4) (ANNEALED)	1,14,20	2
NICAN	2502	NICKEL ALLOY CALITE N	14	333
NICH3	2504	NICKEL ALLOY CHLORIMET 3	14	3333
NICON	2506	NICKEL ALLOY CONSTANTAN (NI45, CU55)	1,2,14,41,47	331
NICOD	2508	NICKEL ALLOY CORROSIST	14	333
NIDAE	2592	NICKEL ALLOY D AND E	1	30
NIDUH	2512	NICKEL ALLOY DURANICKEL (AND -R) (HARD)	1,14,47	333
NIDUS	2510	NICKEL ALLOY DURANICKEL (AND -R) (SOFT)	1,14,47	333
NID20	2514	NICKEL ALLOY DURIMET 20 (CAST)	1	303333
NIHSA	2516	NICKEL ALLOY HASTELLOY A (ANNEALED)	1,14,20	20332
NIHSB	2518	NICKEL ALLOY HASTELLOY B	1,14,20,41,47	300
NIHSC	2520	NICKEL ALLOY HASTELLOY C	1,14,41,47	302
NIHSD	2522	NICKEL ALLOY HASTELLOY D	1,14,41,47	333
NIHSN	2523	NICKEL ALLOY HASTELLOY N AND INOR-8	20,41	330
NIHSR	2524	NICKEL ALLOY HASTELLOY R-235	1,14,20	300
NIHSX	2526	NICKEL ALLOY HASTELLOY X	1,14,20,41	330
NIH80	2528	NICKEL ALLOY HY MU 80	14	200333
NILLG	2530	NICKEL ALLOY ILLIUM G	1,14,20,41,47	2002333
NILLR	2532	NICKEL ALLOY ILLIUM R	1,14,41,47	2000333
NINCL	2534	NICKEL ALLOY INCOLOY	1,14	323
NINC9	2536	NICKEL ALLOY INCOLOY 901	1,20	3310
NINCN	2540	NICKEL ALLOY INCONEL (CAST)	1,14,20,41,47	302
NINCA	2538	NICKEL ALLOY INCONEL (WROUGHT, ANNLD)	1,14,20,41,47	302
NINCW	2542	NICKEL ALLOY INCONEL W	1	333
NINCX	2544	NICKEL ALLOY INCONEL X AND X-750	1,20,41	301
NINC6	2545	NICKEL ALLOY INCONEL 600 (ANNEALED)	1,47	2003330
NINC7	2546	NICKEL ALLOY INCONEL 700	1,14,20,41	330
NINC2	2543	NICKEL ALLOY INCONEL 702 (ANNEALED)	1,20	3320

Table M5.6.1 (continued)

ID	No.	Material	References	Quality Index DCKTHCK[a]
NIN7C	2547	NICKEL ALLOY INCONEL 713C (CAST)	1,20	200320
NINVR	2501	NICKEL ALLOY INVAR (HOT-ROLLED OR FRGD)	6,41,47	20355
COK42	2632	NICKEL ALLOY K-42B	14	3323332
NIMOC	2551	NICKEL ALLOY MONEL (CAST)	1,41	200333
NIMOU	2549	NICKEL ALLOY MONEL (COLD-DRAWN)	1,14,20,41	333
NIMON	2548	NICKEL ALLOY MONEL (HOT-ROLLED)	1,14,41,44,47	0
NIMLH	2552	NICKEL ALLOY MONEL, H (AS CAST)	1,41	220333
NIMHU	2555	NICKEL ALLOY MONEL, H (CAST, VAR COMP)	1,20,41	220333
NIMLK	2554	NICKEL ALLOY MONEL, K (ANNEALED)	1,14,20,41,44	200300
NIMKR	2556	NICKEL ALLOY MONEL, KR (ANNEALED)	1,14	200333
NIMLR	2558	NICKEL ALLOY MONEL, R (HOT-ROLLED)	1,20,41	200330
NIMLS	2560	NICKEL ALLOY MONEL, S (CAST, ALL COND)	1,14,20	200330
NIMOW	2553	NICKEL ALLOY MONEL WELDABLE ALLOY	1	200333
NIM4H	2557	NICKEL ALLOY MONEL 400	47	205533
NIML4	2550	NICKEL ALLOY MONEL 403 (HOT-ROLLED)	1	203333
COMTL	2636	NICKEL ALLOY MULTIMET (N-155) (LOW C)	1,14,20,41	330
COMTM	2634	NICKEL ALLOY MULTIMET (N-155) (WROUGHT)	1,14,20,41	330
NIM25	2561	NICKEL ALLOY M-252 (GE J-1500)	20	3310
NICHR	2562	NICKEL ALLOY NICHROME V (NI80, CR 20)	1,47	23302
NIMND	2564	NICKEL ALLOY NIMONIC DS	47	303333
NIM15	2575	NICKEL ALLOY NIMONIC 105	47	3330
NIM75	2566	NICKEL ALLOY NIMONIC 75	1,14,20	330
NIMSO	2568	NICKEL ALLOY NIMONIC 80	1,14,20,41,47	330
NIM8A	2570	NICKEL ALLOY NIMONIC BOA	1,20,41,47	330
NIM90	2572	NICKEL ALLOY NIMONIC 90	1,14,20,41	330
NIM95	2573	NICKEL ALLOY NIMONIC 95	20,47	303330
NIPER	2574	NICKEL ALLOY PERMANICKEL	1,14	335
NIREN	2576	NICKEL ALLOY RENE 41	20,41	303320
NIUDM	2578	NICKEL ALLOY UDIMET 500 (WROUGHT)	1,20,41	300330
NIWSP	2580	NICKEL ALLOY WASPALLOY	1,20,41	300330
NI330	2582	NICKEL ALLOY 330 (NI99.55) (ANNEALED)	1	335
CNLOX	4218	NICKEL COBALT OXIDE (46NIO.46COO.8LIO)	20,27	3305555
NIOLI	4222	NICKEL LITHIUM OXIDE (95NIO.5LIO)	20,27	3305550
NIOPL	4060	NICKEL OXIDE (NIO) (POLYXTAL, 68-74 D)	20,27,32,47,48,51	0
NIOPX	4058	NICKEL OXIDE (NIO) (POLYXTAL, 88-100 D)	20,27,32,47,48,51	0
NIO	4056	NICKEL OXIDE (NIO) (SINGLE XTAL)	20,27,32,47,48,51	5
CUNIS	2185	NICKEL SILVER (CU BAL, NI 10-20)	1,2,6,41,47	2222555
NIZNF	4226	NICKEL ZINC FERRITE (NI(ZN)O.FE2O3)	20	2025502
NB	1246	NIOBIUM	20,27,32,43,44,42	0
NBTAW	3681	NIOBIUM ALLOY (NB61, TA28, W10, ZR0.5)	20	3300
NBWMO	3684	NIOBIUM ALLOY (NB80, W15, MO5)	20	3300
NBTIZ	3682	NIOBIUM ALLOY (NB85, TI10, ZR5)	20	3300
NBTA5	3683	NIOBIUM ALLOY (NB95, TA5)	20	3303330
NBBED	4714	NIOBIUM BERYLLIDE (NBBE12) (HP, 93-97D)	20,48	2000500
NBBE8	4716	NIOBIUM BERYLLIDE (NB2BE17)	20,48	300530
NBB2	4620	NIOBIUM BORIDE (NBB2) (PRESSED, SNTRD)	20,27,48	2500
NBC	4522	NIOBIUM CARBIDE (NBC)	20,27,48,54	20502
NBN	4434	NIOBIUM NITRIDE (NBN)	20,47,48	505
NB2N	4436	NIOBIUM NITRIDE (NB2N)	20,47,48	300535
NBSI2	4782	NIOBIUM SILICIDE (NBSI2)	20,27	300535
NOGAS	4061	NITRIC OXIDE (NO) (GAS)	1,27	500
NITRR	7141	NITRILE RUBBER	6,39	5555
NITRC	7508	NITROCELLULOSE H.E. (12.7 N)	8	305555
N-GAS	1531	NITROGEN (GAS)	27,2,42,1	0
NO	1467	NOBELIUM		4445555

Table M5.6.1 (continued)

ID	No.	Material	References	Quality Index DCKTHCK[a]
NYLON	7151	NYLON 6, 11, 66, 610 (POLYCAPROLACTAM)	1,6,38	500
NYLGF	7156	NYLON, GLASS FILLED		202555
OBSID	5030	OBSIDIAN GLASS	27,51	305530
ORTHC	4328	ORTHOCLASE (K2O.AL2O3.6SIO2) (CRYSTAL)	27,51	325555
OS	1114	OSMIUM	27,20,42,41	0
O-GAS	1536	OXYGEN (GAS)	27,42,1,2	0
PD	1236	PALLADIUM	20,41,42,27,43	0
E9011	7509	PBX-9011 H.E. (HMX 90, ESTANE 10)	8	555
E9404	7510	PBX-9404-03 H.E. (HMX 94, NC 3, BIND 3)	8,44	511
PETN	7511	PETN H.E.	8	555
PHCAF	7172	PHENOLIC, CAST, ASBESTOS FILLER	6,38	2555
PHCNF	7171	PHENOLIC, CAST, NO FILLER	6,38	222555
PHMHD	7177	PHENOLIC, MOLDED (HIGH DENSITY, K)	6	22555
PHMLD	7176	PHENOLIC, MOLDED (LOW DENSITY, K)	6	22555
PHRPD	7181	PHENOLIC RESIN, PRESSED, TYPES 40, 50	20	305555
PFPPF	7161	PHENOL-FORMALDEHYDE + PHENOL-FURFURAL	20	2225555
PHNXY	7191	PHENOXY	6,38	2000555
P	1321	PHOSPHORUS (WHITE)	27	40005
PLASL	4963	PLASTER, BUILDING (MOLDED, DRY)	1,27	555
PLAMT	7201	PLASTIC LAMINATE, VARIOUS TYPES	6,20	2222555
GLASP	5034	PLATE GLASS	20,51	305532
PT	1116	PLATINUM	20,1,32,27,41,43,42	0
PU	1121	PLUTONIUM	20,31,3,27,43,42,41,	0
PU	1121	PLUTONIUM	+36,44	0
PUSTD	3701	PLUTONIUM ALLOY (DELTA PHASE)	20,27,31,44	200
PUC	4524	PLUTONIUM CARBIDE (PUC) (ARCM OR CAST)	20,48,53,54	2025502
PUN	4438	PLUTONIUM NITRIDE (PUN)	27,48,53	300530
PUP	4762	PLUTONIUM PHOSPHIDE (PUP) (90 PC DENSE)	53	500
PUS	4747	PLUTONIUM SULFIDE	53	550
UPUOX	4242	PLUTONIUM URANIUM OXIDE (PUO2.4UO2) SEE	53	303530
PO	1473	POLONIUM	20,27	20005
PALLO	7211	POLYALLOMER	6,38	22555
PCARB	7221	POLYCARBONATE, VARIOUS FILLERS	6,38	2022555
PESTG	7231	POLYESTER, GLASS FIBER REINFORCED, TAC	20	2555
PETHH	7243	POLYETHYLENE, HIGH DENSITY	6,38	2555
PETHL	7241	POLYETHYLENE, LOW DENSITY	6,38	2555
PETHM	7242	POLYETHYLENE, MEDIUM DENSITY	6,38	2555
PIMHF	7251	POLYIMIDE, H-FILM, KAPTON	6,40	555
MEMAC	7131	POLYMETHYL METHACRYLATE	1,38	25550
PPROC	7262	POLYPROPYLENE, COPOLYMER	6,38	20555
PPROP	7263	POLYPROPYLENE, FILLED	6	20555
PPROM	7261	POLYPROPYLENE, MOPLIN	6,38	555
PSTYF	7271	POLYSTYRENE, FOAMED-IN-PLACE, RIGID	6	2020555
PSTYG	7276	POLYSTYRENE, GENERAL PURPOSE	6,20,38	2550
PSTYM	7281	POLYSTYRENE, MODIFIED	6	22555
PSTYP	7286	POLYSTYRENE, PREFOAMED, RIGID, DOW Q103	6,20	2002550
PSTYL	7287	POLYSTYRENE FOAM (D = 0.038) (1 ATM)	1	20552
PSTYV	7289	POLYSTYRENE FOAM (D = 0.046) (VACUUM)	1	20552
PSTYH	7288	POLYSTYRENE FOAM (D = 0.046) (1 ATM)	1	20552
PSULF	7291	POLYSULFONE	5,6,38	555
PURRF	7302	POLYURETHANE FOAMED-IN-PLACE, RIGID	6,20	2320555
PUREF	7301	POLYURETHANE FOAM, FLEXIBLE	6,20,38	2020555
PURER	7311	POLYURETHANE RUBBER L-100	6,38	20555
PVINA	7321	POLYVINYL ALCOHOL	6	5555
PVINB	7331	POLYVINYL BUTYRAL	6,38	555

Table M5.6.1 (continued)

ID	No.	Material	References	Quality Index DCKTHCK[a]
PVINC	7341	POLYVINYL CARBAZOLE	20	5555
PVCAF	7356	POLYVINYL CHLORIDE ACYTATE, FLEXIBLE	38	2225555
PVCAR	7357	POLYVINYL CHLORIDE ACYTATE, RIGID	38	2225555
PVCFL	7351	POLYVINYL CHLORIDE, FLEXIBLE	6,38,20	2222555
PVCRD	7352	POLYVINYL CHLORIDE, RIGID	6,38,20	2222555
PVTPX	7371	POLYVINYL TPX-R	5,38	5555
PVDCM	7362	POLYVINYLIDENE CHLORIDE	6,38	22555
PVDCF	7361	POLYVINYLIDENE CHLORIDE FILM	6,38	555
PVDCK	7366	POLYVINYLIDENE FLUORIDE (KYNAR)	5,38	5555
PORAL	5281	PORCELAIN, HIGH ALUMINA	20	3005500
PORZR	5282	PORCELAIN, HIGH ZIRCON	20	305535
PORMT	5283	PORCELAIN, MAGNESIUM TITANATE	20,48	305530
PORCE	5286	PORCELAIN, ORDINARY	1,20	3325535
PORBE	5280	PORCELAIN 4811 (BEO)	20	305530
PORC5	5284	PORCELAIN 576	20	325535
K	1226	POTASSIUM	1,27,28,42,41,43,51	0
KLIQ	1227	POTASSIUM (LIQUID)	14,27,28,43,47,51	22
KALUM	4972	POTASSIUM ALUM (K2SO4.AL2(SO4)3.24H2O)	1,27	550
ORTHC	4328	POTASSIUM ALUMINUM SILICATE (ORTHOCLAS)	27,51	325555
KBR	4828	POTASSIUM BROMIDE (KBR) (PRSD 8 KB)	1,27,47	210
KBRX	4830	POTASSIUM BROMIDE (KBR) (SINGLE XTAL)	1,27,47,51	210
KBR50	4833	POTASSIUM BROMIDE (KBR 50, KCL 50)	1,27,47,51	3303330
KBR75	4832	POTASSIUM BROMIDE (KBR 75, KCL 25)	1,27,47,51	3303330
KCL	4836	POTASSIUM CHLORIDE (KCL) (PRSD 8 KB)	1,27,47,51	10
KCLSY	4837	POTASSIUM CHLORIDE (KCL) (SYLVITE XTAL)	1,27,47,51	10
KBR50	4833	POTASSIUM CHLORIDE (KCL 50, KBR 50)	1,27,47,51	3303330
KCL50	4838	POTASSIUM CHLORIDE (KCL 50, NACL 50)	1,27,47,51	303330
KCL75	4834	POTASSIUM CHLORIDE (KCL 75, KBR 25)	1,27,47,51	3303330
KCL90	4835	POTASSIUM CHLORIDE (KCL 90, KBR 10)	1,27,47,51	3303330
KCROM	4233	POTASSIUM CHROMATE (K2O.2CRO3) (M AXIS)	1,27	300050
KCROX	4232	POTASSIUM CHROMATE (K2O.2CRO3) (S AXIS)	1,27	300050
KF	4840	POTASSIUM FLUORIDE (KF) (PRSD 8 KB)	1,27,47	10
KI	4842	POTASSIUM IODIDE (KI) (PRSD 8 KB)	1,27,47	10
KFECN	4974	POTASSIUM FERROCYANIDE (K4FE(CN)6.3H2O)	1,27	550
KNO3	4976	POTASSIUM NITRATE (KNO3) (PR 8000 KB)	1,27	0
PR	1361	PRASEODYMIUM	41,27,20,42	205
PRB6	4628	PRASEODYMIUM BORIDE (PRB6) (95 PC DENS)	48	305555
PM	1421	PROMETHIUM	20,27,42	3332035
PA	1476	PROTACTINIUM	20,27	30005
PYREX	5016	PYREX GLASS	2,20,27,51	500
PYRC6	5018	PYROCERAM 9606 CERAMIC GLASS	20	5500
PYRC8	5019	PYROCERAM 9608 CERAMIC GLASS	20	5500
PYROP	4990	PYROPHYLLITE (PARALLEL TO BEDDING)	27,51	2305530
PYRON	4991	PYROPHYLLITE (PERPEND. TO BEDDING)	27,51	2305530
SIO2A	4066	QUARTZ CRYSTAL, A AXIS (SIO2)	1,2,20,27,37,47,51	2200
SIO2C	4064	QUARTZ CRYSTAL, C AXIS (SIO2)	1,2,20,27,37,47,51	2200
SANQF	6032	QUARTZ FLOUR, FINE (DRY)	51	305535
SANQN	6033	QUARTZ FLOUR, FINE (H2O 21 PC)	51	305555
SIO2	4062	QUARTZ GLASS, FUSED (SIO2)	1,20,27,47,51	2200
SANQP	6039	QUARTZ POWDER, COARSE (H2O 24)	51	305555
SANDY	6034	QUARTZ SAND (DRY) (AV PROP) (SEE REF)	51	2325555
SANDQ	6036	QUARTZ SAND (WET) (H2O 4-23) (AV PROP)	51	2325555
RA	1479	RADIUM	27	2040025
RNGAS	1561	RADON GAS	27	40505
RATTN	8211	RATTAN	44	25555

Table M5.6.1 (continued)

ID	No.	Material	References	Quality Index DCKTHCK[a]
RE	1251	RHENIUM	27,43,41,42	2
RH	1281	RHODIUM	20,27,43,42,41	0
ROCKS	6022	ROCK OR STONE (AVERAGE PROPERTIES)	1,46	3335555
STBRC	7431	RUBBER, BUNA, WITH CARBON BLACK	6,20,39	200555
BUTYR	7031	RUBBER, BUTYL	6,39	555
RUBBD	7382	RUBBER, DIELECTRIC MIX	6,20	550
RUBBK	7383	RUBBER, HIGH K	6,20	550
RUBBN	7381	RUBBER, NATURAL	6	555
RUBBF	7386	RUBBER, NATURAL, FOAM	6,20	320555
NEOPR	7136	RUBBER, NEOPRENE	6,38,39	555
NITRR	7141	RUBBER, NITRILE		5555
PURER	7311	RUBBER, POLYURETHANE ELASTOMER L-100	6,38	20555
RB	1291	RUBIDIUM	1,27,28,42,43,47	40024
RBLIQ	1292	RUBIDIUM (LIQUID)	1,14,27,28,43,47	20022
RBCL	4844	RUBIDIUM CHLORIDE (RBCL) (PRSD 8 KB)	1,27,47	10
RBI	4846	RUBIDIUM IODIDE (RBI) (PRSD 8 KB)	1,27,47	10
RU	1301	RUTHENIUM	20,42,1,27	202020
SM	1371	SAMARIUM	20,27,41,42,43	30205
SMB6	4632	SAMARIUM BORIDE (SMB6) (96.8 PC DENSE)	48	300555
SMS	4748	SAMARIUM SULFIDE (SMS)	20,48	300550
SANDY	6034	SAND (DRY) (D = 1.36 TO 1.84) (AV PROP)	51	2325555
SANDN	6038	SAND, NORTHWAY (H2O 4-10) (AV PROP)	51	2325555
SANDQ	6036	SAND, QUARTZ (WET) (H2O 4-23) (AV PROP)	2,51	2325555
SANDM	6026	SANDSTONE (AV PROP) (SEE REF 51)	2,27,46,51	25555
SANDL	6025	SANDSTONE (LOW DENSITY)	2,27,46,51	25555
ALOXD	4012	SAPPHIRE (AL2O3) (POLYXTAL) (100 PC D)	1,20,27,32,47,48,51	200
ALOXS	4016	SAPPHIRE (AL2O3) (SINGLE XTAL) (AV DIR)	1,20,27,32,47,48,51	202
SC	1341	SCANDIUM	20,27,41,43	30005
SE	1326	SELENIUM (GREY)	27,43,42,1	20005
SHALE	6028	SHALE (AV PROP) (SEE REF 51)	51	2225555
BRISI	5294	SILICA BRICK, HARD FIRED (SIO2 94-95)	20	330
SIO2	4062	SILICA GLASS, FUSED OR VITROUS	1,20,27,47,51	2200
BRISL	5296	SILICEOUS BRICK (SIO2 89, AL2O3 9)(25P)	47	335
SI	1256	SILICON	20,1,27,41,43,42,48	0
SIB4	4614	SILICON BORIDE (SIB4)	27,48	300530
SICAL	4539	SILICON CARBIDE (SIC) (BRICK AL2O3 1.7)	20,27,32,47	2500
SICCF	4535	SILICON CARBIDE (SIC) (CARBOFRAX BRICK)	20,27,32,47	2500
SICFV	4542	SILICON CARBIDE (SIC) (FOAM, IN VACUUM)	20,32,47	2500
SICFB	4536	SILICON CARBIDE (SIC) (FRIT BND BRICK)	20,27,32,47	2500
SICKT	4534	SILICON CARBIDE (SIC) (KT GRADE)	20,27,32,47,48	2500
SICNB	4541	SILICON CARBIDE (SIC) (NITRIDE BONDED)	20,32,47,48	2503
SICPA	4543	SILICON CARBIDE (SIC) (POWDER, IN AIR)	20,32,47	2500
SICPH	4544	SILICON CARBIDE (SIC) (POWDER, IN HE)	20,32,47	2500
SICRD	4540	SILICON CARBIDE (SIC) (REFRACTORY D-30)	20,27,32,47	2500
SICRP	4538	SILICON CARBIDE (SIC) (REXTAL, 65-70 D)	1,20,27,32,47	2500
SICRX	4537	SILICON CARBIDE (SIC) (REXTAL, 80-100 D)	20,27,32,47,48	2500
SICX1	4531	SILICON CARBIDE (SIC) (SINGLE XTAL)	20,27,32,47	22500
SICX2	4532	SILICON CARBIDE (SIC) (SINGLE XTAL)	20,32,47,48	22505
SICSB	4533	SILICON CARBIDE (SIC) (SLF BND, HE ATM)	20,27,32,47	2500
SICSI	5424	SILICON CARBIDE + SI (SIC 76, SI 24)	20	3305550
SI3NL	4444	SILICON NITRIDE (SI3N4) (70 PC DENSE)	20,27,47,48	20502
SI3N4	4442	SILICON NITRIDE (SI3N4) (85 PC DENSE)	20,27,47,48	20502
SIO2F	4068	SILICON OXIDE (SIO2) (FOAM, 1 ATM AIR)	1,20,27,47	2200
SIO2	4062	SILICON OXIDE (SIO2) (FUSED QUARTZ)	1,20,27,47,51	2200
SIO2A	4066	SILICON OXIDE (SIO2) (QUARTZ, A AXIS)	1,2,20,27,37,47,51	2200

Table M5.6.1 (continued)

ID	No.	Material	References	Quality Index DCKTHCK[a]
SIO2C	4064	SILICON OXIDE (SIO2) (QUARTZ, C AXIS)	1,2,20,27,37,47,51	2200
SITE	4936	SILICON TELLURIDE (SITE)	20	305555
SILFF	7401	SILICONE FOAM, FLEXIBLE (LRL)	6,20	2022555
SILFR	7402	SILICONE FOAM, RIGID, VARIOUS	6,20	2022555
SILRH	7423	SILICONE RUBBER, HIGH K (SEE REF 5)	5,6,41,44	220555
SILRL	7421	SILICONE RUBBER, LOW K (SEE REF 5)	5,6,41,44	220555
SILRM	7422	SILICONE RUBBER, MEDIUM K (SEE REF 5)	5,6,41,44	220555
SILR1	7424	SILICONE RUBBER, RTV 521 AND 093-009	5,6,41,44	220555
SILMD	7411	SILICONE, MOLDED, VARIOUS FILLERS	6,20,38	2222555
BRISK	5298	SILLIMANITE BRICK (22 PC POROSITY)	20	300530
AG	1126	SILVER	20,6,1,27,2,32,42,47,	0
AG	1126	SILVER	+14,43	0
AGLIQ	1127	SILVER (LIQUID)	27,32,42,43	30005
SILVA	3751	SILVER ALLOYS, STERLING AND COIN	1	325
SNTE2	4940	SILVER ANTIMONY TELLURIDE (SNTE 25 PC)	20	3305555
AGCL	4848	SILVER CHLORIDE (AGCL) (SINGLE CRYSTAL)	27,47,51	15
AG2SE	4942	SILVER SELENIDE (AG2SE)	20,27,47	20502
SLATE	6030	SLATE (AV PROP) (SEE REF 51)	51	2225555
GLASC	5032	SODA-LIME GLASS	20,27	3325532
NA	1221	SODIUM	2,1,27,28,41,42,43,51	0
NALIQ	1222	SODIUM (LIQUID)	1,14,27,28,42,43,47,	1
NALIQ	1222	SODIUM (LIQUID)	+51	1
ANALC	4329	SODIUM ALUMINUM SILICATE HYDRATE (XTAL)	27,51	305555
NABR	4850	SODIUM BROMIDE (NABR) (PRSD 8 KB)	1,27,47	10
NACLO	4978	SODIUM CHLORATE (NACLO3) (CRYSTAL)	1,27,51	505
NACL	4852	SODIUM CHLORIDE (NACL) (CLEAR CRYSTAL)	1,27,47,51,52	10
NACLR	4854	SODIUM CHLORIDE (NACL) (OPAQUE, IMPURE)	1,27,47,51,52	10
KCL50	4838	SODIUM CHLORIDE (NACL 50, KCL 50)	1,27,47,51	303330
NAF	4856	SODIUM FLUORIDE (NAF) (PRSD 8 KB)	1,27,47	10
SOILS	6046	SOIL (AV PROPS) (SEE REFS)	2,46,51	2225555
SOIL3	6044	SOIL, CLAY (WET)	51	2225555
SANQF	6032	SOIL, FINE QUARTZ FLOUR (DRY)	51	305535
SANQW	6033	SOIL, FINE QUARTZ FLOUR (H2O 21 PC)	51	305555
SOIL1	6042	SOIL, LOAM (DRY) (AV PROP) (SEE REFS)	2,51	2225555
SOIL2	6043	SOIL, LOAM (H2O 4-27 PC) (AV, SEE REFS)	2,51	2225555
SOILM	6048	SOIL, MARS SURFACE (SEE UCRL-50309)		5555
SOLID	6050	SOIL, SANDY DRY	46	5555
SOILW	6052	SOIL, SANDY (H2O 8)	46	5555
ART	7007	SOLID, REGULATING (D=C=K=TM=1,HM=10**9)		0
ART6	9006	SOLID, UNIT LATENT HEAT (D=C=K=TM=HM=1)		0
ART3	9003	SOLID, UNIT PROPERTY (D=C=K=1)		0
SNOWF	8231	SNOW, FRESH	2,27	55
SNOWP	8232	SNOW, PACKED	27,46	55
SOLD1	3611	SOLDER (PB37.5, SN37.5, IN25)	36	3355
SOLD2	3612	SOLDER (PB39.2, SN60.8)	34,41	5
SOLD4	3613	SOLDER (PB50, SN50)	1,41	50
SOLD3	3614	SOLDER (PB60, SN40)	1,41	55
SPINX	4224	SPINEL (MGO.AL2O3) (SINGLE CRYSTAL)	20,27,47,48,51	500
SPINL	4225	SPINEL (MGO.AL2O3) (100 PC DENSE POLYX)	20,27,47,48,51	500
H2OGS	4113	STEAM (H2O) (GAS) (SATD)	1,2,14,27,46	205550
H2OG1	4112	STEAM (H2O) (GAS) (1 ATM)	1,2,14,27,46	200050
STEAT	4326	STEATITE (MGO.SIO2) (COMMERCIAL GRADES)	1,20,27,51	505
STALL	3101	STEEL, ALLOY AND MILD (4130, 4340)	6,41,46	3302
STALC	3106	STEEL, ALLOY, CAST	6	3355
STCAR	3116	STEEL, CARBON, TYPE 1020 (0.2 - 0.6 C)	1,20,37	300

Table M5.6.1 (continued)

ID	No.	Material	References	Quality Index DCKTHCK[a]
STCFC	3111	STEEL, FREE CUTTING, EUTECTOID	2,4,6,20,41	300
STHSP	3121	STEEL, HIGH SPEED (M1, M10, M-2, TI)	20	3303355
COMTL	2636	STEEL, MULTIMET (N-155) (LOW C)	1,14,20,41	330
COMTM	2634	STEEL, MULTIMET (N-155) (WROUGHT)	1,14,20,41	330
STST4	3141	STEEL, STAINLESS (CR 12-13, NI 0-3)	1,2,4,14,20	300
STST3	3131	STEEL, STAINLESS (CR 16-26, NI 8-36)	1,2,4,6,20,37	2023333
SSC08	3208	STEEL, STAINLESS CA15, CA40 (CAST)	1	355
SSC09	3209	STEEL, STAINLESS CB30, CC50 (CAST)	1	355
SSC13	3213	STEEL, STAINLESS CK, CH, HI (CAST)	1	355
SSC12	3212	STEEL, STAINLESS CF (CAST)	1	355
SSC04	3204	STEEL, STAINLESS CN-7M (CAST)	1	355
SSC06	3206	STEEL, STAINLESS HA (CAST)	1	355
SSC07	3207	STEEL, STAINLESS HC, HD (CAST)	1	355
SSC11	3211	STEEL, STAINLESS HE (CAST)	1	355
SSC05	3205	STEEL, STAINLESS HF (CAST)	1	355
SSC10	3210	STEEL, STAINLESS HH, HL, HK (CAST)	1	355
SSC03	3203	STEEL, STAINLESS HT (CAST)	1	355
SSC02	3202	STEEL, STAINLESS HU (CAST)	1	355
SSC01	3201	STEEL, STAINLESS HW (CAST)	1	355
STST3	3131	STEEL, STAINLESS SERIES 300	1,2,4,6,20,37	2023333
STST4	3141	STEEL, STAINLESS SERIES 400	1,2,4,20	300
STPH4	3171	STEEL, STAINLESS 17-4PH	20,14	23302
STPH7	3176	STEEL, STAINLESS 17-7PH	20,14	2003300
ST199	3186	STEEL, STAINLESS 19-9DL	41	2300
STST2	3126	STEEL, STAINLESS 201 AND 202	1	3355
ST304	3133	STEEL, STAINLESS 304	1,4,37	300
ST347	3135	STEEL, STAINLESS 321 AND 347	1,2,4,20,37,14	300
STS4A	3146	STEEL, STAINLESS 430, 430F, AND 431	1,2,4,6,20,14	302
STS4B	3151	STEEL, STAINLESS 446	1,14,20	302
STST5	3161	STEEL, STAINLESS 501 AND 502	2,4	2303330
WCCO2	5453	STEEL, TOOL, TUNGSTEN CARBIDE CA2	20	3300530
WCCO1	5452	STEEL, TOOL, TUNGSTEN CARBIDE CA4	20	3300530
STUHS	3181	STEEL, ULTRA HIGH STRENGTH TYPE 300-M	1	355
SR	1296	STRONTIUM	20,28,42,27	240024
SRS04	4980	STRONTIUM SULFATE (SRSO4) (CRYSTAL)	1,27,51	550
SRTIT	4234	STRONTIUM TITANATE (SRO.TIO2) (100 D)	20,48	500
SRTIP	4235	STRONTIUM TITANATE (SRO.TIO2) (80 D)	20,48	500
STCO1	5426	STRONTIUM TITANATE + CO (CO 10)	20	3300535
STCO2	5427	STRONTIUM TITANATE + CO (CO 20)	20	3300535
STCO3	5428	STRONTIUM TITANATE + CO (CO 30)	20	3300535
STCO4	5429	STRONTIUM TITANATE + CO (CO 40)	20	3300535
STBRC	7431	STYRENE-BUTADIENE RUBBER + CARBON BLK	6,20,39	200555
S	1331	SULFUR	27,1,42,30,2,41	10001
SO2	4071	SULFUR DIOXIDE (SO2) (GAS)	1	5500
TALC	4994	TALC	20,27,51	5505
TA	1161	TANTALUM	20,1,27,32,37,43	20002
TANBV	3784	TANTALUM ALLOY (TA62, NB30, V7.5)	20	3300
TAWHF	3785	TANTALUM ALLOY (TA89, W9, HF2)	20	300
TA10W	3781	TANTALUM ALLOY (TA90, W10)	20,36	500
TACUZ	3783	TANTALUM ALLOY (TA98, CUO.7, ZRO.7)	20	3300
TANB1	3782	TANTALUM ALLOY (TA99.5, NBO.5)	20	3303330
TASB	4944	TANTALUM ANTIMONIDE (TASB)	20	3305552
TABED	4718	TANTALUM BERYLLIDE (TABE12) (HP)	20,48	
TABED	4720	TANTALUM BERYLLIDE (TA2BE17)	20,48	500
TAB	4642	TANTALUM BORIDE (TAB) (PSD, SNTR, 85D)	20,27,47,48	500

Table M5.6.1 (continued)

ID	No.	Material	References	Quality Index DCKTHCK[a]
TAB2	4644	TANTALUM BORIDE (TAB2)	20,27,47,48	2020502
TAC	4562	TANTALUM CARBIDE (TAC)	20,27,48,54	2020502
WCCO5	5456	TANTALUM CARBIDE + WC CERMET K601	49	300530
TAN	4446	TANTALUM NITRIDE (TAN)	20,27,48	2220525
TA2N	4448	TANTALUM NITRIDE (TA2N)	20,27,48	2220522
TASI2	4784	TANTALUM SILICIDE (TASI2)	20,27	300535
TC	1164	TECHNICIUM	27,42	40025
FCTFE	7111	TEFLON	1,6,20,38	2500
FCTFR	7112	TEFLON, REINFORCED	20	2500
TE	1488	TELLURIUM	27,20,42,41,1	20002
TB	1386	TERBIUM	20,27,41,42,43	30205
TBB6	4638	TERBIUM BORIDE (TBB6) (94.3 PC DENSE)	48	305555
TETRL	7512	TETRYL H.E.	8	300555
TL	1336	THALLIUM	41,27,1,42,47	0
TLLIQ	1337	THALLIUM (LIQUID)	1,14,27,42,43,47	55
TH	1166	THORIUM	20,32,34,27,37,43,44,	2
TH	1166	THORIUM	+41	2
THB4	4646	THORIUM BORIDE (THB4)	20,27,48	2002502
THB6	4648	THORIUM BORIDE (THB6)	20,27,48	2000535
THC	4564	THORIUM CARBIDE (THC) (80 PC DENSE)	20,27,48,54	300530
THC2	4565	THORIUM CARBIDE (THC2) (69 PC DENSE)	20,27,48,54	300530
TH02	4072	THORIUM OXIDE (TH02) (96-100 PC DENSE)	1,20,27,47,48,51	2002300
TM	1406	THULIUM	20,27,41,42,43	30005
SN	1171	TIN	2,1,27,32,42,41,47	0
SNLIQ	1172	TIN (LIQUID)	1,14,27,32,41,42,43	0
SOLD1	3611	TIN ALLOY (SN37.5, PB37.5, IN25)	36	3355
SOLD3	3614	TIN ALLOY (SN40, PB60) (SOLDER)	1,41	55
SOLD4	3613	TIN ALLOY (SN50, PB50) (SOLDER)	1,41	50
SOLD2	3612	TIN ALLOY (SN60.8, PB39.2) (SOLDER)	34,41	5
SNO2	4074	TIN OXIDE (SNO2) (93-95 PC DENSE)	1,20,27,47,48	2300
SNTE2	4940	TIN TELLURIDE (SNTE 25, AGSBTE2 75)	20	3305555
SNTE6	4939	TIN TELLURIDE (SNTE 60, AGSBTE2 40)	20	3305555
SNTE8	4938	TIN TELLURIDE (SNTE 80, AGSBTE2 20)	20	3305555
TI	1176	TITANIUM	20,27,32,37,42,43,41,	20002
TI	1176	TITANIUM	+1	20002
TIAL1	2712	TITANIUM ALLOY (TI BAL, AL2, MN2)	20	3303330
TIAL3	2716	TITANIUM ALLOY (TI BAL, AL4, CU2, ZR2)	20	3303330
TIAL7	2730	TITANIUM ALLOY (TI BAL, AL4, CU4, SN2)	20	3303330
TIA11	2732	TITANIUM ALLOY (TI BAL, AL4, MO3, V1)	20	3233323
TIAL5	2720	TITANIUM ALLOY (TI BAL, AL4, V1, MO0.6)	20	3303330
TIAL2	2714	TITANIUM ALLOY (TI BAL, AL4, V2, MO1)	20	3303330
TIAL4	2718	TITANIUM ALLOY (TI BAL, AL4, V3, MO1.5)	20	3303330
TIAL6	2728	TITANIUM ALLOY (TI BAL, AL4, ZR3.5)	20	3303330
TIA12	2736	TITANIUM ALLOY (TI BAL, AL5, SN2.5)	41,45	303330
TI555	2738	TITANIUM ALLOY (TI BAL, AL5, SN5, ZR5)	45	303330
TIA13	2740	TITANIUM ALLOY (TI BAL, AL6, V4)	20,37,45	300
TIA15	2742	TITANIUM ALLOY (TI BAL, AL8, MO1, V1)	45	3330
TIA14	2746	TITANIUM ALLOY (TI BAL, CR3.4, MO2.1)	20	3303330
TIALS	2752	TITANIUM ALLOY (TI BAL, SN4.8, AL4.5)	20	3303330
TIAL9	2754	TITANIUM ALLOY (TI BAL, SN5.5, AL2)	20	3303330
TIV14	2768	TITANIUM ALLOY (TI BAL, V14, CR10, AL4)	20	3003300
TIV15	2766	TITANIUM ALLOY (TI BAL, V15, AL2.8)	20	3003300
TIA10	2770	TITANIUM ALLOY (TI BAL, ZR3, AL2)	20	3303330
TI100	2750	TITANIUM ALLOY C100M (RC130A) (MN7.9)	20	203320
TIH40	2722	TITANIUM ALLOY HYLITE 40 C130AM,RC130B	1,20,41	303330

Table M5.6.1 (continued)

ID	No.	Material	References	Quality Index DCKTHCK[a]
TIH50	2724	TITANIUM ALLOY HYLITE 50 (IMI550)	20,45	303330
TIH51	2726	TITANIUM ALLOY HYLITE 51 (IMI551)	45	303330
TIH55	2760	TITANIUM ALLOY HYLITE 55 (IMI)	20,45	303330
TIH60	2758	TITANIUM ALLOY HYLITE 60 (IMI)	20,45	303330
TIH65	2756	TITANIUM ALLOY HYLITE 65 (IMI)	45	303330
TI679	2764	TITANIUM ALLOY IMI 679 (SN11, ER5, AL2)	45	303330
TI680	2762	TITANIUM ALLOY IMI 680 (SN11, M04, AL2)	45	303330
TI140	2748	TITANIUM ALLOY TI140A (FE2, CR2, MO2)	20	3303330
TI150	2744	TITANIUM ALLOY TI150A (CR2.7, FE1.4)	20	3003300
T1155	2734	TITANIUM ALLOY TI155A (AL5,FE2,CR1,MO1)	1,20	3303330
TIBED	4722	TITANIUM BERYLLIDE (TIBE12) (HP, 95D)	20,48	2500
TIB2	4650	TITANIUM BORIDE (TIB2) (HP, 95 PC DENS)	20,27,47,48	500
TIC93	4567	TITANIUM CARBIDE (TIC) (93 PC DENSE)	20,27,47,48,54	22502
TIC96	4566	TITANIUM CARBIDE (TIC) (96 PC DENSE)	20,27,47,48,54	22502
TICC2	5431	TITANIUM CARBIDE + CO (CO18 NBC,TAC15)	20	3305535
TICC1	5430	TITANIUM CARBIDE + CO (TIC 80, CO 20)	20	305535
TICC3	5432	TITANIUM CARBIDE + NBC + NI	20	3305535
TICCR	5442	TITANIUM CARBIDE + NI OR CO (AVG PROP)	48	2220555
TICC5	5434	TITANIUM CARBIDE CERMET K138A	49	305530
TICC6	5435	TITANIUM CARBIDE CERMET K151A	49	305530
TIC10	5439	TITANIUM CARBIDE CERMET K161B	20	3005500
TICC4	5433	TITANIUM CARBIDE CERMET K162B	49	305530
TICC7	5436	TITANIUM CARBIDE CERMET K163B1	49	305530
TICC8	5437	TITANIUM CARBIDE CERMET K164B	49	305530
TICC9	5438	TITANIUM CARBIDE CERMET K165	49	305530
TINIT	4452	TITANIUM NITRIDE (TIN) (HP, 70-90 DENS)	20,27,47,48	2020502
TIO2A	4084	TITANIUM OXIDE (TIO2) (RUTILE, A AXIS)	1,20,27,32,47,48,51	20202
TIO2C	4082	TITANIUM OXIDE (TIO2) (RUTILE, C AXIS)	1,20,27,32,47,48,51	20202
TIO2	4086	TITANIUM OXIDE (TIO2) (RUTILE, 100 D)	1,20,27,32,47,48,51	200
TNT	7513	TNT H.E. (2, 4, 6-TRINITROTOLUENE) (CAST)	8	555
TOPAZ	4301	TOPAZ (2ALFO.SIO2) (A-AXIS)	27,51	305550
TOPAC	4302	TOPAZ (2ALFO.SIO2) (C-AXIS)	27,51	305551
TOURM	4996	TOURMALINE	27,51	305550
T-GAS	1566	TRITIUM GAS		3335533
W	1181	TUNGSTEN	20,1,32,34,27,37,42,	0
W	1181	TUNGSTEN	+41,43	0
W25RE	3801	TUNGSTEN ALLOY (W75, RE25)		3303330
WNICU	3802	TUNGSTEN ALLOY (W90, NI6, CU2-4)	20	303330
WB	4652	TUNGSTEN BORIDE (WB)	20,27,47,48	2500
WC	4568	TUNGSTEN CARBIDE (WC)	20,27,47,48,54	2500
WCC12	5463	TUNGSTEN CARBIDE CERMET CARBOLOY 883	50	300530
WCC11	5462	TUNGSTEN CARBIDE CERMET CARBOLOY 905	50	300530
WCC10	5461	TUNGSTEN CARBIDE CERMET CARBOLOY 999	50	300530
WCCO2	5453	TUNGSTEN CARBIDE CERMET CA2 TOOL STEEL	20	3300530
WCCO1	5452	TUNGSTEN CARBIDE CERMET CA4 TOOL STEEL	20	3300530
WCCO3	5454	TUNGSTEN CARBIDE CERMET K6 AND K96	20,49	300530
WCCO5	5456	TUNGSTEN CARBIDE CERMET K601	49	300530
WCCO8	5459	TUNGSTEN CARBIDE CERMET X701	49	300530
WCCO9	5460	TUNGSTEN CARBIDE CERMET K801 (WC + NI)	49	300530
WCCO7	5458	TUNGSTEN CARBIDE CERMET K92	49	300530
WCCO6	5457	TUNGSTEN CARBIDE CERMET K94 AND K1	49	300530
WO3	4092	TUNGSTEN OXIDE (WO3) (POLYXTAL. POROUS)	20,27,47,48	20305
WSE2	4946	TUNGSTEN SELENIDE (WSE2)	20,27	3303550
WSI2	4786	TUNGSTEN SILICIDE (WSI2) (HP, 95 DENSE)	20,27,48	2002500
WTE2	4947	TUNGSTEN TELLURIDE (WTE2)	20,27	3303555

Table M5.6.1 (continued)

ID	No.	Material	References	Quality Index DCKTHCK[a]
WTIC5	5470	TUNGSTEN TITANIUM CARBIDE KM	49	300530
WCCO4	5465	TUNGSTEN TITANIUM CARBIDE K2S	20,49	300530
WTIC7	5472	TUNGSTEN TITANIUM CARBIDE K21	49	300530
WTIC6	5471	TUNGSTEN TITANIUM CARBIDE K4H	49	300530
WTIC4	5469	TUNGSTEN TITANIUM CARBIDE K5H	49	300530
WTIC3	5468	TUNGSTEN TITANIUM CARBIDE K81	49	300530
WTIC2	5467	TUNGSTEN TITANIUM CARBIDE K84	49	300530
WTIC1	5466	TUNGSTEN TITANIUM CARBIDE K86, K7H, K3H	49	300530
U	1186	URANIUM	20,31,32,36,27,37,42,	0
U	1186	URANIUM	+41,43,44,34	0
MULBY	3831	URANIUM ALLOY MULBERRY	34,36,37	0
U18ZR	3833	URANIUM ALLOY (U82, ZR18)	20,34	303330
U9OFS	3837	URANIUM ALLOY (U90, FS10)	20	303330
U10MO	3832	URANIUM ALLOY (U90, MO10)	20,35,36	300
UFSZR	3838	URANIUM ALLOY (U93, FS5, ZR2)	20	303330
UCREU	3835	URANIUM ALLOY (U94.4, CR5.6) (EUTECTIC)	20	3003300
UZRO5	3840	URANIUM ALLOY (U95, ZR5)	20	30303330
UO4NB	3834	URANIUM ALLOY (U96, NB4)	20,34	303330
U97FS	3836	URANIUM ALLOY (U97, FS3)	20	303330
UZRO2	3839	URANIUM ALLOY (U98.5, ZR1.5)	20	303330
UBE13	4724	URANIUM BERYLLIDE (UBE13) (SNTRD, 61D)	20,48	305550
UB4	4654	URANIUM BORIDE (UB4)	20,48	300555
UCAMC	4572	URANIUM CARBIDE (UC) (ARCM OR CAST,99D)	20,48,53,54	2502
UCAVG	4574	URANIUM CARBIDE (UC) (AVG, VAR. TYPES)	20,48,53,54	2502
UCSNT	4573	URANIUM CARBIDE (UC) (SINTERED, 90D)	20,48,53,54	2502
UC2	4576	URANIUM CARBIDE (UC2)	20,27,48,54	2000500
UN	4454	URANIUM NITRIDE (UN) (HP, 95-98 DENSE)	20,27,48,PWAC481-65	2500
UO2PX	4096	URANIUM OXIDE (UO2) (POLYXTAL, 97 DENS)	20,27,47,48,51	500
UO2	4094	URANIUM OXIDE (UO2) (SINGLE CRYSTAL)	20,27,47,48,51	500
U3O8L	4099	URANIUM OXIDE (U3O8) (PRSD AT 100 PSI)	1,20,27,47,48	2002500
U3O8H	4098	URANIUM OXIDE (U3O8) (PRSD AT 4200 PSI)	1,20,27,47,48	2002500
UO2CR	5482	URANIUM OXIDE + CR (UO2 80 VOL) (97 D)	20	4305550
UOMO3	5486	URANIUM OXIDE + MO (UO2 70 VOL) (92 D)	20	4305550
UOMO2	5485	URANIUM OXIDE + MO (UO2 80 VOL) (91 D)	20	4305550
UOMO1	5484	URANIUM OXIDE + MO (UO2 80 VOL) (94 D)	20	4305550
UO2NB	5488	URANIUM OXIDE + NB (UO2 80 VOL)	20	4305550
UO2S1	5490	URANIUM OXIDE + ST STEEL (UO2 70 VOL)	20	4305550
UO2S2	5491	URANIUM OXIDE + ST STEEL (UO2 80 VOL)	20	4305550
UO2Z1	5492	URANIUM OXIDE + ZR (UO2 43,ZR 57)(59 P)	20	4305530
UO2Z2	5493	URANIUM OXIDE + ZR (UO2 80,ZR 20)	20	305535
UPUOX	4242	URANIUM PLUTONIUM OXIDE (4UO2.PUO2) SEE	53	303530
U3SI	4788	URANIUM SILICIDE (U3SI)	20,48	20525
URFMA	7442	UREA-FORMALDEHYDE, ALPHA CELLULOSE FLLR	38	25555
URFMN	7441	UREA-FORMALDEHYDE, MOLDED	38	25555
ART2	9002	VACUUM, CONDUCTING (D=C=0, K=10**9)		0
ART1	9001	VACUUM, INSULATING (D=C=K=0)		0
V	1286	VANADIUM	20,32,27,41,42,43	0
VBE12	4726	VANADIUM BERYLLIDE (VBE12) (85 PC DENS)	20,48	505
VB2	4656	VANADIUM BORIDE (VB2)	20,27,48	20555
VC	4578	VANADIUM CARBIDE (VC)	20,27,47,48,54	2022502
VN	4456	VANADIUM NITRIDE (VN) (PR, STRD, 100 D)	20,27,47,48	22505
VERM2	5292	VERMICULITE, EXPANDED (D = 0.19-0.25)	20	305530
VERM3	5293	VERMICULITE, EXPANDED (D = 0.3)	20	305530
VERMI	4986	VERMICULITE BRICK	20	305550
VERMP	4988	VERMICULITE INSULATING POWDER	20	305550

Table M5.6.1 (continued)

ID	No.	Material	References	Quality Index DCKTHCK[a]
SIO2	4062	VITROUS SILICA GLASS	1,20,27,47,51	2200
VYCOR	5036	VYCOR GLASS	20,27	500
H2OGS	4113	WATER (H2O) (GAS) (SATD)	1,2,14,27,46	205550
H2OG1	4112	WATER (H2O) (GAS) (1 ATM)	1,2,14,27,46	200050
WATER	4114	WATER (H2O) (LIQUID)	2,14,27,46	0
ICE	4116	WATER (H2O)(SOLID) (ICE)	27,46,51	0
D2O	4118	WATER, HEAVY (D20) (LIQUID)	14,27	300
GLASW	5028	WINDOW GLASS, LIME	20	305530
BALS1	8516	WOOD, BALSA (ACROSS GRAIN)	1,2,27	305555
BALS2	8517	WOOD, BALSA (ACROSS GRAIN)	1,2,27	305555
CYPRS	8518	WOOD, CYPRESS (ACROSS GRAIN)	1,27	305555
MAHOG	8520	WOOD, MAHOGANY (ACROSS GRAIN)	1,27	305555
MAPLE	8522	WOOD, MAPLE (ACROSS GRAIN)	1,2,27	305555
PINEW	8526	WOOD, NORWAY PINE (ACROSS GRAIN)	1,2,27	305555
OAKLD	8525	WOOD, OAK, RED, BLACK (ACROSS GRAIN)	1,2,27	05555
OAKHD	8524	WOOD, OAK, WHITE, LIVE (ACROSS GRAIN)	1,2,27	05555
PINEL	8527	WOOD, OREGON PINE (ACROSS GRAIN)	1,2,27	305555
PINEW	8529	WOOD, PINE (WITH GRAIN)	1,2,27	305555
WOOD2	18513	WOOD, SPRUCE (ACROSS GRAIN)	46	5555
WOOD1	8512	WOOD, SPRUCE (WITH GRAIN)	46	5555
TEAK	8530	WOOD, TEAK (ACROSS GRAIN)	1,2	305555
PINEV	8528	WOOD, VIRGINIA PINE (ACROSS GRAIN)	1,2,27	305555
FIRWH	8532	WOOD, WHITE FIR (ACROSS GRAIN)	1,2	305555
PINEA	8534	WOOD, WHITE PINE (ACROSS GRAIN)	1,2,27	305555
XE	1541	XENON	27,42	30000
YB	1411	YTTERBIUM	20,27,41,42,43	30205
YBB6	4640	YTTERBIUM BORIDE (YBB6) (90.6 PC DENS)	48	305555
Y	1346	YTTRIUM	41,27,1,20,42,43	20005
YB6	4622	YTTRIUM BORIDE (YB6) (98.4 PC DENSE)	48	300555
Y2O3	4102	YTTRIUM OXIDE (Y2O3) (96-100 PC DENSE)	20,27,47,48	300
ZNFEO	4252	ZINC FERRITE (ZNO.FE203) (PR, FRD, VAC)	20,27	500
ZNO	4104	ZINC OXIDE (ZNO) (PRSD, FIRED, 100 D)	1,20,27,47,48,51	2000
ZNS	4750	ZINC SULFIDE (ZNS) (CUBIC CRYSTAL)	1,27,47,48,51	310
ZINC3	3863	ZINC-ALUMINUM ALLOY ASTM 23	1,6,41	355
ZINC4	3864	ZINC-ALUMINUM-COPPER ALLOY ASTM 25	1,6,41	355
ZIRCN	4330	ZIRCON (ZRO2.SIO2) (SINGLE CRYSTAL)	20,27,48,61	2505
PORZR	5282	ZIRCON PORCELAIN, HIGH	20	305535
ZR	1196	ZIRCONIUM	20,27,32,37,43,42,41	20002
ZR3ZI	3882	ZIRCONIUM ALLOY 3ZI (ZR97,AL1,SN1,MO1)	20	303330
ZIRCA	3881	ZIRCONIUM ALLOYS ZIRCALLOY 2 AND 3	1,6,14	200355
ZRBET	4728	ZIRCONIUM BERYLLIDE (ZRBE13)	20,48	500
ZRB2	4658	ZIRCONIUM BORIDE (ZRB2) (HP, 97 PC DEN)	20,27,47,48	20502
ZRB2B	5496	ZIRCONIUM BORIDE + BORON (BOROLITE 101)	47,48	505
ZRB2Z	5498	ZIRCONIUM BORIDE + MOSI2 (BORIDE Z)	47,48	2000500
ZRC	4580	ZIRCONIUM CARBIDE (ZRC) (HP OR SNT,94D)	20,27,48,54	22502
ZRH12	4892	ZIRCONIUM HYDRIDE (ZRH + ZRH2)	20	2225522
ZRNPF	4458	ZIRCONIUM NITRIDE (ZRN) (PR SR 88-90 D)	20,27,47,48	500
ZRNPS	4459	ZIRCONIUM NITRIDE (ZRN) (PR SR 93 D)	20,27,47,48	20502
ZROYZ	5495	ZIRCONIUM OXIDE (Y203 12, ZR 8) (97 D)	20	4305530
ZRO2	4106	ZIRCONIUM OXIDE (ER02) (NONOC., 100 D)	1,20,27,47,48,51	0
ZRO2C	4108	ZIRCONIUM OXIDE (ZRO2 96, CAO 6, 91 D)	1,20,27,47,48,51	0
ZROTI	5494	ZIRCONIUM OXIDE + TI CERMET ZT-15-M	20	5500
ZIRCN	4330	ZIRCONIUM SILICATE (ZRO2.SIO2) (XTAL)	20,27,48,61	2505
ZIRCP	4332	ZIRCONIUM SILICATE (ZRO2.SIO2) (100 D)	20,27,48,61	2500

[a]See text description of columns 73–79 for explanation of property abbreviation used in each column.

M5.7 MATERIAL DATA LIST

The data for each material are contained on one to seven card-image records. A listing of the material data in the cgs-cal-°C units system may be found in Ref. 1 or read from the appropriate file in the SCALE code package. The following format is used:

MATERIAL IDENTIFICATION CARD:

Columns 1–5

Alphanumeric identifier (same as in material index).

Column 6

Always left blank.

Columns 7–10

Material identification number (same as in material index).

Columns 11–20

Always left blank. (Used in TRUMP program[2] to specify identification numbers of any chemical reactants associated with the material. Such numbers, if required, must be added manually.

Columns 21–25

Number of data pairs listed in the table of specific heat vs temperature. This number does not exceed 12. If the number is not zero, it is always two or more.

Columns 26–30

Number of data pairs listed in the table of thermal conductivity vs temperature. This number does not exceed 12. If this number is not zero, it is always two or more.

Columns 31–40

Density of material in grams per cubic centimeter (g/cm^3). This value is normally the value at or near room temperature or the lowest temperature for which specific heat or thermal conductivity is tabulated, whichever is highest. For use in codes that assume a fixed geometry, both the density and specified dimensions should correspond to the same conditions of temperature and pressure.

Columns 41–50

Specific heat of the material, in cal/g-°C, if constant or if the temperature dependence is unknown. When a table of specific heat vs temperature is listed, the value given here is normally the value at or near room temperature or at the lowest temperature tabulated, whichever is higher.

Columns 51–60

Thermal conductivity of the material, in cal/s-cm-°C, if constant or if the temperature dependence is unknown. When a table of thermal conductivity vs temperature is listed, the value given here is normally the value at or near room temperature or the lowest temperature listed in the table, whichever is higher.

Columns 61–70

Transition temperature of maximum temperature, in °C, at which material may be used. If a latent heat is specified in columns 71–80, this is the transition temperature at which either a phase-change or solid-state transition occurs. If a material has more than one transition with a latent-heat effect, others are included in the table of specific heat vs temperature as a triangular peak superimposed over the actual specific heat curve.' This triangular peak has a base width of 10°C and a height of 115 of the latent heat of transition, in cal/g, and is centered at the transition temperature.

Columns 71–80

Latent heat absorbed by the material, in cal/g, when the temperature is increased past the transition temperature specified in columns 61–70. Other latent-heat effects may be included in the specific heat table as described in the previous description (columns 61–70).

SPECIFIC HEAT TABLE CARDS

Only included if at least two data pairs are listed (no blank cards are needed).

Column 1

Always left blank.

Columns 2–10

Specific heat of the material, in cal/g-°C, at the temperature specified in columns 11–20.

Columns 11–20

Temperature, in °C, at which the material has the specific heat specified in columns 2–10.

Columns 21–30

Specific heat of the material, in cal/g-°C, at the temperature specified in columns 31–40.

Columns 31–40

Temperature, in °C, at which the material has the specific heat specified in columns 21–30. Always equal to or greater than the preceding temperature in the table.

The specific heat table card may list up to four data pairs using ten columns for each value of specific heat or temperature. As many as three cards with the same format can be used to list the number of data pairs specified in columns 21–25.

THERMAL CONDUCTIVITY TABLE CARDS

Only included if at least two data pairs are listed (no blank cards are needed).

Column 1

Always left blank.

Columns 2–10

Thermal conductivity of the material, in cal/s-cm-°C, at the temperature specified in columns 11–20.

Columns 11–20

Temperature, in °C, at which the material has the thermal conductivity specified in columns 2–10.

Columns 21–30

Thermal conductivity of the material, in cal/s-cm-°C, at the temperature specified in columns 31–40.

Columns 31–40

Temperature, in °C, at which the material has the thermal conductivity specified in columns 21–30. Always equal to or greater than the preceding temperature in the table.

The thermal conductivity table card may list up to four data pairs using ten columns for each value of thermal conductivity. As many as three cards with the same format can be used to list the number of data pairs specified in columns 26–30.

M5.8 REFERENCES

1. A. L. Edwards, *A Compilation of Thermal Property Data for Computer Heat-Conduction Calculations,* UCRL-50589, University of California Lawrence Radiation Laboratory, February 24, 1969.

2. A. L. Edwards, *TRUMP: A Computer Program for Transient and Steady-State Temperature Distributions in Multidimensional Systems*, UCRL-14754, Rev. 3, University of California Lawrence Livermore Laboratory, September 1, 1972.

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ORIGEN-S DATA LIBRARIES

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ABSTRACT

The ORIGEN-S code can use three kinds of data libraries: (1) card-image libraries containing nuclear and photon yield data, (2) binary data libraries containing nuclear transition and photon yield data, and (3) the Master Photon Data Base containing detailed photon energy and intensity data.

The first kind of library includes the card-image nuclear data libraries, which contain the basic data required to run ORIGEN-S. The nuclear data libraries are contained in two files. The first file includes decay parameters, natural abundances of nuclides, and radioactivity concentration guides. The second file contains six libraries of which the first three are nuclear data libraries for (a) 689 light elements, (b) 129 actinides, and (c) 879 fission products. Each nuclear data library contains cross sections for four kinds of reactors (HTGR, LWR, LMFBR, and MSBR); the fission-product library also contains fission-product yields from five fissionable nuclides for each kind of reactor. The last three libraries of the second card-image file are photon yield libraries for light-element, actinide, and fission-product nuclides. They contain multigroup photon spectra for decay gamma and X-rays, for prompt and equilibrium fission-product gamma rays from spontaneous fission, for gamma rays associated with (α,n) reactions in oxide fuel, and for bremsstrahlung from decay beta (negatron and positron) particles slowing down in a UO_2 fuel matrix.

The second kind of library is the binary (unformatted) ORIGEN-S data library. It contains the same kinds of data as the card-image nuclear data and photon yield libraries, but for only one kind of reactor (e.g., LWR). The nuclear data are stored in the binary library in the form of a transition matrix, and may be present for one or more burnups, in which case the library is known as a multiburnup binary data library. The binary library format was developed especially for ORIGEN-S and is the kind of library normally used for production runs. It has the significant advantage, as compared to the card-image libraries, that the cross sections in a binary library can be replaced with cross sections derived from detailed multigroup neutronics calculations. Cross-section updating is performed with the COUPLE code which reads the multigroup cross sections from an AMPX-format weighted cross-section library. The SAS2H control module (see Sect. S2) is used for automated generation of burnup-dependent multiburnup binary data libraries. A second advantage is that any portion of the photon yield data from the Master Photon Data Base can be placed in a binary library with any desired energy group structure. A further advantage is that almost any item of data in a binary library can be replaced with a user-specified value by running the COUPLE code.

The third kind of library is the ORNL Master Photon Data Base, originally developed for the ORIGEN2 code. It contains energies and intensities for (a) decay gamma- and X-ray line data, (b) spectra for gamma rays accompanying spontaneous fission and (α,n) reactions, and (c) bremsstrahlung spectra from decay beta (negatron and positron) particles slowing down both in a UO_2 fuel matrix and in water. This is the most comprehensive and up-to-date photon library available to ORIGEN-S. It can be used to generate multigroup photon source spectra, to make card-image photon yield libraries, or to update photon yield data in a binary data library. The multigroup source spectra and photon yield data can be generated in any energy group structure for all light-element, actinide, and fission-product nuclides having photon data. The ORNL Master Photon Data Base is available in both card-image and binary formats.

Noteworthy improvements to the ORIGEN-S data libraries were made at the time of the SCALE-4.2 release both to the decay data and to the structures of the library data files. The number of card-image library files was reduced from six to two, and the file structure for the card-image files was made uniform for all computer systems. The SAS2H method of generating burnup-dependent libraries was improved to combine the data for multiple burnups into a single file. The decay data, including half-lives, branching fractions, and recoverable decay energies, were updated for all but 18 nuclides, principally from ENDF/B-VI data.

This document describes the formats, data sources, and uses of the libraries outlined above.

CONTENTS

LIST OF TABLES

ACKNOWLEDGMENTS

Special thanks are due to S. B. Ludwig of the Oak Ridge National Laboratory (ORNL) Chemical Technology Division, who sponsored the latest update of decay data for both ORIGEN2 and ORIGEN-S, and to P. R. Daniel of the University of Florida, who produced the updated decay libraries from ENDF/B-VI decay data.

M. A. Bjerke wrote the original version of the computer program which retrieves decay data from ENDF/B files. R. W. Roussin and J. E. White of the Radiation Shielding Information Center kindly provided access to the ENDF decay data files. M. J. Martin and M. R. Lay of the ORNL Physics Division provided advice and ENSDF decay data files for many nuclides.

A. G. Croff, K. J. Notz, and C. W. Alexander of the ORNL Chemical Technology Division provided the ORNL Master Photon Data Base originally developed for ORIGEN2.

M. J. Bell developed the original ORIGEN and its nuclear data libraries. C. W. Kee, G. W. Morrison, and R. E. Schenter developed the large light-element and/or fission-product libraries for the original ORIGEN.

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M6.1 INTRODUCTION

The original version of the ORIGEN code[1] used two kinds of data libraries in card-image format. The nuclear data libraries contained decay data, natural abundances of nuclides, radioactivity concentration guides, cross sections, and fission yields. The photon yield libraries contained multigroup photon yields (photons per disintegration) for decay gamma and X-rays, for bremsstrahlung from beta particles slowing down in a UO_2 fuel matrix, and for some gammas accompanying (α,n) reactions in oxide fuels. There were three libraries of each kind: one for 253 light-element nuclides (structural materials and activation products), one for 101 actinide nuclides (fuel materials, transplutonium nuclides, and decay daughters), and one for 461 fission-product nuclides. The nuclear data libraries included cross sections and fission yields for four reactor types: the high-temperature gas-cooled reactor (HTGR), the light-water reactor (LWR), the liquid metal fast breeder reactor (LMFBR), and the molten salt breeder reactor (MSBR). Since the original ORIGEN code and its libraries were primarily intended for use in generic studies of spent fuel and waste characteristics, cross sections for a number of nuclides were adjusted to give agreement between calculated and measured fuel mass balances.

As the ORIGEN code became widely used for more complex applications, two additional data libraries were added. A large light-element library[2,3] for 674 nuclides was created, with cross sections for HTGRs and LWRs. At about the same time, a large fission-product library[3,4] for 821 nuclides, with cross sections and fission yields for LWRs and LMFBRs, was generated from ENDF/B-IV data.[5] Revised versions of these libraries (including a 687-nuclide large light-element library) having updated decay data were generated in the early 1980s and were included in releases of SCALE up through SCALE 4.0. For SCALE 4.1, the small (461 nuclides) fission-product library was removed and the LWR fission-product yields of the large (821 nuclides) library for all nuclides except tritium were updated from ENDF/B-V.[6] New tritium yields were taken from Boumahraz[7] and from Wagemans et al.[8]

A further expansion in the size of the ORIGEN-S libraries and an update[9] in the decay, energy, and fission-product yield data were included for the SCALE-4.2 release. The sizes of the libraries were increased to 689 light-element nuclides, 129 actinides, and 879 fission products; all smaller libraries were removed. Decay data, principally from ENDF/B-VI,[10] were used to update half-lives, branching fractions, and recoverable energies per disintegration. Fission-product yields for all of the fissile nuclides included for the four reactor types (HTGR, LWR, LMFBR, and MSBR) were updated from ENDF/B-V. Although the decay data update was undertaken primarily for the ORIGEN2 code, the resulting decay data base is now used to generate decay libraries with the same nuclides for ORIGEN-S and ORIGEN2.

Most revisions of the card-image nuclear data libraries have involved updating decay data. Most cross-section data have been left the same as in the original ORIGEN libraries. Updating of cross-section data for the binary data libraries discussed later is performed with the COUPLE code (Sect. F6), using problem-dependent multigroup cross sections from a detailed neutronics calculation. The photon-yield libraries have data taken from the ORNL Master Photon Data Base[11] discussed later. In addition to using the photon-yield libraries described in this report, the user of ORIGEN-S can generate photon-yield libraries in any desired energy-group structure (Sect. F7.6).

In addition to the card-image nuclear data and photon-yield libraries, the ORIGEN-S code can use data from two other kinds of libraries: a binary (unformatted) data library and the ORNL Master Photon Data Base.

The use of a binary library is perhaps the most significant feature of ORIGEN-S. A binary data library is generated with the COUPLE code (Sect. F6). It contains, in a single library, the same kinds of data as the card-image nuclear data and photon-yield libraries, but for only one reactor type. The ORIGEN-S code

is typically run with a multiburnup binary data library for the reactor type of interest. The binary data library has many advantages over the card-image data libraries. Its principal advantage is that the cross sections within the library can be replaced with cross sections derived from a detailed multigroup neutronics (e.g., unit cell) calculation. Cross-section updating is performed with the COUPLE code which reads the multigroup cross sections from an AMPX[12] weighted (working) cross-section library (Sect. F2.3.8). Automated generation of time-dependent (i.e., burnup-dependent) binary data libraries can be performed with the SAS2H control module (Sect. S2), which invokes the BONAMI, NITAWL-II, XSDRNPM, COUPLE, and ORIGEN-S codes (Sects. F1, F2, F3, F6, and F7, respectively). Another advantage is that any portion of the photon-yield data from the ORNL Master Photon Data Base can be placed in the binary library with any desired energy group structure. Furthermore, most data items in a binary library can be replaced with user-specified values by running the COUPLE code.

The ENDF/B-IV photon-yield library formerly distributed with ORIGEN-S has been removed because improved and more complete data described below are available.

The ORNL Master Photon Data Base[11] was originally developed for the ORIGEN2 code.[13] In its card-image form, it consists of six data files for six kinds of photon sources. One file contains decay gamma- and X-ray line data from the Evaluated Nuclear Structure Data File (ENSDF).[14,15] Another file contains spectra for gamma rays accompanying spontaneous fission and (α,n) reactions. Two files contain bremsstrahlung spectra from decay beta (negatron and positron) particles slowing down in a UO_2 fuel matrix. The last two files contain bremsstrahlung spectra from decay betas slowing down in water. These files can be concatenated in any user-chosen combination to form a card-image master photon data base for use with ORIGEN-S. In addition, ORIGEN-S can be used (Sect. F7.6) to create a binary (unformatted) master photon data base, containing data from any combination of the card-image data files, for use in subsequent ORIGEN-S runs. It has been customary at ORNL to run ORIGEN-S with a binary master photon data base, since execution is somewhat more efficient for that mode of operation. The ORNL Master Photon Data Base is the most comprehensive and up-to-date photon library available to ORIGEN-S. It can be used (Sect. F7.6) to generate multigroup photon source spectra, to make card-image photon-yield libraries, or to update photon-yield data in a binary data library. The spectra and photon-yield data can be generated in any energy group structure for all light-element, actinide, and fission-product nuclides having photon data.

The remainder of this document describes in detail the file structures, formats, data sources, and uses of the different kinds of ORIGEN-S libraries outlined above.

M6.1.1 FILE STRUCTURE OF CARD-IMAGE LIBRARIES

The ORIGEN-S card-image libraries are divided between two data files. The first file contains the decay data library, which includes natural nuclide abundances and radioactivity concentration guides in addition to decay parameters. The second file contains the following six libraries in the order specified:

1. the light-element cross-section library,
2. the actinide cross-section library,
3. the fission-product cross-section and yield library,
4. the light-element photon-yield library,
5. the actinide photon-yield library, and
6. the fission-product photon-yield library.

The card-image libraries are divided into two broad classifications. The decay data library and the cross-section and fission-yield libraries are called the nuclear data libraries and are described in Sect. M6.2. The second category is just the photon yield libraries, which are described in Sect. M6.3.

M6.1.2 MULTIBURNUP BINARY DATA LIBRARY

A multiburnup binary data library is a binary (unformatted) data library containing multiple sets of updated cross sections for different burnups.

A typical sequence of steps to produce a multiburnup library is as follows. First, data for a specific type of reactor from the card-image libraries is converted to a binary ORIGEN-S library by running the COUPLE code. Next, using that binary library as input, the SAS2H control module is executed to update the cross sections of all nuclides having data in the SCALE 27-group depletion library. This SAS2H case typically uses a single burnup interval for the entire lifetime of a fuel assembly. The resulting library is called a preliminary SAS2H, or preSAS, binary data library. The preSAS library, in turn, is used as the standard input ORIGEN-S binary data library for SAS2H cases for the same reactor type. An example of a preSAS case is shown in Sect. M6.7.4.

The multiburnup binary data library is produced by running a SAS2H case having multiple burnup intervals or cycles. The preSAS library is used as input, and cross sections are updated for user-specified nuclides of interest. The resulting multiburnup binary data library contains (within a single file) updated cross-section data for each burnup interval or cycle specified in the input power history.

A multiburnup binary data library is obviously useful as input to a wide variety of ORIGEN-S cases. An important advantage of the multiburnup format is that it requires less effort to keep track of a single library with many burnups than it does to keep track of many libraries with a single burnup.

M6.2 CARD-IMAGE NUCLEAR DATA LIBRARIES

The card-image nuclear data libraries consist of three cross-section libraries and the decay data library. The cross-section libraries are (1) a light-element library for 689 nuclides, (2) an actinide library for 129 nuclides, and (3) a fission-product library for 879 nuclides. The decay data base contains (for all nuclides in the three cross-section libraries) decay data, percent natural abundances, and radioactivity concentration guides. The decay data for a nuclide include the half-life, branching fractions, recoverable energy per decay, and the fraction of recoverable energy from photons. The data for each nuclide in the cross-section libraries are contained on five card-image records. The first card-image record contains information identifying the nuclide. The last four card images contain cross-section, and for fission-product nuclides, fission-yield data for four reactor types (HTGR, LWR, LMFBR, and MSBR), with one card image for each reactor type.

The card-image nuclear data libraries are the basic libraries for ORIGEN-S. The code can be run using these libraries directly, or it can be run from a binary data library which (prior to any cross-section or other nuclear data updating) was created by running the COUPLE code (Sect. F6) to convert the data for a specific reactor type.

When ORIGEN-S is run with these card-image libraries, the customary procedure is to use the light-element library, the actinide library, and the fission-product library. However, ORIGEN-S can be run with only one or two nuclear data libraries if the user wishes (Sect. F7.6). All the decay data are obtained from a separate data file referenced by unit 27. The card-image cross-section data and photon-yield libraries are referenced by another logical unit number. The libraries are read in the following order: light-element, actinide, and fission-product decay and cross-section data libraries, followed by light-element, actinide, and fission-product photon-yield libraries.

The remainder of this section is devoted to describing the data formats and sources for the decay data library and the three cross-section data libraries. Much of the description has been taken from the original ORIGEN report.

M6.2.1 DECAY DATA LIBRARY

The decay data library contains decay data, atom percent natural abundances, and radioactivity concentration guides for both air and water. These data are in a single data file broken into three segments: light elements, actinides, and fission products. There is an exact one-to-one correspondence in the order of the decay-data-library nuclides and those in the three cross-section libraries. In processing these nuclear data libraries, first the nuclide identification (ID) number is read into variable NUCL(I) from the cross-section library, next the data from the decay data library for the same nuclide are read, and then the cross-section data for the specified type of reactor are read. The decay data are read with a list-directed read statement as follows:

```
READ(LIBDEC,*) LIB, NUC1, IU, HALFL, FB1, FP, FP1, FA, FT, LI2,
   *FSF, FN, Q(I), ABUND(I), AMPC(I), WMPC(I), LI3, FG(I), FB .
```

During the processing, the nuclide data are stored in several arrays at locations indicated by the index I. The value of the ID number in both NUCL(I) and NUC1 is given by

$$NUCL(I) = Z * 10000 + W * 10 + IS , \qquad (M6.2.1)$$

where Z is the atomic number, W is the atomic mass number, and IS is 0 for a ground state or 1 for the first metastable state. In principle, IS could be greater than 1 for a nuclide in a higher metastable state, but none of the libraries currently contain data for any such nuclides.

The variable HALFL is the physical half-life in units designated by the variable IU, as shown in Table M6.2.1. The definitions of eight variables for branching fractions are given in Table M6.2.2.

The variable Q(I) is the total amount of recoverable energy (MeV) per disintegration released by radioactive decay. It does not include the energy of neutrinos emitted during beta decay transitions.

The variable FG(I) is the fraction of recoverable energy per disintegration that comes from gamma and X rays. In the ORIGEN-S libraries this fraction includes the energy from all decay gamma and X rays and from all gamma rays associated with spontaneous fission. Using an approximation[11] for the combined spectra of prompt and equilibrium fission-product gamma rays from spontaneous fission, a value of 12.56 MeV per spontaneous fission transition was calculated for use in determining FG for any nuclide having a spontaneous fission fraction exceeding 10^{-7}. Note that the definition of FG is not the same as that for the original ORIGEN libraries. In those libraries,[1] FG included only those photons with energies greater than 200 keV. In addition, it included the bremsstrahlung radiation from beta particles slowing down in a UO_2 fuel matrix. Bremsstrahlung radiation is **not** included in the values of FG in the ORIGEN-S libraries, since the bremsstrahlung spectrum depends on the medium that contains the decaying nuclide. Neither is the energy from gamma rays accompanying (α,n) reactions included, since it too depends on the medium.

The variable ABUND(I) is the atom percent abundance of naturally occurring isotopes. It is read by ORIGEN-S for light-element nuclides but is ignored for the actinide and fission-product nuclides.

The variables WMPC(I) and AMPC(I) are the radioactivity concentration guides for continuous ingestion (from water) and inhalation (from air) in unrestricted areas, in units of curies per cubic meter (Ci m^{-3}). The RCG values, as defined in the pre-1991 version of Part 10, Title 20, of the *Code of Federal Regulations*[16] (10CFR20), specify the maximum permissible concentrations of an isotope in soluble and insoluble forms, for both ingestion and inhalation, and for occupational and unrestricted exposure. When the activity (in curies) of a given isotope is divided by WMPC (or AMPC) for that isotope, the result is the volume of water (or air) required to dilute that quantity of the isotope to its maximum permissible concentration. The dilution volume is a measure of the radioactive toxicity of the nuclide for cases of direct ingestion or inhalation. The values of WMPC and AMPC are defined to be the smaller (i.e., more toxic) of the values for soluble and insoluble forms of the isotope.

The variables LIB, LI2, and LI3 contain the library ID numbers read first from each card image. They are for accounting purposes and may be ignored.

M6.2.2 LIGHT-ELEMENT CROSS-SECTION LIBRARY

The light-element card-image cross-section data library contains data for structural materials, activation products, and their decay daughters. The library has data for 689 nuclides.

As indicated earlier, there are five card-image records for each nuclide. The first record contains the nuclide ID number defined by Eq. (M6.2.1) in an I7 format plus other information not used by the code. The next four records contain data for neutron-induced reactions, with one record for each of the four reactor types. The data in these four records are referred to collectively as cross-section data, even though some items are not cross sections. The data are read using the following READ statement and FORMAT:

```
  150 READ(L,11500) SIGTH, FNG1, FNA, FNP, RITH, FINA,
     *FINP, SIGMEV, FN2N1, FFNA, FFNP, IT

11500 FORMAT(7X, F9.2, 3F5.3, F9.2, 2F5.3, F9.2, 3F5.3, 5X, I1) .
```

Table M6.2.1 Units of half-life indicated by the variable IU

IU	Units of half-life
1	seconds
2	minutes
3	hours
4	days
5	years
6	stable
7	10^3 years
8	10^6 years
9	10^9 years

Table M6.2.2 Definitions of branching fraction variables

Variable name	Definition
FB	Fraction of decay transitions that take place by beta (negatron) emission and lead to a product nuclide in the ground state
FB1	Fraction of decay transitions that take place by beta emission and lead to a product nuclide in an excited (metastable) nuclear state
FP	Fraction of decay transitions that take place by positron emission or orbital electron capture and lead to a product nuclide in the ground state
FP1	Fraction of decay transitions that take place by positron emission or orbital electron capture and lead to a product nuclide in an excited nuclear state
FA	Fraction of decay transitions that take place by alpha particle emission
FT	Fraction of decay transitions that take place by isomeric transition
FSF	Fraction of decay transitions that take place by spontaneous fission
FN	Fraction of decay transitions that take place by the emission of both a beta particle and a neutron

Definitions of the nuclear data variables are given in Table M6.2.3 for the case of a thermal reactor (HTGR, LWR, or MSBR). For an LMFBR, the cross-section variables have different definitions than those of Table M6.2.3. In that case, either SIGTH or RITH is the spectrum-averaged radiative capture (n,γ) cross section. When one is nonzero, the other is always zero. The variable SIGMEV is the sum of the spectrum-averaged (n,2n), (n,α), and (n,p) cross sections.

Table M6.2.3 Definitions of nuclear data variables in light-element libraries for a thermal reactor

Variable name	Definition
SIGTH	Total absorption cross section (barns) for thermal (2200 m s^{-1}) neutrons
FNG1	Fraction of radiative capture (n,γ) reactions that produce a product nuclide in an excited (metastable) nuclear state
FNA	Fraction of SIGTH that produces (n,α) reactions
FNP	Fraction of SIGTH that produces (n,p) reactions
RITH	Resonance integral (barns) for all epithermal (above 0.5 eV) neutron absorption, $\int_{0.5\ eV}^{\infty} \frac{1}{E}\ \sigma_a(E)\ dE$
FINA	Fraction of RITH that produces (n,α) reactions
FINP	Fraction of RITH that produces (n;p) reactions
SIGMEV	Fission-spectrum-averaged cross section (barns) for all reactions with a threshold above 1 MeV
FN2N1	Fraction of (n,2n) reactions that produce a product nuclide in an excited (metastable) nuclear state
FFNA	Fraction of SIGMEV that produces (n,α) reactions
FFNP	Fraction of SIGMEV that produces (n,p) reactions

The last variable on the card-image record, IT, is used to indicate the reactor type for which the data have been compiled. Possible values are shown in Table M6.2.4. In the original ORIGEN libraries, a value of zero for IT indicated that no data were present for that reactor type. In the ORIGEN-S libraries, a

Table M6.2.4 Reactor type as a function of variable IT

IT	Reactor type
1	HTGR
2	LWR
3	LMFBR
4	MSBR

nonzero value is always used, even if all other data on the card-image record are zero. This gives the same number of nuclides for every reactor type, which is necessary for full utilization of the blended fuel option in ORIGEN-S.

Three additional pieces of data are computed from the data on the card image, as shown in the following equations:

$$FNG = 1.0 - FNA - FNP , \tag{M6.2.3}$$

$$FING = 1.0 - FINA - FINP , \tag{M6.2.4}$$

and

$$FN2N = 1.0 - FFNA - FFNP . \tag{M6.2.5}$$

In these equations, FNG and FING are the fractions of SIGTH and RITH, respectively, which produce (n,γ) reactions. The variable FN2N is the fraction of SIGMEV which produces (n,2n) reactions.

For all reactor types, the effective one-group cross sections are obtained by weighting the cross sections from the card-image record, as described below. The (n,α), (n,p), (n,γ), and (n,2n) cross sections are given by

$$\sigma_{n,\alpha} = THERM * SIGTH * FNA + RES * RITH * FINA + FAST * SIGMEV * FFNA , \tag{M6.2.6}$$

$$\sigma_{n,p} = THERM * SIGTH * FNP + RES * RITH * FINP + FAST * SIGMEV * FFNP , \tag{M6.2.7}$$

$$\sigma_{n,\gamma} = THERM * SIGTH * FNG + RES * RITH * FING , \tag{M6.2.8}$$

and

$$\sigma_{n,2n} = FAST * SIGMEV * FN2N . \tag{M6.2.9}$$

The (n,γ) and (n,2n) cross sections are further divided into cross sections for product nuclides in ground and excited states by using the variables FNG1 and FN2N1. The total capture cross section is computed from the relation

$$\sigma_c = \sigma_{n,\alpha} + \sigma_{n,p} + \sigma_{n,\gamma} + \sigma_{n,2n} . \tag{M6.2.10}$$

For thermal reactors, the variables THERM, RES, and FAST in Eqs. (M6.2.6) through (M6.2.9) are spectral indices (weight factors) defined in Table M6.2.5. It can be seen that all reaction rates for thermal reactors are computed with the thermal neutron flux. A more complete discussion of THERM, RES, and FAST for thermal reactors and alternative definitions based upon the use of multigroup neutron fluxes and cross sections are given in both the COUPLE (Sect. F6.2.1) and ORIGEN-S (Sects. F7.2.6 and F7.2.12) documentation.

Table M6.2.5 Definitions of spectral indices for thermal reactors

Index (weight factor)	Definition
THERM	Ratio of the neutron reaction rate for a 1/v absorber with a population of neutrons that has a Maxwell-Boltzmann distribution at absolute temperature T, to the reaction rate given by the product of the thermal neutron flux and the 2200 m s^{-1} cross section
RES	Ratio of the resonance neutron flux per unit lethargy to the thermal neutron flux
FAST	1.45 times the ratio of the neutron flux above 1 MeV to the thermal neutron flux

For the LMFBR, the spectral indices are all equal to 1.0 since the cross sections are already spectrum-averaged. In this case, all reaction rates are computed with the total neutron flux. The values of FNA, FNP, FINA, and FINP are always zero for the LMFBR, since SIGTH (or RITH) is only the (n,γ) cross section.

Three steps are used in reading the nuclear data for each nuclide in the library. First, the card-image record containing only the nuclide ID number is read from the cross-section library. Second, the decay data are read from the decay library. Then, the card-image records containing cross-section data are read from the cross-section library until the value of the variable IT is equal to the value of the input parameter NLIBE (Sect. F7.6.10). The remaining records, if any, containing cross-section data are then processed as described in Sect. M6.2.5. When data for all nuclides in the library have been read, processing of the actinide and/or fission-product libraries begins.

M6.2.3 ACTINIDE CROSS-SECTION LIBRARY

The actinide library contains data for 129 fuel, transplutonium, and decay daughter nuclides. Again, the first card-image record for each nuclide contains the ID and the last four records contain cross-section data for four reactor types. These cross-section data are read with the following READ and FORMAT statements:

```
      READ(L,11700) SIGNG, RING, FNG1, SIGF, RIF, SIGFF,
     *SIGN2N, FN2N1, SIGN3N, IT

11700 FORMAT(7X, 2F9.2, F5.3, 4F9.2, F4.3, F9.2,I1)   .
```

Definitions of the nuclear data variables for thermal reactors are given in Table M6.2.6. For an LMFBR, the variables RING, RIF, and SIGFF are not used. In addition, the variables SIGNG, SIGF, SIGN2N, and SIGN3N are then reactor-spectrum-averaged cross sections for (n,γ), fission, (n,2n), and (n,3n) reactions, respectively.

Table M6.2.6 Definitions of nuclear data variables in the actinide library for a thermal reactor

Variable name	Definition
SIGNG	Radiative capture (n,γ) cross section (barns) for thermal ($2200\ m\ s^{-1}$) neutrons
RING	Resonance integral (barns) for (n,γ) reaction
FNG1	Fraction of (n,γ) reactions that produce a product nuclide in an excited (metastable) nuclear state
SIGF	Thermal neutron (n,fission) cross section (barns)
RIF	Resonance integral (barns) for (n,fission) reaction
SIGFF	Fission-spectrum-averaged (n,fission) cross section (barns) for nuclides having a high-energy threshold for fission
SIGN2N	Fission-spectrum-averaged (n,2n) cross section (barns)
FN2N1	Fraction of (n,2n) reactions that produce a product nuclide in an excited (metastable) nuclear state
SIGN3N	Fission-spectrum-averaged (n,3n) cross section (barns)

The variable IT identifies the reactor type, as explained in Sect. M6.2.2 (Table M6.2.4).

If the input variable LPU (Sect. F7.6.10) is greater than zero, the cross-section data for LPU actinide nuclides, whose ID numbers are specified in the input array NEWCX, are read from cards in the input stream. These data are read with a READ statement and FORMAT identical to the ones for the card-image library, as described above.

Again, the effective one-group cross sections are obtained by weighting the cross sections from the card-image record. The (n,γ), (n,fission), (n,2n), and (n,3n) cross sections are given by

$$\sigma_{n,\gamma} = \text{THERM} * \text{SIGNG} + \text{RES} * \text{RING}\ , \qquad \text{(M6.2.11)}$$

$$\sigma_{f} = \text{THERM} * \text{SIGF} + \text{RES} * \text{RIF} + \text{FAST} * \text{SIGFF}\ , \qquad \text{(M6.2.12)}$$

$$\sigma_{n,2n} = \text{FAST} * \text{SIGN2N}\,, \qquad \text{(M6.2.13)}$$

and

$$\sigma_{n,3n} = \text{FAST} * \text{SIGN3N}\,. \qquad \text{(M6.2.14)}$$

As for the light-element library, the (n,γ) and (n,2n) cross sections are divided into cross sections for product nuclides in ground and excited states by using the variables FNG1 and FN2N1. The total capture cross section is found from

$$\sigma_c = \sigma_{n,\gamma} + \sigma_f + \sigma_{n,2n} + \sigma_{n,3n}\,. \qquad \text{(M6.2.15)}$$

For thermal reactors, the variables THERM, RES, and FAST are the spectral indices, as defined in Table M6.2.5. Again, these indices are all 1.0 for an LMFBR, since the cross sections on the card-image record are already spectrum-averaged.

The nuclear data records for the actinide library are read and processed in the same manner as those for the light-element library.

M6.2.4 FISSION-PRODUCT CROSS-SECTION AND FISSION-YIELD LIBRARY

The fission-product library contains data for 879 fission-product nuclides. As for the light-element and actinide libraries, the first card-image record for each nuclide contains the ID. In the fission-product libraries, the last four records contain fission yield as well as cross-section data. These data are read with the following READ and FORMAT statements:

```
  620 READ(L, 11800) SIGNG, RING, FNG1, (Y(I), I=1,5), IT
11800 FORMAT(7X, 2F9.2, F5.3, 5F9.2, 4X,I1) .
```

All the nuclear data variables except Y have the same definitions as for the actinide library (Table M6.2.6). Radiative capture is the only neutron absorption reaction considered for fission products, and the effective one-group (n,γ) cross section is given by Eq. (M6.2.11). As in the actinide library, the variable RING is not used for the LMFBR, and the spectral indices are all 1.0 for that reactor. As before, the variable FNG1 is used to divide the one-group (n,γ) cross section into cross sections for product nuclides in ground and excited states.

The array Y contains energy-dependent direct fission-product yields for five fissionable nuclides. The fissionable nuclides for the four reactor types are shown in Table M6.2.7.

Table M6.2.7 Fissionable nuclides having yield data

Reactor	Y(1)	Y(2)	Y(3)	Y(4)	Y(5)
HTGR	^{233}U	^{235}U	$^{232}Th^a$	$^{238}U^a$	^{239}Pu
LWR	^{233}U	^{235}U	^{241}Pu	$^{238}U^a$	^{239}Pu
LMFBR	$^{241}Pu^a$	$^{235}U^a$	$^{240}Pu^a$	$^{238}U^a$	$^{239}Pu^a$
MSBR	^{233}U	^{235}U	$^{232}Th^a$	$^{238}U^a$	^{239}Pu

[a]Yield is for fission-spectrum-energy neutrons.

In the table, any yields not footnoted "*a*" are for thermal-neutron-induced fission. All fission-product yields for all nuclides except ^{3}H, ^{6}Li, ^{7}Li, ^{9}Be, ^{10}Be, and ^{14}C are from ENDF/B-V.[6] The tritium yield from ^{238}U fission is the average of data from Boumahraz.[7] The tritium yields from fission of ^{233}U, ^{235}U, ^{239}Pu, and ^{241}Pu are from measurements described by Wagemans et al.[8] Yield data for ^{6}Li, ^{7}Li, ^{9}Be, ^{10}Be, and ^{14}C were taken from the ORIGEN2 fission-product yield library.[13]

The nuclear data records for the fission-product libraries are read and processed in the same manner as for the light-element and actinide libraries.

M6.2.5 CONSTRUCTION OF THE TRANSITION MATRIX

In general, the ORIGEN-S code solves a coupled set of linear, nonhomogeneous, first-order differential equations with constant coefficients (Sect. F7.2) which can be written in matrix form as

$$\dot{\underset{\sim}{N}} = \underset{\approx}{A}\,\underset{\sim}{N} + \underset{\sim}{B} \; . \qquad \text{(M6.2.16)}$$

In this equation, $\underset{\sim}{N}$ is a vector of nuclide concentrations, $\underset{\approx}{A}$ is the transition matrix, and $\underset{\sim}{B}$ is a vector of user-specified rate changes (which are zero if the chemical processing options are not used).

In the transition matrix, each element a_{ij} is the first-order rate constant for the formation of nuclide i from nuclide j. Each rate constant is defined by one of the following equations:

$$a_{ij} = \ell_{ij}\,\lambda_j \; , \qquad \text{(M6.2.17)}$$

$$a_{ij} = f_{ij}\,\sigma_j\,\phi \; , \qquad \text{(M6.2.18)}$$

or

$$a_{ii} = -\,(\lambda_i + \sigma_i\phi) \; . \qquad \text{(M6.2.19)}$$

In these equations, λ_i is the radioactive decay constant (s^{-1}) for nuclide j, σ_i is the effective one-group neutron absorption (total capture) cross section (cm^2), and ϕ is the neutron flux ($cm^{-2}\,s^{-1}$). The variables ℓ_{ij} and f_{ij} are the fractions of radioactive decay and neutron absorption of nuclide j which lead to the formation of nuclide i. Note that the term $f_{ij}\,\sigma_j$ in Eq. (M6.2.18) is general enough to include the formation of fission-product nuclides as well as the daughter products of any other kind of neutron capture reaction.

The transition matrix elements are constructed from the information in the card-image nuclear data libraries described in the preceding subsections. In addition, the nuclear data in an ORIGEN-S binary data library are stored in transition matrix format. Therefore, this subsection is devoted to a description of how the transition matrix and its associated nuclide locator vectors are constructed. These operations are performed in subroutine XNUDAT of ORIGEN-S or COUPLE.

Since the transition matrix is normally very sparse, and since straightforward construction of this matrix would require the storage of a very large number of matrix elements (~2.9 million words for the large libraries), a different approach was taken when the original ORIGEN code[1] was developed. Only the diagonal elements and nonzero off-diagonal elements of the matrix are stored. The location of each nonzero off-diagonal element (i.e., row and column in the full transition matrix) is recorded using three nuclide locator vectors.

The information needed to construct the diagonal elements a_{ii} is stored in two one-dimensional (1-D) arrays. The radioactive decay constant λ_i, computed from the half-life, is stored in array element DIS(I). The total capture cross section for nuclide i is stored in array element TOCAP(I).

The processing of information for the nonzero off-diagonal elements a_{ij} is described below. The first-order rate constant for a decay transition is calculated by multiplying the decay constant λ_j of the parent nuclide by the fraction of transitions to the final state of interest. Next, the product nuclide of the transition is identified by addition of a suitable constant to the six-digit identification number NUCL(J). For example, NUCL(J)+10000 identifies the product nuclide following β^- decay of nuclide j, and NUCL(J)-1 identifies the product of isomeric transition. Two temporary arrays are constructed. In the first, each element NPROD(M,J) contains the six-digit identifier of the product nuclide formed by transition M of nuclide J. In the second array, the element COEFF(M, J) contains the first-order rate constant for the corresponding transition.

For nonfission neutron capture transitions, a slightly different procedure is followed. Since the neutron flux is not known, only that portion of the rate constant given by $f_{ij}\sigma_j$ is computed. For example, the product of FN2N1 and the one-group (n,2n) cross section gives $f_{ij}\sigma_j$ for an (n,2n) transition from nuclide j to metastable product nuclide i. Again, the product nuclide identifier is found by adding a suitable constant to the six-digit parent nuclide identifier NUCL(J). For the example under consideration, the metastable product nuclide from the (n,2n) reaction is given by NUCL(J)-9. As before, the temporary array element NPROD(M, J) contains the six-digit product nuclide identifier. For neutron capture transitions, the element COEFF(M, J) of the second array contains only the $f_{ij}\sigma_j$ portion of the rate constant.

After the arrays NPROD and COEFF have been constructed, a search is made of the NPROD array to identify all the parents of a given nuclide I. Nuclide J is a parent of I if NPROD(M,J) equals NUCL(I) for any reaction type M. When a parent of nuclide I has been located, the value of the corresponding transition matrix element a_{ij} is just COEFF(M, J). The nonzero, off-diagonal matrix elements a_{ij} are stored sequentially in a 1-D array A. Each time a matrix element is stored in array element A(N), the index N is incremented by one. At the same time, the value of J identifying the parent nuclide is stored in array element LOC(N) of a second 1-D array. The total number of parents for production of nuclide I is stored in array element I of a third array NON0. Finally, the number of parents for production of nuclide I by radioactive decay is stored in array element I of the last locator vector KD.

When the nonzero, off-diagonal matrix elements for nuclide I are stored in array A, all those for radioactive decay transitions are grouped first. These elements are followed by those for formation of I by neutron capture. The number of neutron capture transitions for formation of nuclide I is given by NON0(I)-KD(I).

Since the matrix elements for nuclide I are grouped by transition type, the information in the locator vectors LOC, NON0, and KD is sufficient to identify the location of any array element A(N) in the expanded transition matrix. Note that NON0(I) is the number of nonzero, off-diagonal elements in row I of the expanded matrix and LOC(N) is the column number of array element A(N).

After the matrix elements for all nuclides have been stored, the elements of the NON0 array are converted (in subroutine XORIGN of ORIGEN-S) to indicate the cumulative number of matrix elements for all nuclides up to and including the nuclide of interest. The array element NON0(I+1) is set equal to NON0(I) + NON0(I+1) for all I greater than 1. The elements of the KD array are also adjusted such that NON0(I) - KD(1) still gives the number of neutron capture transitions for formation of nuclide I.

The construction of the matrix elements a_{ij} corresponding to the production of fission-product nuclides is slightly different. When the yield Y_{ij} (for direct formation of nuclide i from fission of nuclide j) is multiplied by the fission cross section σ_{fj}, the result is just the $f_{ij}\sigma_j$ portion of the first-order rate constant a_{ij}. The product $Y_{ij}\sigma_{fj}$ is entered directly into the proper array element A(N), J is entered into LOC(N), and there is no need for the temporary arrays NPROD and COEFF.

M6.2.6 SOURCES OF DECAY DATA

An extensive decay-data update[9] was completed prior to the release of the SCALE-4.2 version of ORIGEN-S. The primary source of the radioactive decay data was ENDF/B-VI.[10] Approximately 24% of the library nuclides are stable. About 66% of the nuclides were completely updated with decay half-lives, branching fractions, recoverable energy per decay, and gamma energy per decay from ENDF/B-VI. The decay data for most of the remaining nuclides were taken from ENSDF.[14,15] Only 21 nuclides were not fully updated. Here, the number of nuclides represents the number of nuclide positions or locations in the libraries. The number of unique nuclides would be smaller because some isotopes or isomers are included in more than one of the three library segments (light elements, actinides, and fission products).

Improved decay data were placed in the ORIGEN-S and ORIGEN2 libraries during the same project.[9] The decay data libraries of both codes were made the same size, and the same data were put into each library, with one exception. The ORIGEN2 data for each nuclide are read from two card images. A third card image is added in the ORIGEN-S library that contains the library ID, the β^- (negatron) branching fraction, and the fraction of the recoverable photon energy per decay. At the time this is written, ORIGEN2 calculates the negatron branching fraction from the other branching fractions and does not compute recoverable photon energies. However, all decay data common to both codes are identical.

Table M6.2.8 summarizes nuclides according to their change status (updated or unchanged), their decay data source, and their decay nature (stable or radioactive). The nature of ^{204}Pb was changed to stable because it was reevaluated since the previous update. Most nuclides were updated from ENDF/B-VI data files. Nuclides that were updated from ENSDF data are listed in Table M6.2.9. The half-life of ^{79}Se (from ENDF/B-VI) was changed because it was determined to be in error. It was discovered that the conversion of measured disintegrations per second to half-life in one of the source reports for ^{79}Se was in error by a factor of 10. Also, the half-life of ^{86m}Br was changed back to the initial value because it was inadvertently given the ^{86}Br value. The corrected half-lives were placed in the ORIGEN-S decay library prior to the release of SCALE 4.3.

All the remaining nuclides for which all data items were not updated, or which were given special treatment, are listed in Table M6.2.10. Although these are taken from the last 26 nuclides in the listing in Table M6.2.8, note that only 22 are shown in Table M6.2.10. The reason for the difference in numbers is because four of the different nuclides in Table M6.2.10 are in two library segments, and the values in Table M6.2.8 represent the number of nuclide positions in the entire library. The pseudonuclides ^{155m}Gd and ^{250}S are not real nuclides, but are locations for neutron counters used by ORIGEN2. The special purpose of ^{4}H is explained in Sect. M6.2.8. The decay data for nuclides in Table M6.2.10 which are not specifically footnoted were taken from either the library for the original version of ORIGEN[1] or the first expansion of the light-element and fission-product libraries.[2,4] The source of most of the decay data in those libraries was either the Table of Isotopes[20] or the Chart of the Nuclides,[21] although the source of some of the data remains unknown.

A part of the recoverable energy per decay not included in the ENDF/B-VI and ENSDF data was that from spontaneous fission. This quantity was calculated as the product of spontaneous fission branching fraction and recoverable energy per fission and added to the ENDF or ENSDF recoverable energy. A value (consistent with that used in unchanged data) of 200 MeV per fission[11] was assumed. A value of 12.56-MeV gamma energy per fission[11] was used in computing the fraction of recoverable energy from photons.

In addition to radioactive decay data, the decay database contains two other kinds of data. Atom percent natural isotopic abundances were taken from Holden,[22] and maximum permissible radioactivity concentration guides (RCGs) for air and water were taken from the *Code of Federal Regulations*, 10 CFR 20.[16]

Table M6.2.8 Summary of decay data sources

Number of nuclides	Stability, change status, and data source
404	Stable, unchanged
1126	Radioactive, updated (ENDF/B-VI[10])
2	Radioactive, required half-life revision after ENDF/B-VI update
139	Radioactive, updated (ENSDF[14,18,19])
1	Stable, updated (*Table of Radioactive Isotopes*[a])
21	Radioactive, partial[b] or no change (prior ORIGEN2[c])
4	Special purpose (pseudonuclide) positions, unchanged
1697	Total library size

[a]Taken from Ref. 17.
[b]Not all data items were changed.
[c]Taken from Ref. 11.

Table M6.2.9 Unique nuclides updated with decay data from ENSDF

4Be 11	25Mn 57	58Ce139m	72Hf178m	78Pt195m
5 B 12	25Mn 58	59Pr139	72Hf179m	78Pt197m
7 N 13	27Co 58m	59Pr140	72Hf180m	78Pt197
6 C 15	27Co 61	60Nd141	73Ta180	80Hg197m
11Na 24m	27Co 62	63Eu149	72Hf181	89Hg197
11Na 25	28Ni 65	66Dy157	73Ta182m	78Pt199m
13Al 29	28Ni 66	66Dy159	73Ta183	78Pt199
13Al 30	29Cu 67	67Ho163	74 W183m	79Au199
14Si 32	30Zn 69m	68Er163	74 W185m	79Au200
15 P 33	30Zn 69	68Er165	76Os185	80Hg205
15 P 34	31Ga 70	68Er169	74 W188	84Po211m
16 S 35	30Zn 71	70Yb169	75Re188m	88Ra222
16 S 37	30Zn 71m	69Tm170	75Re188	90Th226
17Cl 38m	32Ge 71	68Er171	74 W189	92 U230
17Cl 38	32Ge 71m	69Tm171	75Re189	92 U231
19 K 43	45Rh102	68Er172	76Os190m	91Pa235
19 K 44	47Ag106	69Tm172	76Os191m	93Np235
21Sc 46m	55Cs131	69Tm173	76Os191	95Am239
20Ca 49	56Ba131	70Yb175	78Pt191	93Np241
21Sc 49	56Ba131m	72Hf175	77Ir192	94Pu246
21Sc 50	55Cs132	71Lu176m	77Ir192m	95Am246
23 V 53	56Ba133m	70Yb177	76Os193	96Cm251
23 V 54	58Ce137	71Lu177m	78Pt193m	99Es254
24Cr 55	58Ce139	71Lu177	77Ir194m	

Table M6.2.10 Nuclides not updated with decay data or changed to stable

1H4[a]	58Ce137m[c]	65Tb163m	96Cm250	99Es255
4Be 8[b]	58Ce142	69Tm170m	97Bk251	S250[a]
23V50[c]	62Sm149	70Yb175m	98Cf254	
34Se85m	65Tb162m	92 U241	99Es254m[e]	
35Br86m	64Gd155m[a]	82Pb204[d]	98Cf255	

[a]Special purpose pseudonuclides with no physical decay data.
[b]Half-life increased from 6.7×10^{-17} s to 2×10^{-6} s to require fewer changes in PC version.
[c]Half-lives and recoverable energies from ENSDF.
[d]The decay nature was specified as stable in Ref. 17.
[e]Gamma energies from Ref. 17.

M6.2.7 SOURCES OF CROSS-SECTION DATA

With the exception of the nuclides discussed later, all cross-section and fission-yield data for the HTGR, LMFBR, and MSBR were taken from the ORIGEN libraries.[1-4] However, some rearrangement of these data was undertaken at the time (early 1980s) of the first major data update, as explained below.

Cross sections were transferred from the small light-element library to the large light-element library for those nuclide and reactor-type combinations that previously had no cross-section data in the large light-element library.

The cross sections for those nuclide and reactor-type combinations that were already present in the large light-element library were transferred to the small light-element library, since these data were from more recent sources[2,4] than those data originally in the small library.

Cross sections for ^{129}I were transferred from the original small fission-product library to the large (now the only) fission-product library for the HTGR and MSBR, since the large library had no data for these cases.

When data were transferred from the large to the small libraries, the transfers were performed only for those nuclides originally in the small libraries. No nuclides were added. As mentioned earlier in Sect. M6.2.2, 13 nuclides from the small light-element library were added to the original large light-element library during the updating.

The net result of all the transfers of cross-section data was to make the small light-element library a subset of the large light-element library. The small libraries were retired at the release of SCALE 4.2.

Later, cross-section data for ^{133}Cs were replaced for the HTGR, LWR, and MSBR in the large light-element and fission-product libraries. Values of the thermal (2200 m s^{-1}) (n,γ) cross section and the (n,γ) resonance integral were taken from an ENDF/B-V compilation.[23] For the LWR only, those cross sections were adjusted slightly to give an effective one-group (n,γ) cross section of 117 b for ^{133}Cs when used with the "typical" values of 0.632 for THERM and 0.333 for RES. This one-group cross section is more representative of a modern LWR than the old value, which consistently led to an overestimate of the afterheat power from ^{134}Cs.

The value of FINP for ^{3}He in the old light-element libraries was erroneously given as zero. The correct value of 1.0 was used for the new libraries.

The values of (n,α) cross sections for the HTGR and LWR in the old light-element libraries were replaced for the following 11 nuclides: ^{1}H, ^{2}H, ^{6}Li, ^{7}Li, ^{9}Be, ^{10}B, ^{11}B, ^{12}C, ^{14}N, ^{16}O, and ^{19}F. The sum of the (n,α) and the (n,2n) cross sections from the original reference[24] had been misinterpreted as just the (n,α) cross

section, leading to erroneously high values for the (n,α) cross sections in the libraries. New cross-section data were taken either from a compilation[25] of ENDF/B-IV thermal cross sections and resonance integrals or from a collapse of the SCALE 218-group library (Sect. M4). A 1/E weighting in the resonance region and a fission spectrum weighting in the fast region were used for the collapse.

The thermal cross sections and resonance integrals for the (n,γ) and (n,fission) reactions were updated for the following nuclides in the actinide library: ^{242m}Am, ^{242}Am, ^{242}Cm, ^{243}Cm, and ^{245}Cm. New values were placed in the library for the HTGR, LWR, and MSBR. The new data were taken from an ENDF/B-V compilation.[23] Cross sections for these nuclides are sometimes not updated before running an ORIGEN-S case, and the new values should give better nuclide concentrations and neutron sources than those from the old actinide library.

M6.2.8 SPECIAL TREATMENT OF CERTAIN NUCLIDES

The data for certain nuclides in the ORIGEN-S card-image nuclear data libraries are not the same as the data taken from the original sources. Because this situation is potentially confusing to the user, explanations of these cases are presented here.

The first special case is that of the fictitious nuclide ^{4}H. This nuclide has been added to the light-element library, so the following reaction can be represented for the HTGR and LWR:

$$^{7}_{3}\mathrm{Li} + ^{1}_{0}\mathrm{n} \rightarrow ^{3}_{1}\mathrm{H} + ^{4}_{2}\mathrm{He} + ^{1}_{0}\mathrm{n} \; . \qquad \text{(M6.2.20)}$$

Since this fictitious nuclide is represented as being stable with a large (9.9×10^{10} b) (n,2n) cross section, the reaction of Eq. (M6.2.20) can be represented by the following two reactions:

$$^{7}_{3}\mathrm{Li} + ^{1}_{0}\mathrm{n} \rightarrow ^{4}_{1}\mathrm{H} + ^{4}_{2}\mathrm{He} \; , \qquad \text{(M6.2.21)}$$

$$^{4}_{1}\mathrm{H} + ^{1}_{0}\mathrm{n} \rightarrow 2^{1}_{0}\mathrm{n} + ^{3}_{1}\mathrm{H} \; . \qquad \text{(M6.2.22)}$$

If the reaction of Eq. (M6.2.21) is given the same cross section as that of Eq. (M6.2.20), then the sum of the reactions of Eqs. (M6.2.21) and (M6.2.22) is a good approximation of the reaction in Eq. (M6.2.20).

The second special case is that of ^{92}Nb in the light-element library. The decay data shown for ^{92}Nb are actually the data for ^{92m}Nb, which is formed by the reaction

$$^{92}_{42}\mathrm{Mo} + ^{1}_{0}\mathrm{n} \rightarrow ^{1}_{1}\mathrm{H} + ^{92\,m}_{41}\mathrm{Nb} \; . \qquad \text{(M6.2.23)}$$

Since there is no provision for representing an (n,p) reaction leading to a metastable product nuclide, ^{92m}Nb has been represented as ^{92}Nb.

The third special treatment of certain nuclides involves the request for the option to solve for the time integral of fission-product concentrations (Sect. F7.2.7) during the decay-only type of time interval. The option is requested in ORIGEN-S input by specifying a nonzero value for NVERT, the 32nd entry in the 3$ data array (Sect. F7.6.10). The model for the integral option requires that fission-product nuclides do not decay by the (β,n) or the α modes of decay. If the integral option is requested, the code sets the α decay and the (β,n) decay branching fractions to zero when processing the card-image libraries and does not change other branching fractions of the decay of the nuclide. The option is not permitted during irradiation, when the (β,n) emission can be important. Following the first hour after a reactor power shutdown, the nuclides that have (β,n)

emission have diminished to insignificance because their half-lives do not exceed 1 minute. The fission products that decay by α emission are ^{142}Ce, ^{144}Nd, ^{146}Sm, ^{147}Sm, ^{148}Sm, ^{149}Sm, and ^{152}Gd. The shortest half-life of these nuclides (for ^{146}Sm) exceeds 10^8 years.

M6.3 CARD-IMAGE PHOTON YIELD LIBRARIES

The original card-image photon yield libraries for ORIGEN[1] contained multigroup photon yields (photons per disintegration) for decay gamma and X rays, for bremsstrahlung from decay beta rays slowing down in a UO_2 fuel matrix, and for some gammas accompanying (α,n) reactions in oxide fuels. The yields for light elements and fission products were given in the 12-group structure of the PHOEBE code.[26] For the actinide library, the lowest energy group was divided into seven smaller groups with energies down to 20 keV, giving 18 groups in all.

There are three card-image photon yield libraries that were generated specifically for ORIGEN-S: (1) a light-element library for 323 nuclides, (2) an actinide library for 114 nuclides, and (3) a fission-product library for 298 nuclides. The photon yields in these libraries include decay gamma and X rays, prompt and equilibrium fission-product gamma rays from spontaneous fission, gamma rays accompanying (α,n) reactions in oxide fuel, and bremsstrahlung from decay beta rays slowing down in a UO_2 fuel matrix. The light-element and fission-product photon yields were generated in a 12-group structure, and the actinide photon yields are given in an 18-group structure. Both group structures are shown in Table M6.3.1.

Table M6.3.1 Group structures for ORIGEN-S photon yield libraries

Group No.		Lower energy	Average energy
LE,FP	ACT	(MeV)	(MeV)
	1	0.00	0.01
	2	0.02	0.03
	3	0.04	0.055
	4	0.07	0.085
	5	0.10	0.12
	6	0.14	0.17
1	7	0.20	0.30
2	8	0.40	0.65
3	9	0.90	1.125
4	10	1.35	1.575
5	11	1.80	2.00
6	12	2.20	2.40
7	13	2.60	2.80
8	14	3.00	3.25
9	15	3.50	3.75
10	16	4.00	4.25
11	17	4.50	4.75
12	18	5.00	5.50

The lower energy bounds for the light-element and fission-product libraries are the same as in the original ORIGEN libraries. For the actinide library, the lower bounds are the same as in the original library for groups 8 to 18, but the group bounds have been revised for the seven lowest energy groups. The revised boundaries were chosen to give a relatively flat spectrum in these low energy groups.

The standard setup for all computers is for the three nuclear data libraries and the three photon yield libraries to reside in a single data file, separated by blank cards, and to be referenced by a single logical unit number.

Note that the user can generate his own card-image photon yield libraries by the use of various options in ORIGEN-S (Sect. F7.6.10). Because of programming considerations, the number of energy groups in the light-element and fission-product libraries must be less than or equal to 12, and the number of groups in the actinide library must be in the range 10 to 18. Any energy group boundaries can be used.

Other ORIGEN-S options (Sect. F7.6.10) allow multigroup photon yield data to be placed in a binary data library (Sect. M6.7). In a binary data library, there are no limits on the number of energy groups which can be used.

The remainder of this section is devoted to describing (1) the data formats for the original libraries and for the ORIGEN-S photon libraries and (2) the data source for the ORIGEN-S libraries.

M6.3.1 FORMATS

The photon yields are read from the card-image libraries with a READ statement such as the following:

```
READ(NDSET, FOR, END=350) NUCLID, (GFRAC(N), N=1, NGP) ,
```

where NUCLID is the nuclide identification number of Eq. (M6.2.1), GFRAC(N) is the yield in group N, and NGP is the number of groups. The READ statement used for photon libraries in the input stream does not have the "END=" option. The FORMAT used is given in array FOR and varies according to the library being read. The FORMATS used for the original ORIGEN libraries are given in Table M6.3.2.

Table M6.3.2 FORMATS for original photon yield libraries

Library	FORMAT
Light element or fission product	(I6,12F6.4)
Actinide	(I6,9E8.2,2X/6X,9E8.2)

If the value of NUCLID on the first record is negative, subroutine XPHOLB assumes that an ORIGEN-S photon yield library is being used. The number of groups is -NUCLID. The FORMAT to be used in the READ statement above is then read in with the following statements:

```
      READ(NDSET, 11000) FOR
11000 FORMAT(18A4) .
```

The FORMAT read into array FOR is read from the second record of an ORIGEN-S light-element or fission-product library. In an ORIGEN-S actinide photon library, the second record is ignored, and the FORMAT of array FOR is read from the third record.

Once the proper FORMAT has been set, the remaining records of a photon yield library are read by the first READ statement given above, for both the original ORIGEN and the ORIGEN-S libraries.

Any format compatible with the number of energy groups can be used for an ORIGEN-S photon yield library. The current ORIGEN-S libraries were generated by ORIGEN-S itself, using the FORMATS shown in Table M6.3.3.

Table M6.3.3 FORMATS for current ORIGEN-S photon yield libraries

Library	FORMAT
Light element	(I6,6E12.5,2X/6X,6E12.5)
Actinide	(I6,6E12.5,2X/6X,6E12.5,2X/6X,6E12.5)
Fission product	(I6,6E12.5,2X/6X,6E12.5)

M6.3.2 SOURCE OF DATA

The ORIGEN-S card-image photon yield libraries were generated by ORIGEN-S itself from data in the ORNL Master Photon Data Base described in Sect. M6.5.

As an aid to those who may wish to generate their own libraries, and for completeness in documentation, the ORIGEN-S input data to generate these libraries are presented below:

```
#shell
  cat $ORCARD/mpdkxgam $ORCARD/mpsfangm $ORCARD/mpbru* > ft60f001
  rm ft35f001 ft36f001 ft37f001
  touch ft35f001
  touch ft36f001
  touch ft37f001
end
#origens
0$$ a9 60 e
  1t
case makes 12-group card-image light element photon library
3$$  a33 12  4** 0.632 0.333 2 e  2t
35$$ 0  4t
56$$ 0 1 a13 1 a16 35 4  e  5t
60**  1
73$$  190400 74** 1 75$$ 1
81$$ 8 a3 60  e
83** 6000000.0 5000000.0 4500000.0 4000000.0 3500000.0 3000000.0
     2600000.0 2200000.0 1800000.0 1350000.0  900000.0  400000.0
      200000.0  6t
12-group card-image light element photon library

56$$ f0 t
end
#origens
0$$ a9 60 e
  1t
case makes 18-group card-image actinide photon library
3$$  a33 18  4** 0.632 0.333 2 e  2t
35$$ 0  4t
56$$ 0 1 a13 1 a16 36 4  e  5t
60**  1
```

```
73$$  922380 74** 1 75$$ 2
81$$ 9 a3 60  e
83** 6000000.0 5000000.0 4500000.0 4000000.0 3500000.0 3000000.0
     2600000.0 2200000.0 1800000.0 1350000.0  900000.0  400000.0
      200000.0  140000.0  100000.0   70000.0   40000.0   20000.0
           0.0  6t
18-group card-image actinide photon library

56$$ f0 t
end
#origens
0$$ a9 60 e
  1t
case makes 12-group card-image fission product photon library
3$$  a33 12  4** 0.632 0.333 2 e  2t
35$$ 0  4t
56$$ 0 1 a13 1 a16 37 4  e  5t
60**  1
73$$  360850 74** 1 75$$ 3
81$$ 10 a3 60  e
83** 6000000.0 5000000.0 4500000.0 4000000.0 3500000.0 3000000.0
     2600000.0 2200000.0 1800000.0 1350000.0  900000.0  400000.0
      200000.0  6t
12-group card-image fission product photon library

56$$ f0 t
end
#shell
  cp ft35f001 $RTNDIR/12_group_light_element_photon_lib
  cp ft36f001 $RTNDIR/18_group_actinide_photon_lib
  cp ft37f001 $RTNDIR/12_group_fission_product_photon_lib
end
```

All three cases shown in the input data are run back to back. Each case simulates a 1-day decay of some nuclide in the library of interest since ORIGEN-S must perform some calculation before generating a new library. The large light-element, actinide, and fission-product nuclear data libraries are read on unit 28. The card-image master photon data base for these runs was formed by concatenating the data sets for (1) decay gamma and X rays, (2) gamma rays accompanying spontaneous fission and (α,n) reactions, and (3) bremsstrahlung for betas and positrons slowing down in UO_2. This card-image master photon data base is read on unit 60. The light-element, actinide, and fission-product card-image photon yield libraries are written on units 35, 36, and 37, respectively. Further details of the input data may be found by studying Sect. F7.6 of the ORIGEN-S documentation.

When the data from the ORNL Master Photon Data Base[11] (Sect. M6.5) are converted to multigroup yields by ORIGEN-S, the intensities of the photons are adjusted to ensure conservation of the photon energy release rates calculated by ORIGEN-S. Experience has shown that conservation of energy yields photon dose rates outside shipping casks that are in better agreement with experiment than does conservation of photons. The adjusted group intensity is given by:

$$I_g = I_a(E_a/E_g) \ , \qquad \text{(M6.3.1)}$$

where

I_g = group photon intensity (photons per disintegration),

I_a = actual photon intensity from the ORNL Master Photon Data Base (photons per disintegration),
E_a = actual photon energy (MeV), and
E_g = mean energy of the group (MeV).

If the actual photon energy E_a is near a group boundary, the group intensity may be split between two groups. To determine when this split occurs, a factor f is computed as

$$f = \frac{E_a - E_\ell}{E_u - E_\ell} , \qquad \text{(M6.3.2)}$$

where

E_ℓ = lower energy bound of the group (MeV), and
E_u = upper energy bound of the group (MeV).

If $f \leq 0.03$, the intensity I_g is split equally between group g and the next lower energy group, unless group g is the lowest group. If $f \geq 0.97$, the intensity I_g is split equally between group g and the next higher energy group, unless group g is the highest group. If $0.03 < f < 0.97$, the intensity I_g is not split between adjacent groups.

M6.4 DATA PROGRAMMED INTO ORIGEN-S AND COUPLE

Several items of nuclear data are programmed directly into ORIGEN-S and COUPLE. Descriptions of these data are presented here. Although these data are not part of the ORIGEN-S libraries, the user may on occasion wish to change these data or to understand explicitly how they are used.

The arrays EACTGP and EGROUP are defined by DATA statements in subroutine FLXDIM in ORIGEN-S and in subroutine CARDIM in COUPLE. The array EACTGP contains the average energies of the 18 groups in the original card-image actinide photon yield library. The array EGROUP contains the average energies of the 12 groups in the original card-image light-element and fission-product photon yield libraries. These are the average energies of Table M6.3.1. Note that the arrays EACTGP, EGROUP, and EFPGRP can be read as input data in the 36*, 37*, and 39* arrays of ORIGEN-S (Sect. F7.6.10) or COUPLE (Sect. F6.5.8). When read as input data, these arrays contain the energy group boundaries (**not** the average group energies) for the card-image light-element, actinide, and fission-product photon yield libraries. These data should be read in **only** when the user has made his own card-image photon yield libraries to be read using the **original** ORIGEN library FORMATS of Table M6.3.3, and then **only** if different energy group boundaries have been used. These data should **not** be read when photon yield libraries with the new ORIGEN-S variable FORMATS are used.

A number of data in the ORIGEN-S COMMON/SPECDT/ are defined by DATA statements in the BLOCK DATA ORGENS subroutine of ORIGEN-S. These data, used in the calculation of spontaneous fission and (α,n) neutron sources in UO_2 (Sect. F7.2.8), are described below in their order of appearance in the COMMON block.

1. The variable NGAL is the number of energy groups in which neutron spectra data are provided for (α,n) neutron sources due to ^{242}Cm, ^{244}Cm, and ^{238}Pu.
2. The variable NGSP is the number of energy groups in which neutron spectra data are provided for spontaneous fission neutron sources from ^{242}Cm and ^{244}Cm.
3. The array GRPAL contains the energy group boundaries (MeV) for neutron spectra from (α,n) reactions.
4. The array GRPSP contains the energy group boundaries (MeV) for neutron spectra from spontaneous fission.
5. The array SA38 contains the neutron spectrum from (α,n) reactions due to alpha decays in ^{238}Pu.
6. The array SA42 contains the neutron spectrum from (α,n) reactions due to alpha decays in ^{242}Cm.
7. The array SA44 contains the neutron spectrum from (α,n) reactions due to alpha decays in ^{244}Cm.
8. The array SS42 contains the neutron spectrum from spontaneous fission of ^{242}Cm.
9. The array SS44 contains the neutron spectrum from spontaneous fission of ^{244}Cm.
10. The array EALPH contains the mean alpha energies (MeV) for those actinides which decay by alpha emission.
11. The array FA contains the alpha decay branching fractions for the actinides.
12. The array SPONU contains the values of the spontaneous fission yield, ν_{SF}, for those actinides that have measured data.
13. The array HALFSP contains spontaneous fission half-lives (years) for a number of actinides.
14. The array AEK contains data for an empirical formula used to estimate the spontaneous fission yield for those actinides having no measured value of ν_{SF}.

Data having the same variable names as those in COMMON/SPECDT/ are also present in COMMON/SPEBOR/. They are defined by DATA statements in the BLOCK DATA BORSIL subroutine of ORIGEN-S. These data are used in the calculation of (α,n) neutron sources in borosilicate glass.

The arrays YLD1, YLD2, YLD3, YLD4, and YLD5 from COMMON/NEUTYL/ of ORIGEN-S are defined in the BLOCK DATA BORSIL subroutine. These arrays contain spectrally dependent (α,n) neutron yields in borosilicate glass for the 54 lightest elements in the ORIGEN-S libraries.

The arrays ST1, ST2, ST3, ST4, ST5, and ST6 from COMMON/STPOWR/ of ORIGEN-S are also defined in the BLOCK DATA BORSIL subroutine. They contain spectrally dependent stopping power data for alpha particles for the 99 elements in the ORIGEN-S libraries.

The array MSRS in subroutine FLXDI1 in ORIGEN-S, and in subroutine CARDIM in COUPLE, contains the identification numbers of the fissionable nuclides which have fission-product yield data in the card-image nuclear data libraries (Table M6.2.7).

A number of arrays defined by DATA statements in subroutine POWERF in ORIGEN-S contain data used to compute the recoverable energy (MeV per fission) for converting power to flux. The array IDL contains the identification numbers of ten light-element nuclides having values of recoverable energy per neutron capture in the array QCLIT. The array QNFISS contains values of recoverable energy per (n,fission) reaction for 30 actinides whose identification numbers are given in array IDA. The array QCACT contains values of recoverable energy per neutron capture for the same 30 actinides. The array IDF has identification numbers for 30 fission products whose values of recoverable energy per neutron capture are given in the array QCFPR. The recoverable energy values in arrays QCLIT, QCACT, QNFISS, and QCFPR were taken primarily from ENDF.[5,6] The recoverable energy per neutron capture is assumed to be 5.0 MeV for all nuclides for which data are not given in the DATA statements.

Finally, the arrays YTNEUT, YRNEUT, and YFNEUT are defined by DATA statements in subroutine XNUDAT in ORIGEN-S and in COUPLE. These arrays contain values of ν (neutrons per fission) for the thermal, resonance, and fast energy groups, respectively, for all 129 nuclides. These values are used in ORIGEN-S if the option to compute the infinite medium neutron multiplication factor has been invoked. The user has the option to read in his own values as input data in the 121*, 122*, and 123* arrays of ORIGEN-S (Sect. F7.6.10).

M6.5 MASTER PHOTON DATA BASE

The ORNL Master Photon Data Base[11] was originally developed for the ORIGEN2 code.[13] It is maintained as six card-image data sets for ease in updating. However, ORIGEN-S can be used (Sect. F7.6.10) to create a binary (unformatted) master photon data base for use in subsequent ORIGEN-S runs. It has been customary at ORNL to run ORIGEN-S with a binary master photon data base, since execution is somewhat more efficient for that mode of operation. The ORNL Master Photon Data Base is the most comprehensive and up-to-date photon library available to ORIGEN-S. It can be used (Sect. F7.6.10) to generate multigroup photon source spectra, to make card-image photon yield libraries, or to update photon yield data in a binary data library. The spectra and photon yield data can be generated in any energy group structure for all light-element, actinide, and fission-product nuclides having photon data. The ORNL Master Photon Data Base is described in detail in Ref. 11. The remainder of this section is devoted to a summary description of the formats, data sources, and uses of this data base.

M6.5.1 CARD-IMAGE DATA BASES

There are six card-image data sets for six categories of photon sources. The first data set contains decay gamma and X-ray line data from ENSDF.[14,15]

The second data set contains spectra for gamma rays accompanying spontaneous fission and for gamma rays accompanying (α,n) reactions in oxide fuels. The combined spectra for prompt and equilibrium fission-product gamma rays from spontaneous fission are computed from the following approximation:[11]

$$\begin{aligned} N(E) &\cong 11.5 && , 0.1 \le E < 0.6 \text{ MeV}, \\ &\cong 35.4 \exp(-1.78E), && 0.6 \le E < 1.5 \text{ MeV}, \\ &\cong 12.6 \exp(-1.09E), && 1.5 \le E \le 10.5 \text{ MeV}, \\ &\cong 0 && , E < 0.1;\ E > 10.5 \text{ MeV}, \end{aligned} \qquad \text{(M6.5.1)}$$

where

$N(E)$ = number of photons per unit energy per fission (photons MeV^{-1} per fission) at energy E,

and

E = photon energy (MeV).

The spectrum of gamma rays accompanying (α,n) reactions is computed from the following approximation:[11]

$$N(E) \cong 2.13 \times 10^{-8} \exp(-1.38E)\ , \qquad \text{(M6.5.2)}$$

where

$N(E)$ = number of photons per unit energy per alpha decay (photons MeV^{-1} per disintegration) at energy E,

and

E = photon energy (MeV).

Two data sets contain bremsstrahlung spectra from decay negatrons and positrons slowing down in a UO_2 fuel matrix. The last two data sets contain bremsstrahlung spectra from decay negatrons and positrons slowing down in water. According to Ref. 11, all bremsstrahlung spectra were calculated using a computer program developed by Dillman et al.,[27] using beta spectra derived from ENSDF[14,15] decay data with a computer program written by Gove and Martin.[28]

The six data sets described above can be concatenated in any user-chosen combination to form a card-image master photon data base for use with ORIGEN-S. All six data sets are constructed in the same card-image format. The data are read in subroutine GSMAST of ORIGEN-S by READ and FORMAT statements such as

```
      READ(NLIB, 10000, END=320) NUC, (RE(J), RI(J), J=1, 3)
 1000 FORMAT(I6, 4X, 6F10.0) .
```

In the READ statement, NUC is the nuclide identification number, RE is the photon energy (MeV), and RI is the photon intensity (photons per disintegration).

There are several cards for each nuclide. The first card contains a nonzero value of NUC, and zero values for all the RE and RI entries. The remaining cards for a nuclide contain a zero entry for NUC and nonzero entries for the RE and RI values. These cards are repeated until all photon data for a nuclide have been given.

M6.5.2 BINARY DATA BASES

As mentioned earlier, a binary master photon data base can be created by ORIGEN-S from any combination of the six card-image data sets. All data in a binary master photon data base are read in subroutine GSMAST of ORIGEN-S by the following unformatted READ statement:

```
READ(NLIB, END=310) NUC, LINES, (RE(J), RI(J), J=1, LINES).
```

In this READ statement, LINES is the total number of entries for the nuclide. The variables NUC, RE, and RI have the same meanings as for a card-image master photon data base.

Three binary master photon data bases have been generated for use at ORNL. Each contains decay gamma and X-ray line data and the spectra for gamma rays accompanying spontaneous fission and (α,n) reactions. One contains no bremsstrahlung data, another contains bremsstrahlung spectra for a UO_2 fuel matrix, and the last contains bremsstrahlung spectra for a water medium.

The ORIGEN-S input data to create the three standard binary master photon data bases are given below. For each of the three cases, a card-image master photon data base is read on unit 59, 61, or 62. The card-image data base is then converted to a binary master photon data base written on unit 23, 24, or 26. The large light-element, actinide, and large fission-product card-image nuclear data and photon yield libraries are read on unit 28. Details of the input data can be determined by studying Sect. F7.6.10 of the ORIGEN-S documentation.

```
#shell
  cat $ORCARD/mpdkxgam $ORCARD/mpsfangm $ORCARD/mpbru* > ft59f001
  cat $ORCARD/mpdkxgam $ORCARD/mpsfangm $ORCARD/mpbrh* > ft61f001
  cat $ORCARD/mpdkxgam $ORCARD/mpsfangm  > ft62f001
  rm  ft23f001 ft24f001 ft26f001
  touch ft23f001
  touch ft24f001
  touch ft26f001
end
#origens
0$$ a4 0 28 a9 59 a11 26 e 1t
new card-image nuclear data libraries
3$$ 28  a33 12 e
4** 0.632 0.333 2 e 2t
4t
56$$ a2 1 a5 1 0 a13 1 a15 1 a17 1 e 5t

60** 1 73$$ 922380 74** 1 75$$ 2 81$$ 15 a3 59 e 6t
making binary master photon library with uo2 bremsstrahlung
1$$ 0 1t
end
#origens
0$$ a4 0 28 a9 61 a11 24 e 1t
new card-image nuclear data libraries
3$$ 28  a33 12 e
4** 0.632 0.333 2 e 2t
4t
56$$ a2 1 a5 1 0 a13 1 a15 1 a17 1 e 5t

60** 1 73$$ 922380 74** 1 75$$ 2 81$$ 15 a3 61 e 6t
making binary master photon library with h2o bremsstrahlung
1$$ 0 1t
end
#origens
0$$ a4 0 28 a9 62 a11 23 e 1t
new card-image nuclear data libraries
3$$ 28  a33 12 e
4** 0.632 0.333 2 e 2t
 4t
56$$ a2 1 a5 1 0 a13 1 a15 1 a17 1 e 5t

60** 1 73$$ 922380 74** 1 75$$ 2 81$$ 15 a3 62 e 6t
making binary master photon library with no bremsstrahlung
1$$ 0 1t
end
#shell
   cp ft23f001 $DATA/maphnobr
   cp ft24f001 $DATA/maphh2ob
   cp ft26f001 $DATA/maphuo2b
end
```

M6.6 ENDF/B-IV FISSION-PRODUCT DATA BASE

The ORIGEN-S card-image libraries formerly included an ENDF/B-IV fission-product data base containing fission-product decay data in ENDF/B-IV card-image format.[29] These data had been processed from file (MF) 1, reaction type (MT) 457 of the ENDF/B-IV fission-product tapes.[5]

It was possible for ORIGEN-S (Sect. F7.6.10) to use this library to generate multigroup fission-product photon source spectra, or to make a card-image or binary (unformatted) photon yield library for fission products.

As of the release of SCALE 4.3, this library has been removed from the ORIGEN-S card-image libraries, since it contained old data that were rarely used. The user should note that the ORIGEN-S routines which read those data will not work for decay data in ENDF/B-V[6] or ENDF/B-VI[10] formats, since the data formats are not the same as those for ENDF/B-IV.[29]

M6.7 BINARY ORIGEN-S DATA LIBRARIES

The use of a binary data library is perhaps the most significant feature of ORIGEN-S. A binary data library is made or updated with the COUPLE code (Sect. F6). It contains, in a single library, the same kinds of data as the card-image nuclear data and photon yield libraries, but for only one reactor type. The ORIGEN-S code is normally run with one or more (time-dependent) binary data libraries for the reactor type of interest, since a binary data library has many advantages over the card-image libraries. Its principal advantage is that the cross sections in the library can be replaced by cross sections derived from a detailed multigroup neutronics (e.g., unit cell) calculation. Cross-section updating is performed by COUPLE, which reads the multigroup cross sections from an AMPX[12] weighted (working) cross-section library (Sect. F2.3.8). Automated generation of a multitime-dependent (i.e., multiburnup-dependent) binary data library can be performed with the SAS2H control module (Sect. S2) which invokes the BONAMI, NITAWL, XSDRNPM, COUPLE, and ORIGEN-S codes (Sects. F1, F2, F3, F6, and F7, respectively). Another advantage is that any portion of the photon yield data from the ORNL Master Photon Data Base can be placed in the binary data library with any energy group structure. In addition, any item of data other than ν in a binary data library can be replaced by a user-specified value by using COUPLE (Sect. F6.5.8).

The remainder of this section gives the description and formats of the two kinds of binary data libraries, as well as the input data necessary to generate some of the binary data libraries in use at ORNL.

M6.7.1 DESCRIPTION

There are two kinds of binary data libraries. A binary master library contains all the kinds of data present in the card-image nuclear data and photon yield libraries for a single reactor type. It does not contain one-group flux-weighted cross sections, so it cannot be used as an input library to run ORIGEN-S. A master library can be made by direct conversion from card-image libraries or by updating another master library using COUPLE with card-image data input by the user.

A binary working library contains all the data of a master library. In addition, it contains effective one-group flux-weighted cross sections that apply at one or more burnups so it can be used as an input library to run ORIGEN-S. It can be made by direct conversion from card-image libraries, by direct conversion from a master library, by updating either form of binary library with data input from card images, or by updating either form of binary library with cross sections from an AMPX weighted cross-section library. A multiburnup binary working library may be produced by the SAS2H control module (Sect. S2) of SCALE.

Every binary data library has a library identification number given by the variable NEWID. A master library has a value of NEWID < 950. A working library has a value of NEWID > 1000.

A binary data library is subdivided (unless deleted by special options) into three kinds of libraries: Library 1 for light elements, Library 2 for actinides, and Library 3 for fission products. The designations of Library 1, 2, or 3 are used in the discussion of different updating options in COUPLE (Sect. F6.5.8).

Additional details about the definitions, uses, and updating of binary data libraries are given in Sect. F6.5 of the COUPLE documentation.

M6.7.2 FORMATS

A master library contains 36 binary (unformatted) records; at least 40 binary records are found in a working library. A working library is identical to a master library except for the addition of at least four records containing effective one-group flux-weighted data. A working library produced by converting a card-image library contains only one set of an additional four records. However, if the library is produced during a SAS2H case, there is an additional set of four records for each burnup interval or cycle specified in the power history input to the SAS2H case.

The first records of a binary data library contain the header information described in Table M6.7.1. A summary description of the data in all the records of a binary data library is given in Table M6.7.2. Most of these data have been described in earlier sections of this report.

Table M6.7.1 Data in first record of binary data library

Variable name	Description
ITOT or ITMAX	Total number of nuclides in library
ILITE or ILMAX	Number of light-element nuclides in library
IACT or IAMAX	Number of actinide nuclides in library
IFP or IFMAX	Number of fission-product nuclides in library
NON or IZMAX	Number of nonzero off-diagonal elements in the transition matrix
NREACT	Maximum number of transitions for any single nuclide
NFISO	Number of fissionable nuclides for which fission-product yields are given
NELEM	Largest atomic number of nuclides in library
NMO	Month library was made
NDAY	Day of month library was made
NYR	Year library was made
NENAC	Number of energy groups for actinide photon yields
NENLE	Number of energy groups for light-element photon yields
NENFP	Number of energy groups for fission-product photon yields
THERM	Thermal group flux weighting factor for first burnup interval
RES	Resonance group flux weighting factor for first burnup interval
FAST	Fast-group flux weighting factor for first burnup interval
ERR	Truncation error limit below which values computed by ORIGEN-S are considered to be zero
IDREFS	ID number of nuclide in AMPX weighted cross-section library containing the weighting spectrum used to obtain the flux weighting factors THERM, RES, and FAST
NEWID	ID number of binary data library
ENERHI	Upper bound of resonance energy region (eV) for first burnup interval
ENERLO	Lower bound of resonance energy region (eV) for first burnup interval
FLXRAT	Ratio of total flux to thermal flux for first burnup interval

Table M6.7.2 Structure of binary data library

Record length[a]		Array	Description
1	23	---	Header information of Table M6.7.1
2	20*NTIT[b]	TITLE	Title cards containing descriptive information
3	NFISO	NUCFIS	ID numbers of fissionable nuclides having fission-product yields
4	3*NFISO	SIGFIS	Three-group fission cross sections for nuclides in NUCFIS array in the order ((SIGFIS(N,I), N=1,3),I=1,NFISO)
5	ITOT	NUCL	ID numbers for all nuclides in library
6	ITOT	KD[c]	KD(I) is the number of parents for production of nuclide I by decay transitions
7	ITOT	NON0[c]	NON0(I) is the total number of parents for nuclide I
8	NON	LOC[c]	LOC(J) is the position in array NUCL of the parent of the transition stored in position J of the compressed transition matrix A
9	NON	A_1[c]	Compressed transition matrix for thermal group neutron capture transitions
10	ITOT	$TOCAP_1$[c]	Thermal group total capture cross sections
11	IACT	$FISS_1$	Thermal group fission cross sections
12	ILITE+IACT	$GENNEU_1$	Thermal group neutron yields, expressed as the sum of the product of neutrons per capture reaction times the capture cross section for that reaction, summed over all neutron-producing reactions
13	NON	A_2[c]	Compressed transition matrix for resonance group neutron capture transitions
14	ITOT	$TOCAP_2$[c]	Resonance group total capture cross sections
15	IACT	$FISS_2$	Resonance group fission cross sections
16	ILITE+IACT	$GENNEU_2$	Resonance group neutron yields
17	NON	A_3[c]	Compressed transition matrix for fast group neutron capture transitions
18	ITOT	$TOCAP_3$[c]	Fast group total capture cross sections
19	IACT	$FISS_3$	Fast group fission cross sections
20	ILITE+IACT	$GENNEU_3$	Fast group neutron yields
21	NON	A_λ[c]	Compressed transition matrix for decay transitions
22	ITOT	DIS[c]	Radioactive decay constants
23[e]	NON	A[c,d]	Compressed transition matrix for effective one-group neutron capture transitions of first burnup interval and for decay transitions
24[e]	ITOT	TOCAP[c,d]	Effective one-group capture cross sections of first burnup interval
25[e]	IACT	FISS[d]	Effective one-group fission cross sections of first burnup interval
26[e]	ITOT+IACT	GENNEU[d]	Effective one-group neutron yields of first burnup interval

Table M6.7.2 (continued)

Record length[a]		Array	Description
27	ITOT	Q[f]	Recoverable energy values
28	ITOT	FG[f]	Fractions of Q-values due to photons
29	ITOT	AMPC[f]	RCG values for air
30	ITOT	WMPC[f]	RCG values for water
31	ILITE	ABUND[f]	Natural abundances of light-element nuclides
32	IACT	SPONF	Values of the product of the decay constant times the spontaneous fission branching fraction times Avagadro's number (no longer used)
33	IACT	ALPHAN	Values of the product of the decay constant times the alpha decay branching fraction times Avagadro's number times the number of neutrons per alpha decay (no longer used)
34	NENLE+1	EGROUP	Mean photon group energies (NENLE values) for light-element photon yield data, ordered from low energy to high. The last value is the lower energy bound of group 1.
35	NENAC+1	EACTGP	Mean photon group energies (NENAC values) for actinide photon yield data, ordered from low energy to high. The last value is the lower energy bound of group 1.
36	NENFP+1	EFPGRP	Mean photon group energies (NENFP values) for fission-product photon yield data, ordered from low energy to high. The last value is the lower energy bound of group 1.
37	NENAC	SFGAMA	Multigroup photon yields for gamma rays accompanying spontaneous fission, in the group structure specified by EACTGP. See Sect. M6.4 for details.
38	NENLE*ILITE	GAMGRP	Multigroup light-element photon yields, in the order ((GAMGRP(N,I),N=1,NENLE),I=1,ILITE)
39	NENFP*IFP	GFPGRP	Multigroup fission-product photon yields, in the order ((GFPGRP(N,I),N=1,NENFP),I=1,IFP)
40	NENAC*IACT	ACTGRP	Multigroup actinide photon yields, in the order ((ACTGRP(N,I),N=1,NENAC),I=1,IACT)
41[g,h]	NON	A[c,d]	Compressed transition matrix for effective one-group neutron capture transitions of the second burnup interval and for decay transitions
	6		THERM, RES, FAST, ENERHI, ENERLO, FLXRAT for second burnup interval
42[g]	ITOT	TOCAP[c,d]	Effective one-group capture cross sections of second burnup interval

Table M6.7.2 (continued)

Record length[a]		Array	Description
43[g]	IACT	FISS[d]	Effective one-group fission cross sections of second burnup interval
44[g]	ILITE+IACT	GENNEU[d]	Effective one-group neutron yields of second burnup interval.
			.
			.
			.

(This last set of four records is continued for the third, fourth, and/or higher burnup intervals or cycles of the SAS2H power history producing the library, until the last burnup interval is completed.)

[a]Length in single-precision words.
[b]NTIT is the number of title cards.
[c]These arrays are discussed in Sect. M6.2.5.
[d]Effective one-group values for the burnup interval given.
[e]Records 23 through 26 are present only in a binary working library.
[f]These variables are defined in Sect. M6.2.1.
[g]Records 41 and above are present only in a multiburnup binary working library.
[h]Libraries created with older versions of SCALE may not contain the second part of Record 41 containing the six items given in the description column. These items are added by SAS2H. Their purpose is to allow conversion of one-group cross sections from a thermal flux basis to a total flux basis. Beginning in SCALE 4.4, these items are required by ORIGEN-S and ORIGEN-ARP.

M6.7.3 LIBRARY CONVERSION PROGRAMS

Two simple utility programs are distributed with SCALE to allow transmission of ORIGEN-S binary data libraries between different computer systems.

The OSBICO (ORIGEN-S Binary Library Converter) program converts one or more binary libraries to a card-image format which is readable on any computer system. The OSBIRE (ORIGEN-S Binary Library Restorer) program restores converted libraries to a binary format.

The input data for both programs are read as list-directed input. Input descriptions are provided in Tables M6.7.3 and M6.7.4. Although unit numbers and file names of binary and card-image libraries can be specified as input, a simplified input which suffices for most users and is identical for both programs is as follows:

```
n
/
/
.
```

where line 1 contains an integer n that specifies the number of libraries to convert and is followed by twice that number of lines which have a / in column one. To convert or restore five libraries, the input is the following:

```
5
/
/
/
/
/
/
/
/
/
/
```

The maximum number of datasets which can be converted/restored with one execution of OSBICO/OSBIRE is twenty. Binary datasets are automatically allocated and incremented by one, beginning at unit number 30 (file ft30f001) and going to a maximum of unit number 49 (file ft49f001). Card-image files are automatically allocated and incremented by one beginning at unit number 50 (file ft50f001) and going to a maximum of unit number 69 (file ft69f001).

To use a binary library dataset in ORIGEN-S, it should be allocated to the file number specified by NDSET in the $3 array. Because the BWR and PWR libraries are contained in multiple-library datasets, then the position of the library within the dataset must be specified by NTYPE in the $3 array.

Table M6.7.3 Input description for OSBICO

Record[a]	Variable	Description
1	NLIB	Number of libraries to convert
2	LIBTYP	Binary library type: 0 = SCALE 4.3 or before 1 = SCALE 4.4 or later (default)
2	BIFILE	Binary library file name (default = "ft30f001")
2	UNITBI	Binary library unit number (default = 30)
3	FRMSEL	Format selector for converted ASCII library: <0 = A4 format for all data 0 = 8I10 for integer, 1P5E14.6 for real, and 20A4 for character >0 = Z8 format for all data
3	CVFILE	Converted ASCII library file name (default = "ft50f001")
3	UNITCV	Converted ASCII library unit number (default = 50)

[a]Repeat records 2 and 3 for each library up to a maximum of 20. Default unit numbers and filenames are automatically incremented by one.

Table M6.7.4 Input description for OSBIRE

Record[a]	Variable	Description
1	NLIB	Number of libraries to restore
2	BIFILE	Binary library file name (default = "ft30f001")
	UNITBI	Binary library unit number (default = 30)
3	CVFILE	Converted ASCII library file name (default = "ft50f001")
	UNITCV	Converted ASCII library unit number (default = 50)

[a]Repeat records 2 and 3 for each library up to a maximum of 20. Default unit numbers and filenames are automatically incremented by one.

M6.7.4 GENERATION OF SOME USEFUL LIBRARIES

As an aid to the beginning user, this section presents the input data for COUPLE, ORIGEN-S, and SAS2H cases to generate some binary data libraries that have been useful at ORNL.

The user may find this section helpful in understanding part of the installation of a new version of SCALE on a computer. After the SCALE system is installed, it is typically executed by using a predefined procedure (e.g., a script). Some data for SCALE, required to be in the card-image mode for portability, are more efficiently utilized after conversion to the binary mode. Indeed, SCALE cases will not execute properly unless certain required files have been made. Several cases using COUPLE, ORIGEN-S, and SAS2H, required to install SCALE, have been combined into two somewhat large cases to make the various binary libraries referenced in a SCALE procedure. The user does not need to know the details or purposes of the large cases to perform the SCALE installation. The user needs to change only items such as names of files or volumes and other installation-dependent parameters in the case's job control language or script for the case to run properly. However, the user who would like to understand the purposes of the conversion cases may wish to read this section and the input instructions of the codes. Although the examples given here may not be precisely the same as the cases used in the installation of SCALE, the purposes of the cases are the same.

The first example contains back-to-back runs of COUPLE, ORIGEN-S, and SAS2H. The first COUPLE case converts the data in the card-image library to a binary working library for an LWR. The flux weighting factors used are THERM=0.632, RES=0.333, and FAST=2.0. The card-image cross-section data and photon-yield libraries are read from unit 28, and the decay data file is read from unit 27. The binary working library generated by this case is written on unit 42. The second COUPLE case generates an edit of the cross-section transitions in the binary working library on unit 42.

The ORIGEN-S case replaces the photon yield data in the binary working library with 18-group photon yields for the light elements, actinides, and fission products. The 18-group energy boundaries are those of Table M6.3.2. The photon yield data are read from a binary master photon data base on unit 26 which includes decay gamma and X rays, gamma rays accompanying spontaneous fission and (α,n) reactions, and bremsstrahlung for a UO_2 fuel matrix. The input binary working library from COUPLE is read from unit 42. The final binary working library is written by ORIGEN-S on unit 21. Details of the input data given below can be determined by studying Sect. F6.5.8 of the COUPLE document and Sect. F7.6.10 of the ORIGEN-S document.

The SAS2H case in this example is commonly known as a "preSAS" case. The purpose of a preSAS case is to make the Preliminary LWR ORIGEN-S Binary Working Library to be input to subsequent SAS2H cases for LWR fuel assembly depletion analyses. The case updates all of the (more than 200) nuclides having cross-section data on the SCALE 44-group ENDF/B-V library, using the input design data for a typical modern PWR. Most SAS2H cases update only a fraction of the nuclides having data available in the SCALE depletion library. Thus, the remaining nuclides, updated on the preliminary library, will have data that are substantially improved over that on the initial card-image nuclear data libraries.

The SAS2H case in this example generates a single-burnup-interval binary working library at the mid-time of an 800-day cycle for a 466.3-kgU, 17 × 17 pin assembly. The total burnup is 31.69 GWd/MTU, and the initial ^{235}U enrichment of the fuel is 3.0 wt %. Densities, temperatures, design dimensions, and standard composition specifications for the nuclides to be updated are shown in the input for the case given below:

```
#shell
  rm ft21f001 ft33f001 ft71f001
  touch ft21f001
  touch ft33f001
  touch ft71f001
end
#couple
*********************************************************************************
*                                                                               *
*            prelim lwr origen-s binary working library--id = 1143              *
*                   made from card-image origen-s libraries                     *
*      data from the light element, actinide, and fission product libraries     *
*        decay data, including gamma and total energy, are from endf/b-vi       *
*                                                                               *
*      neutron flux spectrum factors and cross sections were produced from      *
*     the "presas2" case updating all nuclides on the scale "burnup" library    *
*                                                                               *
*                  fission product yields are from endf/b-v                     *
*                                                                               *
*              photon libraries use an 18-energy-group structure                *
*             the photon data are from the master photon data base,             *
*              produced to include bremsstrahlung from uo2 matrix               *
*                                                                               *
*        see information above this box (if present) for later updates          *
*                                                                               *
*********************************************************************************

0$$ a2 28 a6 42 e
1$$ 2r1 a11 1142 e 2** a2 0.632 0.333 2.0 e 1t
3$$ 28 e 5$$ 2 3t
35$$ 0 5t
edit

0$$ a4 42 e
1$$ a2 1 a5 1 a13 -1 e 1t
done
end
#origens
0$$ a4 42 a8 26 a11 21 e 1t

3$$ 42 a3 1 a6 1 a33 18 2t
4t
56$$ a2 1 a5 2z a13 1 a17 1 e 5t
60** 1 73$$ 922380 74** 1 75$$ 2 81$$ 11 a3 26 1 e 82$$ 21
83** 6+6 5+6 4.5+6 4+6 3.5+6 3+6 2.6+6 2.2+6 1.8+6 1.35+6 9+5
     4+5 2+5 1.4+5 1+5 7+4 4+4 2+4 0 6t
*                                                                               *
1$$ 0 1t
end
```

```
#sas2     parm='halt01,skipshipdata,size=300000'
presas2 case: typical pwr 17x17 plant, 31.69 gwd/mtu, 466.3 kgu/assmb.
'
' - - - - - - (june 1, 1993)- - - - - - - - - - - by o. w. hermann
'
'   mixtures of fuel-pin-unit-cell:
'
44group    latticecell
uo2  1 0.9485 901 92234 0.025 92235 3.0 92236 0.014 92238 96.961  end
  d       1 0 1-20 901  end  h-3      1 0 1-20 901  end
  he      1 0 1-20 901  end
  li-6    1 0 1-20 901  end
  li-7    1 0 1-20 901  end  si       1 0 1-20 901  end
  be      1 0 1-20 901  end  cl       1 0 1-20 901  end
  c       1 0 1-20 901  end  k        1 0 1-20 901  end
  n       1 0 1-20 901  end  ca       1 0 1-20 901  end
  f       1 0 1-20 901  end  ti       1 0 1-20 901  end
  na      1 0 1-20 901  end  mg       1 0 1-20 901  end
  ge-72   1 0 1-20 901  end      sb-124  1 0 1-20 901  end
  ge-73   1 0 1-20 901  end      sb-125  1 0 1-20 901  end
  ge-74   1 0 1-20 901  end      sb-126  1 0 1-20 901  end
                                 te-120  1 0 1-20 901  end
  ge-76   1 0 1-20 901  end      te-122  1 0 1-20 901  end
  as-75   1 0 1-20 901  end      te-123  1 0 1-20 901  end
  se-76   1 0 1-20 901  end      te-124  1 0 1-20 901  end
  se-77   1 0 1-20 901  end      te-125  1 0 1-20 901  end
  se-78   1 0 1-20 901  end      te-126  1 0 1-20 901  end
  se-80   1 0 1-20 901  end      te-127m 1 0 1-20 901  end
  se-82   1 0 1-20 901  end      te-128  1 0 1-20 901  end
  br-79   1 0 1-20 901  end      te-129m 1 0 1-20 901  end
  br-81   1 0 1-20 901  end      te-130  1 0 1-20 901  end
  kr-80   1 0 1-20 901  end      te-132  1 0 1-20 901  end
  kr-82   1 0 1-20 901  end       i-127  1 0 1-20 901  end
  kr-83   1 0 1-20 901  end       i-129  1 0 1-20 901  end
  kr-84   1 0 1-20 901  end       i-130  1 0 1-20 901  end
  kr-85   1 0 1-20 901  end       i-131  1 0 1-20 901  end
  kr-86   1 0 1-20 901  end       i-135  1 0 1-20 901  end
  xe-124  1 0 1-20 901  end      xe-126  1 0 1-20 901  end
  rb-85   1 0 1-20 901  end      xe-128  1 0 1-20 901  end
  rb-86   1 0 1-20 901  end      xe-129  1 0 1-20 901  end
  rb-87   1 0 1-20 901  end      xe-130  1 0 1-20 901  end
  sr-84   1 0 1-20 901  end      xe-131  1 0 1-20 901  end
  sr-86   1 0 1-20 901  end      xe-132  1 0 1-20 901  end
  sr-87   1 0 1-20 901  end      xe-133  1 0 1-20 901  end
  sr-88   1 0 1-20 901  end      xe-134  1 0 1-20 901  end
  sr-89   1 0 1-20 901  end      xe-135  1 0 1-20 901  end
  sr-90   1 0 1-20 901  end      xe-136  1 0 1-20 901  end
   y-89   1 0 1-20 901  end      cs-134  1 0 1-20 901  end
   y-90   1 0 1-20 901  end      cs-135  1 0 1-20 901  end
   y-91   1 0 1-20 901  end      cs-136  1 0 1-20 901  end
  zr-90   1 0 1-20 901  end      cs-137  1 0 1-20 901  end
  zr-91   1 0 1-20 901  end      ba-134  1 0 1-20 901  end
  zr-92   1 0 1-20 901  end      ba-135  1 0 1-20 901  end
  zr-93   1 0 1-20 901  end      ba-136  1 0 1-20 901  end
  zr-94   1 0 1-20 901  end      ba-137  1 0 1-20 901  end
  zr-95   1 0 1-20 901  end      ba-138  1 0 1-20 901  end
  zr-96   1 0 1-20 901  end      ba-140  1 0 1-20 901  end
  nb-93   1 0 1-20 901  end      la-139  1 0 1-20 901  end
  nb-94   1 0 1-20 901  end      la-140  1 0 1-20 901  end
  nb-95   1 0 1-20 901  end      ce-140  1 0 1-20 901  end
  mo-92   1 0 1-20 901  end
  mo-94   1 0 1-20 901  end      ce-141  1 0 1-20 901  end
  mo-95   1 0 1-20 901  end      ce-142  1 0 1-20 901  end
  mo-96   1 0 1-20 901  end      ce-143  1 0 1-20 901  end
  mo-97   1 0 1-20 901  end      ce-144  1 0 1-20 901  end
  mo-98   1 0 1-20 901  end      pr-141  1 0 1-20 901  end
```

```
  mo-99    1 0 1-20 901  end      pr-142   1 0 1-20 901  end
  mo-100   1 0 1-20 901  end      pr-143   1 0 1-20 901  end
  tc-99    1 0 1-20 901  end      nd-142   1 0 1-20 901  end
  ru-96    1 0 1-20 901  end      ru-98    1 0 1-20 901  end
  ru-99    1 0 1-20 901  end      nd-143   1 0 1-20 901  end
  ru-100   1 0 1-20 901  end      nd-144   1 0 1-20 901  end
  ru-101   1 0 1-20 901  end      nd-145   1 0 1-20 901  end
  ru-102   1 0 1-20 901  end      nd-146   1 0 1-20 901  end
  ru-103   1 0 1-20 901  end      nd-147   1 0 1-20 901  end
  ru-104   1 0 1-20 901  end      nd-148   1 0 1-20 901  end
  ru-105   1 0 1-20 901  end      nd-150   1 0 1-20 901  end
  ru-106   1 0 1-20 901  end      pm-147   1 0 1-20 901  end
  rh-103   1 0 1-20 901  end      pm-148   1 0 1-20 901  end
  rh-105   1 0 1-20 901  end      pm-149   1 0 1-20 901  end
  pd-102   1 0 1-20 901  end      pm-151   1 0 1-20 901  end
  pd-104   1 0 1-20 901  end      sm-144   1 0 1-20 901  end
  pd-105   1 0 1-20 901  end      sm-147   1 0 1-20 901  end
  pd-106   1 0 1-20 901  end      sm-148   1 0 1-20 901  end
  pd-107   1 0 1-20 901  end      sm-149   1 0 1-20 901  end
  pd-108   1 0 1-20 901  end      sm-150   1 0 1-20 901  end
  pd-110   1 0 1-20 901  end      sm-151   1 0 1-20 901  end
  ag-107   1 0 1-20 901  end      sm-152   1 0 1-20 901  end
  ag-109   1 0 1-20 901  end      sm-153   1 0 1-20 901  end
  ag-111   1 0 1-20 901  end      sm-154   1 0 1-20 901  end
  cd-106   1 0 1-20 901  end      eu-151   1 0 1-20 901  end
  cd-108   1 0 1-20 901  end      eu-152   1 0 1-20 901  end
  cd-110   1 0 1-20 901  end      eu-153   1 0 1-20 901  end
  cd-111   1 0 1-20 901  end      eu-154   1 0 1-20 901  end
  cd-112   1 0 1-20 901  end      eu-155   1 0 1-20 901  end
  cd-113   1 0 1-20 901  end      eu-156   1 0 1-20 901  end
  cd-114   1 0 1-20 901  end      eu-157   1 0 1-20 901  end
  cd-115m  1 0 1-20 901  end      gd-152   1 0 1-20 901  end
  cd-116   1 0 1-20 901  end      gd-154   1 0 1-20 901  end
  in-113   1 0 1-20 901  end      gd-155   1 0 1-20 901  end
  in-115   1 0 1-20 901  end      gd-156   1 0 1-20 901  end
  sn-112   1 0 1-20 901  end      sn-114   1 0 1-20 901  end
  sn-115   1 0 1-20 901  end      gd-157   1 0 1-20 901  end
  sn-116   1 0 1-20 901  end      gd-158   1 0 1-20 901  end
  sn-117   1 0 1-20 901  end      gd-160   1 0 1-20 901  end
  sn-118   1 0 1-20 901  end      tb-159   1 0 1-20 901  end
  sn-119   1 0 1-20 901  end      tb-160   1 0 1-20 901  end
  sn-120   1 0 1-20 901  end      dy-160   1 0 1-20 901  end
  sn-122   1 0 1-20 901  end      dy-161   1 0 1-20 901  end
  sn-123   1 0 1-20 901  end      dy-162   1 0 1-20 901  end
  sn-124   1 0 1-20 901  end      dy-163   1 0 1-20 901  end
  sn-125   1 0 1-20 901  end      dy-164   1 0 1-20 901  end
  sn-126   1 0 1-20 901  end      ho-165   1 0 1-20 901  end
  sb-121   1 0 1-20 901  end      er-166   1 0 1-20 901  end
  sb-123   1 0 1-20 901  end      er-167   1 0 1-20 901  end
  lu-175   1 0 1-20 901  end      re-185   1 0 1-20 901  end
  lu-176   1 0 1-20 901  end      re-187   1 0 1-20 901  end
  ta-181   1 0 1-20 901  end      au       1 0 1-20 901  end
   w-182   1 0 1-20 901  end      th-232   1 0 1-20 901  end
   w-183   1 0 1-20 901  end      pa-231   1 0 1-20 901  end
   w-184   1 0 1-20 901  end      pa-233   1 0 1-20 901  end
   w-186   1 0 1-20 901  end       u-233   1 0 1-20 901  end
  th-230   1 0 1-20 901  end       u-232   1 0 1-20 901  end
zirc2   2 1   628    end
h2o   3 den=0.7149   1   579 end
  al       3 0 1-20 579  end
  p        3 0 1-20 579  end
  mn       3 0 1-20 579  end
  co-59    3 0 1-20 579  end
  pb       3 0 1-20 579  end
  bi-209   3 0 1-20 579  end
arbm-bormod   0.7149 1 1 0 0 5000 100 3 600.0e-6   579   end
```

```
'
'    600 pm(wt) boron
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
end comp
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'      fuel-pin-cell geometry:
'
squarepitch   1.25984 0.81915 1 3 0.94966 2 0.83566 0  end
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
more data   szf=0.6  end
'
'    assembly and cycle parameters:
'
npin/assm=264 fuelnght=365.76 ncycles=1  nlib/cyc=1
printlevel=4 lightel=9  inplevel=1 ortube=0.61214 srtube=0.5715
numinstr=1  facmesh=0.65   end
power=18.4715  burn=800  down=1826.25   end
  o  63  cr  2.8  mn  0.15
  fe 6.0 co 0.035 ni  4.6
  zr 103 nb  0.33 sn  1.7
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
end
=shell
   cp ft33f001 $RTNDIR/prlimlwr
end
```

The second example is a SAS2H run to generate a three-burnup-interval binary working library for a "typical" PWR fuel assembly with a burnup of 33 GWd/MTU and the initial uranium composition of Table M6.7.5. The irradiation history is divided into three cycles having 80% full power irradiation at 37.5 MW/MTU and 20% downtime. Updated cross sections are computed from a 44-group unit cell calculation, at the midpoint of each irradiation cycle, for the nuclides given in Table M6.7.6. The resonance cross-section processing and unit cell calculations are performed for the geometry and operating conditions of a 17 × 17 PWR fuel assembly. The cross sections used in the calculations are read from the SCALE 44-group ENDF/B-V library (Sect. M4). The input binary library is the Preliminary LWR ORIGEN-S Binary Working Library generated in the example outlined above, which is read on unit 21. The burnup-dependent binary working libraries for cycles 1, 2, and 3 are written on unit 33. None of these libraries can be used with the integral option. Details of the SAS2H method and input data requirements can be found in Sects. S2.2 and S2.5, respectively, of the SAS2H documentation.

Table M6.7.5 Initial uranium composition of typical PWR assembly

Nuclide	Weight percent
^{234}U	0.028
^{235}U	3.200
^{236}U	0.015
^{238}U	96.757

Table M6.7.6 Nuclides with updated cross sections in typical PWR and BWR libraries

^{1}H	^{105}Rh	^{143}Nd	^{235}U
^{10}B	^{106}Ru	^{144}Ce	^{236}U
^{11}B	^{124}Sb	^{145}Nd	^{238}U
^{16}O	^{131}Xe	^{147}Nd	^{237}Np
^{59}Co	^{132}Xe	^{147}Pm	^{238}Pu
^{85}Kr	^{135}Xe	^{147}Sm	^{239}Pu
^{90}Sr	^{136}Xe	^{149}Sm	^{240}Pu
^{89}Y	^{133}Cs	^{151}Sm	^{241}Pu
^{94}Zr	^{134}Cs	^{152}Sm	^{242}Pu
^{95}Zr	^{137}Cs	^{153}Eu	^{241}Am
^{94}Nb	^{136}Ba	^{154}Eu	^{243}Am
^{99}Tc	^{139}La	^{155}Eu	^{244}Cm
^{103}Rh	^{143}Pr	^{234}U	

The input data for this SAS2H case are given below.

```
#shell
  rm ft33f001 ft71f001
  touch ft33f001
  touch ft71f001
end
#sas2h    parm='halt03,skipshipdata'
pwr typical irradiation history - 3.2% enrich - 33 gwd/mtu
44group  latticecell
uo2  1  0.90180  811 92234 0.028 92235 3.2 92236 0.015 92238 96.757 end
kr-85   1  0  1-20  811   end
sr-90   1  0  1-20  811   end
y-89    1  0  1-20  811   end
zr-94   1  0  1-20  811   end
zr-95   1  0  1-20  811   end
nb-94   1  0  1-20  811   end
tc-99   1  0  1-20  811   end
rh-103  1  0  1-20  811   end
rh-105  1  0  1-20  811   end
ru-106  1  0  1-20  811   end
sb-124  1  0  1-20  811   end
xe-131  1  0  1-20  811   end
xe-132  1  0  1-20  811   end
xe-135  1  0  8.72-9  811   end
xe-136  1  0  1-20  811   end
cs-134  1  0  1-20  811   end
cs-137  1  0  1-20  811   end
ba-136  1  0  1-20  811   end
la-139  1  0  1-20  811   end
pr-143  1  0  1-20  811   end
nd-143  1  0  1-20  811   end
ce-144  1  0  1-20  811   end
nd-145  1  0  1-20  811   end
pm-147  1  0  1-20  811   end
nd-147  1  0  1-20  811   end
sm-147  1  0  1-20  811   end
sm-149  1  0  1-20  811   end
sm-151  1  0  1-20  811   end
sm-152  1  0  1-20  811   end
```

```
eu-153   1   0   1-20   811    end
eu-154   1   0   1-20   811    end
eu-155   1   0   1-20   811    end
zirc2    2   1          620   end
b-10     3  0 4.190-6  570   end
b-11     3  0 1.824-5  570   end
h2o      3  0.73411    570   end
co-59    3   0   1-20   570   end
end comp
squarepitch    1.25984 0.83566 1 3 0.94996 2 end
more data  szf=0.7       end
npin/assm=264  fuelngth=365.76 ncycles=3  nlib/cyc=1
printlevel=5
lightel=16
inplevel=1
numins=1 ortube=0.61214 srtube=0.57150 end
power=17.3025  burn=293.3333  down=73.33333  end
power=17.3025  burn=293.3333  down=73.33333  end
power=17.3025  burn=293.3333  down=1826.25   end
c  0.059994  n  0.033766  o  62.136  al  0.045689
si  0.065864  p  0.14216  ti  0.049833  cr  2.3398
mn  0.10963  fe  4.5992  co  0.033444  ni  4.4022
zr  100.84  nb  0.32754  mo  0.18156  sn  1.6519
end
#shell
   cp ft33f001 $DATA/pwr33gwd
   cp ft71f001 $DATA/pwr33f71.sas1inp
end
```

M6.8 ORIGEN-S LIBRARIES AT ORNL

This section gives a summary description of the card-image and binary ORIGEN-S libraries available on ORNL computing systems. Complete descriptions of most of these libraries were given in earlier sections of this report.

All libraries are maintained as separate data files on workstations and PCs. Names and descriptions of card-image libraries are given in Table M6.8.1; those for binary libraries are given in Table M6.8.2.

Table M6.8.1 Card-image ORIGEN-S libraries at ORNL

Library name[a]	Description
END6DEC	Decay data for the light elements, actinides, and fission products
MPBRH2OM	Master photon data for bremsstrahlung from negatrons slowing down in water
MPBRH2OP	Master photon data for bremsstrahlung from positrons slowing down in water
MPBRUO2M	Master photon data for bremsstrahlung from negatrons slowing down in UO_2
MPBRUO2P	Master photon data for bremsstrahlung from positrons slowing down in UO_2
MPDKXGAM	Master photon decay X- and gamma-ray line data
MPSFANGM	Master photon gamma ray spectra from spontaneous fission and (α,n) reactions
XSECTPHO	Nuclear data libraries and photon-yield libraries for the light elements, actinides, and fission products

[a] Filename on a workstation or PC.

Table M6.8.2 Some binary ORIGEN-S libraries at ORNL

Library name[a]	Description
PRLIMLWR	Preliminary LWR ORIGEN-S Binary Working Library described in Sect. M6.7.4. It has (β,n) decay data for fission products, so it cannot be used with the integral option.
BASLMFBR	Basic LMFBR ORIGEN-S Binary Working Library. This library was converted from the large light-element, actinide, and large fission-product card-image nuclear data libraries. It has the same (β,n) decay data and photon yield data as the Basic LWR Binary Working Library. It cannot be used with the integral option.
MAPHH2OB	Binary Master Photon Library with the photon data from members MPDKXGAM, MPSFANGM, MPBRH2OM, and MPBRH2OP of the card-image library
MAPHNOBR	Binary Master Photon Library with the photon data from members MPDKXGAM and MPSFANGM of the card-image library
MAPHUO2B	Binary Master Photon Library with the photon data from members MPDKXGAM, MPSFANGM, MPBRUO2M, and MPBRUO2P of the card-image library
PWR33GWD	Multi-burnup binary working library produced from the typical PWR 33-GWd/MTU SAS2H case described in Sect. M6.7.4

[a] Filename on a workstation or PC.

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THE MATERIAL INFORMATION PROCESSOR FOR SCALE

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ABSTRACT

The Material Information Processor was developed to utilize free-form input data consisting of easily visualized engineering parameters to derive and prepare input data for many of the functional modules used in SCALE. The processor creates an AMPX master format cross-section library that contains only those nuclides utilized in the problem. This library can then be used to create a problem-dependent cross-section library in the AMPX working format for use by SCALE modules.

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ACKNOWLEDGMENTS

The concept of a Material Information Processor using alphanumeric material specifications was initially proposed and developed by R. M. Westfall. J. R. Knight and J. A. Bucholz expanded and refined the Material Information Processor. J. R. Knight developed the Standard Composition Library and many of the associated data-processing routines. He also developed routines to calculate the Dancoff factor and other resonance parameters needed by the Material Information Processor. J. A. Bucholz implemented the Material Information Processor in CSAS1 and CSAS2. This work forms the basis of the current version of the Material Information Processor.

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M7.1 INTRODUCTION

The Material Information Processor was developed to utilize standardized engineering-type input data and standardized procedures to provide data to create problem-dependent cross-section libraries for use by the SCALE functional modules. Information provided by the Standard Compositions Library is used by the Material Information Processor to calculate the number densities (atoms/b-cm) of each material specified in the problem, to develop data used by the resonance processors, and to utilize the automatic mesh-generator to calculate the mesh intervals used in the cell-weighting calculation.

M7.2 TECHNIQUES

M7.2.1 MATERIAL INFORMATION PROCESSOR FEATURES

The Material Information Processor reads and checks a unified set of engineering-type data and performs the calculations that are necessary to create binary input data files for use by the codes BONAMI, NITAWL, and, optionally, XSDRNPM and/or ICE to provide a problem-dependent cross-section library. If the control sequence that activates the Material Information Processor activates XSDRNPM, the eigenvalue for the designated problem is calculated. The control sequences that utilize the Material Information Processor and the codes they activate are listed in Table M7.2.1. The engineering-type data read by the Material Information Processor include (1) the standard composition data (a standardized alphanumeric name, mixture number, and other data to define materials, including volume fraction or percent theoretical density, temperature, and isotopic distribution) which is used in the standardized number density calculations, and (2) unit cell description defining the materials, dimensions, and boundary conditions of the geometry that will be used in the Dancoff factor calculations, the resonance self-shielding calculations, and the flux-weighting cell calculations used in cross-section processing.

Table M7.2.1 Control sequences and their associated functional modules

Control sequence	Cross-section processing codes				Criticality, shielding, and burnup/decay codes		
CSASI	BONAMI-S	NITAWL-II[a]		ICE-S			
CSASIX	BONAMI-S	NITAWL-II	XSDRNPM-S	ICE-S			
CSASN	BONAMI-S	NITAWL-II					
CSAS1X	BONAMI-S	NITAWL-II	XSDRNPM-S				
CSAS25	BONAMI-S	NITAWL-II			KENO V.a		
CSAS2X	BONAMI-S	NITAWL-II	XSDRNPM-S		KENO V.a		
CSAS4	BONAMI-S	NITAWL-II			KENO V.a	MODIFY[b]	
CSAS4X	BONAMI-S	NITAWL-II	XSDRNPM-S		KENO V.a	MODIFY[b]	
SAS1	BONAMI-S	NITAWL-II			XSDRNPM-S	XSDOSE	
SAS1X	BONAMI-S	NITAWL-II	XSDRNPM-S		XSDRNPM-S	XSDOSE	
SAS2	BONAMI-S	NITAWL-II	XSDRNPM-S		COUPLE	ORIGEN-S	XSDRNPM-S
SAS3	BONAMI-S	NITAWL-II		ICE-S	MORSE-SGC/S	XSDOSE	
SAS3X	BONAMI-S	NITAWL-II	XSDRNPM-S	ICE-S	MORSE-SGC/S		
SAS4	BONAMI-S	NITAWL-II	XSDRNPM-S		MORSE-SGC/S		

[a]Although the text of this section (M7) refers only to NITAWL, the version available beginning with the SCALE-4 release is NITAWL-II.

[b]MODIFY is a control module.

M7.2.2 APPLICABILITY OF THE MATERIAL INFORMATION PROCESSOR

The Material Information Processor is primarily used to prepare data for creating the problem-dependent cross-section libraries required by the criticality safety and/or shielding sequences listed in Table M7.2.1. The Material Information Processor creates the binary input files for the cross-section processing codes. It provides only a limited set of code options to these codes; thus, the options that are exercised are considerably more limited than when the codes are executed in a "stand-alone" mode. These problem-dependent cross-section libraries can be used with any code that requires (1) a microscopic or macroscopic AMPX working format library or (2) a Monte Carlo formatted macroscopic cross-section library in the MORSE/KENO format. The Material Information Processor is particularly applicable for large homogeneous systems and large regular lattices of slabs, pins, or spheres. In the case of large regular lattices, it can prepare data that allow the cross-section processing codes to create a homogenized cell-weighted cross section, denoted as mixture 500, that is capable of representing a heterogeneous array of cells as a homogeneous mixture. This capability allows the three-dimensional (3-D) heterogeneous system to be modeled as a single region composed of mixture 500, the homogenized cell-weighted mixture. The Material Information Processor can create data for only one cell-weighted mixture per problem. Other limitations are discussed in this section.

M7.2.3 NUMBER DENSITY CRITERIA OF THE MATERIAL INFORMATION PROCESSOR

A primary function of the Material Information Processor is to calculate the "number density" (atoms/b-cm) of every nuclide in each mixture defined in the problem. Known limitations in this process are listed below:

1. The available nuclides are limited to those nuclides that are included in the Standard Composition Library, and then only to those available in the specified cross-section library with the correct nuclide identifier (ID). Section M8.2 lists the available nuclides. A new Standard Composition Library containing additional nuclides can be created by using COMPOZ. See Sect. M14 for additional information.

2. Temperature data are not available for any of the solution standard compositions except uranyl nitrate (SOLNUO2(NO3)2). Data for all other solutions are given at room temperature. Note that if the specific gravity of the solution is known at a temperature other than room temperature, and it is entered in the standard composition specification using SPG=, the temperature effect is accounted for in the calculated number densities. The temperature should still be entered in the standard composition data so it can be used in the resonance calculations for the individual nuclides. A solution standard composition is one whose standard composition name begins with SOLN. The available solutions are listed in Table M8.3.1 of the standard composition section of the SCALE document.

3. Mixed-oxide (MOX) solutions are particularly difficult to describe in a manner that will provide correct number densities. It is possible to obtain correct number densities if the specific gravity and molarity of the mixed solution are known and the mixture is described using a SOLN standard composition name for both solutions. The volume fractions of the two SOLN standard composition specifications must sum to 1.000. The volume fraction of the uranium solution must be entered as the weight fraction of the

fuel density that is uranium, and the volume fraction of the plutonium solution must be entered as the weight fraction of the fuel density that is plutonium. See Sect. M7.5.5.6, example 1, for a MOX solution specification.

M7.2.4 GEOMETRICAL CRITERIA OF THE MATERIAL INFORMATION PROCESSOR

The Material Information Processor offers three types of calculations: INFHOMMEDIU, LATTICECELL, and MULTIREGION. The method of specifying the desired calculation type is described in Sects. M7.4.3 and M7.5.4.

The Material Information Processor utilizes a unit cell description to provide information for the resonance self-shielding corrections and the Dancoff corrections that are applied to the cross sections to create a problem-dependent cross-section library.

M7.2.4.1 INFHOMMEDIUM (Infinite Homogeneous Medium) Treatment

The INFHOMMEDIUM treatment is best suited for large masses of materials where the size of each material is large compared with the average mean-free path of the material or where the fraction of the material that is a mean-free path from the surface of the material is very small. When the infinite homogeneous medium treatment is specified, every material specified in the problem is treated as an infinite lump. Systems composed of small fuel lumps should not be treated as an infinite homogeneous medium.

M7.2.4.2 LATTICECELL Treatment

The LATTICECELL treatment is appropriate for large arrays of slabs, fuel pins, or spherical pellets. Examples showing the use of the LATTICECELL treatment are given in Sect. M7.5.6.2. The input data are described in Sect. M7.4.6. When the LATTICECELL treatment is used, the mixtures specified in the cell have resonance self-shielding with Dancoff corrections applied to the cross sections of the nuclides utilized in the cell. All other mixtures and their nuclides are treated as INFHOMMEDIUM unless the appropriate resonance and Dancoff data are explicitly entered in the optional parameter data as described in Sects. M7.4.8, M7.5.7, and M7.5.10. Limitations of the LATTICECELL treatment are listed below:

1. The cell description is limited to a one-dimensional (1-D) cell. Most physical systems consist of 3-D geometry, but in many instances a 1-D representation is adequate, as in the case of a large array of spheres in a regular lattice, a large array of slabs, or a large array of long uniform pins in a regular lattice. A 1-D representation is inadequate for systems that exhibit a two-dimensional (2-D) or 3-D spatial dependence.

2. Only one cell description is allowed in a problem. This limitation can be circumvented by entering the appropriate data in the optional parameter data. See Sects. M7.4.8 and M7.5.10 for details.

3. The LATTICECELL treatment assumes an infinite array of 1-D cells. This assumption is an excellent approximation for large arrays of long fuel pins or large arrays of spherical pellets. The approximation becomes less rigorous for short fuel pins and/or small arrays where multidimensional spatial dependence can become important.

4. The choices of cell configurations are strictly limited. The available options are described in detail in Sect. M7.4.6 and are summarized below:

   a. The first option is an infinite planar array of pin cells or an infinite array of spherical pellets. Cylindrical pins or spherical pellets consist of fuel, gap, clad, and moderator where the gap and clad are optional. The configuration of the cell requires that the innermost region must be the fuel, with subsequent regions being the gap, clad, and moderator in that order. The moderator fills the volume between the pins or pellets and the outer boundaries of the cell. The gap is the only component of the unit cell that can be a void, specified as mixture 0.

   b. The second option is an infinite planar array of annular pin cells or an infinite array of annular spherical pellets. The annular cylindrical pins or annular spherical pellets have an annular fuel region with an optional gap and/or optional clad on both sides of the fuel. The second moderator is defined to be the innermost region, and the first moderator is present outside the other regions and inside the outer boundaries of the cell. The thickness and material of the gap are required to be the same on both sides of the fuel, as are the thickness and material of the clad. The moderator materials and the thicknesses of the two moderators need not be the same.

   c. The third option is an infinite symmetric array of slabs, called a symmetrical slab cell. The configuration of a symmetric slab cell requires the fuel region to be the innermost region with an optional gap and/or optional clad outside the fuel region followed by a moderator region. The cell is defined to extend from the centerline of the fuel region to the center of the moderator region.

   d. The fourth option is an infinite asymmetric array of slabs, called an asymmetrical slab cell. The configuration of an asymmetric slab cell requires the fuel region to be the innermost region with an optional gap and/or optional clad outside the fuel region. A moderator region exists on each side of the fuel/gap/clad region. The moderator materials and the thickness of the two moderators need not be the same. The cell is defined to extend from the centerline of one moderator region to the centerline of the second moderator region.

M7.2.4.3 MULTIREGION Treatment

The MULTIREGION treatment is appropriate for 1-D geometric regions where the geometry effects may be important, but the infinite homogeneous media treatment or LATTICECELL treatment are inappropriate. The MULTIREGION unit cell allows more flexibility in the placement of the fuel, but requires all regions of the cell to have the same geometric shape (i.e., slab, cylinder, sphere, buckled slab, or buckled cylinder). See Sects. M7.4.7 and M7.5.6.3 for more details. Limitations of the MULTIREGION cell treatment are listed below:

1. A MULTIREGION cell is limited to a 1-D approximation of the system being represented. This constraint is appropriate for a sphere, an infinitely long cylinder, a slab, or an infinite array of slabs.

2. The shape of the outer boundary of the MULTIREGION cell is the same as the shape of the inner regions. Cells with curved outer surfaces cannot be stacked to represent arrays.

3. The boundary conditions available in a MULTIREGION problem include vacuum (eliminated at the boundary), reflected (reflected about the normal to the surface at the point of impact), periodic (a particle exiting the surface effectively enters an identical cell having the same orientation and continues traveling in the same direction), and white (isotropic return about the point of impact). Reflected and periodic boundary conditions on a slab can represent a real physical situation, but are not valid on a curved outer surface.

4. A MULTIREGION cell represents a single cell if the outer boundary has a vacuum boundary condition applied to it. The cross-section treatment then uses an interlump Dancoff factor of zero in the geometric correction calculations.

5. If the outer boundary of a MULTIREGION cell has a boundary condition other than vacuum, the interlump Dancoff correction is approximated by homogenizing the adjacent zones and computing the transmission through the homogenized material. This value is correct for a slab having a reflected or periodic boundary condition, but is inexact for a curved surface.

6. The intralump Dancoff factor is determined using homogenized interior zones.

M7.2.5 APPLICABILITY OF PROBLEM-DEPENDENT CROSS-SECTION PREPARATION

Cross-section processing is briefly discussed here because the Material Information Processor is indirectly involved in cross-section processing by virtue of providing binary input data files to the cross-section processing codes. The problem-dependent AMPX working format cross-section library is created by executing BONAMI and NITAWL and, optionally, ICE and/or XSDRNPM.

The cross-section processing in SCALE utilizes the Bondarenko (or shielding factor) method[1] and the Nordheim Integral Treatment.[2] With the exception of the 16-group Hansen-Roach library, SCALE uses BONAMI primarily to shield unresolved resonances, while NITAWL is used for the resolved resonances. The assumptions and limitations shared by these methods include:

1. The simple two-zone model used in the formulation is not valid where strong 2-D effects occur [boiling-water reactor (BWR) fuel assemblies] or where double levels of heterogeneity exist (fuel grains in some gas reactor fuels).

2. The assumption of a spatially flat flux may not be good, especially at the peak of a large resonance.

3. Thermal upscatter into the resonance range cannot be accounted for. This may be important for the 0.3-eV resonance in ^{239}Pu and/or the 1.0-eV resonance in ^{240}Pu. For example, at 550 K, hydrogen may supply the 0.3-eV ^{239}Pu resonance with approximately 40% as many neutrons via upscatter as via downscatter. Incoherent scattering with hydrogen may scatter neutrons up as high as 2.0 eV. Upscatter effects are also important when the moderating nuclide is bound in a crystalline lattice such as graphite or beryllium.

M7.2.5.1 Applicability of the Bondarenko Method

The Bondarenko method is basically an "infinite medium" method that parameterizes cross sections for a nuclide as a function of temperature, T, and σ_0, the "background" cross section of all the other nuclides mixed with the nuclide. Section F1.2 contains a more-detailed discussion of this method. Simplistically, if the temperature and cross-section values are known, the self-shielded cross sections are determined by interpolating the tabulated parameterized data. Because self-shielding causes changes in the background cross sections that apply to a nuclide, an iterative procedure is used for each nuclide in the problem.

To account for geometric effects, the σ_0 value is augmented by an escape cross section, σ_e. This escape cross-section value is a function of the geometry and the total cross-section value in the medium. Many implementations of this approach use either the Wigner rational approximation ($\sigma_e = 1/\ell N_i$), or a modified form. BONAMI uses "exact" values of escape probabilities for the three simple geometries (slabs, cylinders, and spheres) as developed by Case, de Hoffman, and Placzek.[3] These "exact" values are based on the assumption that the flux in each region is spatially flat and the scattering is isotropic. Multizone situations such as reactor lattices are accounted for by the use of Dancoff factors, which are used to modify the escape probability and, hence, the value of σ_e.

Several of the approximations used in the Bondarenko method are known to be inadequate in some situations. At low energies, many nuclides have resonances that are wide when compared with the scattering ranges for the mixtures in a particular configuration. This discrepancy typically leads to cross-section values that are too high in the resonances. Systems with nuclides whose resonances overlap also cause inaccuracies. In SCALE, the Bondarenko factors are used primarily in the unresolved energy region where the resonances are too narrow to be resolved into sets of resonance parameters. Although the flat flux and isotropic scattering approximations used to determine escape probabilities may have an effect on the group-averaged values, a potentially larger effect is possible because of the procedures used to generate the original Bondarenko factor tables. These tables may not have included all of the resonance-resonance overlap terms. However, given proper Bondarenko factors for the unresolved range, the treatment is probably adequate for treating an "unresolved" region.

SCALE uses the Bondarenko method to shield its 16-group Hansen-Roach cross-section library. As originally distributed, this library contained several sets of data for importance resonance nuclides that were characterized by various values of background cross sections, σ_0. The basic sets were generated using narrow resonance approximations, and were adjusted to make them accurately calculate the multiplication factor for a variety of critical experiments. This adjustment accounts for the success of the Hansen-Roach library in accurately calculating many types of criticality problems. This library was converted into Bondarenko format by dividing the "shielded" cross-section sets by a reference infinite dilution set. Advantages of converting them to Bondarenko format include:

1. The user does not have to determine the appropriate value of σ_0 because BONAMI does it automatically.

2. Because σ_0 varies as a function of energy, the user is not restricted to a single set of data.

3. The σ_0 values can be interpolated rather than using only a set of discrete values.

4. σ_0 is modified to account for lattice and two-region geometrical effects.

Although there are many approximations in the basic cross sections used to create the 16-group Bondarenko factors, the Bondarenko treatment has significantly increased its utility for SCALE users.

M7.2.5.2 Applicability of the Nordheim Integral Method

The Nordheim Integral treatment is discussed in detail in Sect. F2.2. It is basically a two-region integral transport theory method for a fuel lump surrounded by a moderator region. The moderator region is assumed to have an asymptotic (1/E) flux at all energies and over all space. Escape probabilities are used to account for coupling between the two regions. As with BONAMI, NITAWL uses exact escape probabilities for slabs, cylinders, and spheres as developed by Case, de Hoffman, and Placzek,[3] but which are based on the assumption of a flat flux and isotropic scattering in the fuel lump. To account for lattice effects, a Dancoff factor can be specified, though it is a single value that must be used at all energies. The Nordheim Integral Treatment considers only one resonance nuclide in its calculation (i.e., the overlap between resonances of different nuclides is not treated), and a separate calculation is performed for each resonance using the assumption that the resonances of a nuclide do not overlap.

Because NITAWL does not include resonance-resonance overlap, it does not accurately treat nuclides having large low-energy resonances (^{233}U and ^{241}Pu) or multinuclide systems that contain many overlapping resonances such as (1) systems containing MOXs of uranium and plutonium ,and (2) advanced thorium converter systems. For fast reactor systems, the effects are not as severe as might be expected for criticality studies because the most important energy region is high relative to the resolved energy regions for most nuclides. For systems involving primarily ^{235}U and ^{238}U, such as the light-water reactor (LWR), the Nordheim treatment is quite good because the resonance overlap effect for these two nuclides is small.

An area in which the Nordheim method is particularly weak is that of calculating small, tightly packed lattices, where the flux in the moderator is significantly different from the assumed asymptotic value, for example, gas-reactor fuel where tiny fuel pellets are coated with a graphite moderator.

The use of escape probabilities based on the flat flux and isotropic scattering assumptions used in NITAWL introduce errors in some cases. Fix-ups[4,5] (not available in NITAWL) involving the use of transport corrections to the scattering have been tried but have not been entirely satisfactory. Cohen[6] derived probabilities based on a hyperbolic cosine-shaped source which should be more accurate for some cases.

The fact that the Nordheim method only treats free atom elastic scattering may introduce errors where inelastic sources are important or where upscattering effects for low-energy resonances are important. The Nordheim treatment as implemented in SCALE has been shown to be adequate for treating a variety of critical experiment problems and other problems. *The user should be aware of the limitations inherent in the Material Information Processor and the cross-section processing performed by SCALE and use them accordingly.*

M7.2.5.3 Applicability of the Dancoff Factor

The Nordheim method was designed to treat a single fuel lump in an infinite moderator. To account for the heterogeneous effects of a lattice of fuel lumps, a correction known as the Dancoff factor is applied to the leakage probability from the lump. The interlump Dancoff factor (C) is the probability that a neutron emitted isotropically from the surface of one absorber lump will pass through the external media and enter a nearby absorber lump. In the case of an annular region, the total Dancoff factor is a weighted sum of the interlump factor and the probability of a neutron emitted on the inner surface of the annulus reentering the annulus without experiencing a collision. The weighting factors are the inner and outer surface areas of the annular region.

$$C = (A_o C_o + A_i C_i)/(A_o + A_i), \qquad \text{(M7.2.1)}$$

where

C is the total Dancoff factor,

A_o is the outer surface area of the region,

C_o is the Dancoff factor associated with the outer surface,

A_i is the inner surface area of the region,

C_i is the Dancoff factor associated with the inner surface.

Interaction probabilities are calculated for lattices of spheres, infinitely long cylinders, or infinite slabs. The algorithms used in SCALE for LATTICECELL problems were developed in SUPERDAN,[7] a program that uses a double numerical integration to analytically determine the Dancoff factor of spheres, cylinders, and slabs. In each case, the program accounts for any cladding that might be present. For a particular fuel lump, the total Dancoff factor (C) is calculated for the appropriate lattice. The overshadowing of one neighboring lump by another is accounted for analytically and includes all nearest and second-nearest neighbors. Figure M7.2.1 represents cylindrical pins in a square lattice, and Fig. M7.2.2 represents cylindrical pins in a triangular lattice. The Dancoff factor is the summation of the Dancoff factors of all fuel regions visible to the lump. See Table M7.2.2 for the appropriate equations used to determine the Dancoff factor.

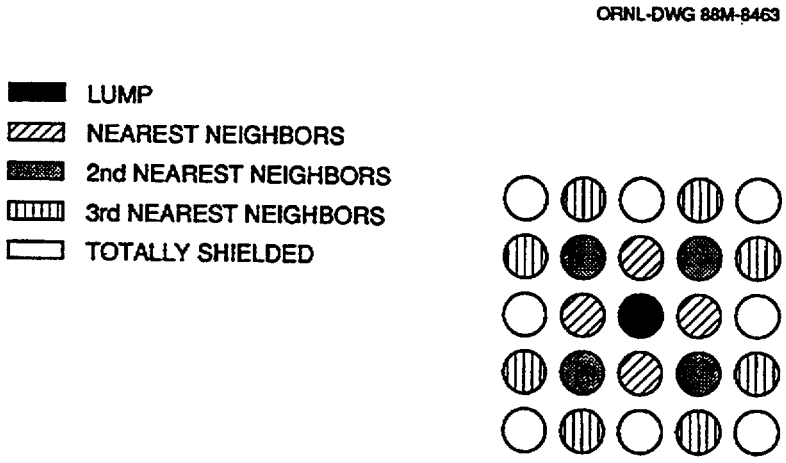

Figure M7.2.1 Representation of a lump and its neighbor for cylindrical pins in a square lattice

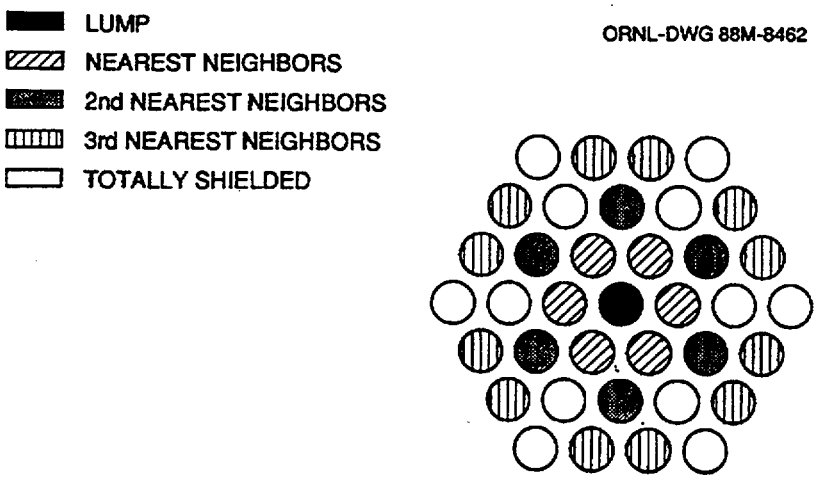

Figure M7.2.2 Representation of a lump and its neighbors for cylindrical pins in a triangular-pitch lattice

Table M7.2.2 Dancoff factor equations for various geometries

Fuel lump	Type of lattice pitch	Number of neighbors: Nearest	Second nearest	Third nearest	Dancoff
Cylinder	Square	4	4	8[a]	$C = \sum_{i=1}^{8} C_i$
Cylinder	Triangular	6	6	12[a]	$C = \sum_{i=1}^{12} C_i$
Sphere	Square	6	12	8	$C = \sum_{i=1}^{26} C_i$
Sphere	Triangular	12	6	8	$C = \sum_{i=1}^{26} C_i$
Slab	-	2	-	-	$C = \sum_{i=1}^{2} C_i$

[a]Not included in the SUPERDAN treatment.

In order to treat the interaction to the third and subsequent nearest neighbors, a correction factor, CF, is added to the Dancoff factor, C, calculated using the SUPERDAN algorithm. The CF is determined by repeating the Dancoff calculation using a void in the place of the moderator. This computation yields a Dancoff factor, D_0, which represents the fraction of the solid angle that is being treated by the SUPERDAN algorithm. Since the true solid angle should be 1.0, the untreated solid angle is $1.0 - D_0$. An exponential attenuation based on the total cross section, Σ_T, of the moderating media and an estimated distance $\bar{\ell}$ is applied to the untreated solid angle, that is,

$$CF = (1.0 - D_0)\, e^{-\Sigma_{T_m} \bar{\ell}}, \qquad \text{(M7.2.2)}$$

$$DF = C + CF, \qquad \text{(M7.2.3)}$$

where $\bar{\ell}$ is given in Table M7.2.3 and the untreated fraction of the solid angle is shown graphically in Fig. M7.2.3.

Table M7.2.3 $\bar{\ell}$ used in the Dancoff correction

System geometry	$\bar{\ell}$
Cylindrical square pitch	Pitch × $\sqrt{5}$
Cylindrical triangular pitch	Pitch × $\sqrt{7}$
Spherical square pitch	Pitch × $(\sqrt{5} + \sqrt{7})/2$
Spherical triangular pitch	Pitch × $\sqrt{3}$

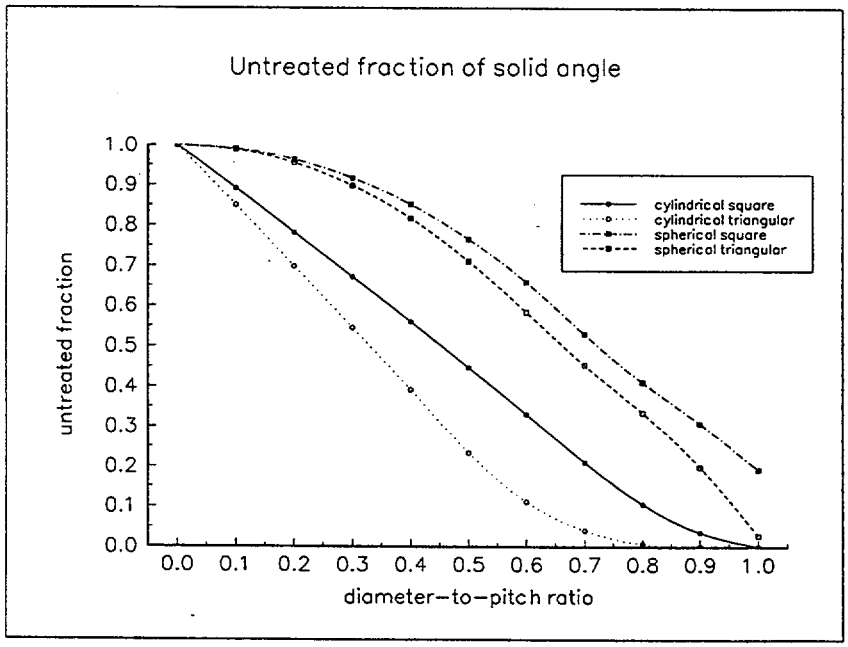

Figure M7.2.3 Untreated fraction of solid angle $d = (0.710446)\lambda_{TR}$

The magnitude of the correction, CF, and the effect on a calculated k_{eff} will depend on both the geometry of the system and the moderator cross section. This Dancoff treatment calculates the correct limits for cases in which the particle size and/or the moderator cross section are very small. The ratio CF/(1-DF) provides a quantity that can be used to estimate the importance of the correction. For a typical LWR lattice, this ratio is on the order of 10^{-3}, with a change in k_∞ of $< 10^{-5}$. Other studies with LWR fuel indicate ratios less than 0.01 lead to changes in k_∞ less than 0.1%, and ratios less than 0.2 lead to changes in k_∞ of less than 2%.

M7.2.5.4 The One-Dimensional Approximation With/Without Buckling

The Material Information Processor assumes that the physical system may be adequately represented in one dimension. For most LATTICECELL calculations, this is a reasonable approximation since the leakage out the ends of a fuel rod is almost negligible and the effect of neighboring fuel rods may be accounted for by using the appropriate boundary condition. For MULTIREGION calculations, however, the implications of the approximation should be examined more carefully. In 1-D calculations, cylinders are assumed to be infinitely long and slabs are assumed to be of infinite extent in both of the transverse directions. Hence, a true 1-D calculation in these geometries would tend to overestimate the k_{eff} of the physical system.

To partially alleviate this difficulty, it is possible to use a buckling correction that accounts for the leakage out of the system in the transverse direction(s). To do this, the leakage in each group is calculated as $D_g B_g^2 \phi_g$ and treated as an absorption term in the transport equation. Here, D_g is the diffusion coefficient:

$$D_g = 1/(3\,\Sigma_{TR_g})\,, \tag{M7.2.4}$$

and the buckling, B_g^2, is given by

$$B_g^2 = (\pi/DY_g^*)^2 + (\pi/DZ_g^*)^2 \tag{M7.2.5}$$

in slab geometry, and

$$B_g^2 = (\pi/DY_g^*)^2 \tag{M7.2.6}$$

in cylindrical geometry. DY_g^* and DZ_g^* are the extrapolated dimensions of the assembly defined by

$$DY_g^* = DY + 2d_g\,, \tag{M7.2.7}$$

and

$$DZ_g^* = DZ + 2d_g\,, \tag{M7.2.8}$$

where DY and DZ are the actual dimensions of the assembly and d_g is the extrapolation distance from the surface of the assembly. For a semi-infinite system in planar geometry, the analytic solution to the Milne

problem yields d = $(0.710446)\lambda_{TR}$. For smaller systems, d can be shown to lie between $(0.7104)\lambda_{TR}$ and $(1.3333)\lambda_{TR}$. Within the XSDRNPM code, d is calculated as

$$d_g = (\tfrac{1}{2})(BKL)\,\lambda_{TR_g} = (\tfrac{1}{2})(BKL)(1/\Sigma_{TR_g}), \qquad (M7.2.9)$$

where BKL is an optional parameter that the user may supply. A default value of BKL = 1.420892 is typically supplied by the control module. Even though it is true that underestimating the extrapolation distance (i.e., using a value of BKL that is too small) will cause a buckling-corrected transport calculation to underestimate k_{eff} by a slight amount, that is nearly always a second- or third-order effect. In systems with transverse dimensions small enough for d to be much greater than $(0.7104)\lambda_{TR}$, the 1-D approximation is no longer valid and a 2-D model of the physical system is probably required.

M7.2.5.5 Use of XSDRNPM by the Material Information Processor

The Material Information Processor prepares data that are used by the 1-D discrete-ordinates code XSDRNPM. XSDRNPM performs the dual functions of (1) criticality safety analyses and (2) cross-section processing to create a homogenized cell-weighted mixture cross section. The Material Information Processor utilizes an automatic mesh generator and an automatic quadrature generator to supply data for XSDRNPM. The automatic mesh generator creates a mesh across the material zones used to calculate the fluxes that are used in calculating λ, the neutron multiplication factor, and in creating the homogenized cell-weighted mixture cross section. The angular quadrature is used to divide the directions of the angular flux into discrete bins defined by the direction cosines. Appropriate weights are defined to be used in the numerical integration of the angular-dependent flux to obtain a scalar flux used in the calculation.

M7.2.5.6 The Automatic Mesh Generator

The Material Information Processor determines the number and location of mesh boundaries within a zone using an algorithm based on the total epithermal cross section and asymptotic diffusion length in each mixture. The number of mesh intervals used in a calculation may be increased or decreased by entering a value for the parameter SZF= in the optional parameter data.

Within a particular material zone, the mesh boundaries are logarithmically symmetric about the midpoint of the zone as shown in Fig. M7.2.4.

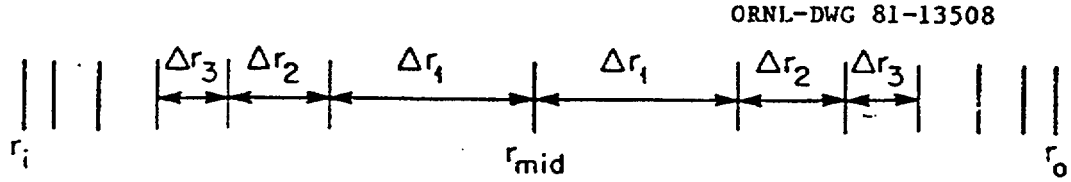

Figure M7.2.4 Mesh spacing scheme used in material zone

Assuming a total of N mesh intervals in a zone, the size of each mesh interval (Δr_n) is given by

$$\Delta r_n = 0.5(r_o r_i)\log_{10}\{[N + 18(n)]/[N + 18(n - 1)]\} \; . \; n=1,2,...,N/2 \; . \qquad \text{(M7.2.10)}$$

This logarithmically symmetric distribution has the advantage of providing more mesh intervals near the material zone interfaces where greater flux gradients are likely to exist. To determine N, the size of the largest mesh interval must be less than some specified number of mean free paths or asymptotic diffusion lengths. Specifically, N is determined by applying the requirement that

$$\begin{aligned} &(\Delta r_{max}) \le (SZF)(0.06)(\lambda_T) \text{ for LATTICECELL calculations, or} \\ &(\Delta r_{max}) \le (SZF)(0.25)(L) \text{ for MULTIREGION calculations,} \end{aligned} \qquad \text{(M7.2.11)}$$

where the size factor (SZF) is an optional control parameter that may be specified by the user, and L is the asymptotic diffusion length for the mixture defined by

$$(1/L)^2 = 3\Sigma_A \Sigma_S(1 - \bar{\mu})(1 - 4\Sigma_A/5\Sigma_T) \; . \qquad \text{(M7.2.12)}$$

The asymptotic diffusion length is computed using epithermal cross-section data from the Standard Composition Library (see Sect. M8). The constants [0.06 and 0.25 in Eq. (M7.2.11)] were chosen to ensure an adequate mesh size when SZF is set to its default value of 1.0. The size of the largest mesh interval can be adjusted by entering a value for SZF in the optional parameter data. For LATTICECELL calculations, the number of mesh intervals in a zone is given by

$$N = 18/(10^x - 1) \; , \qquad \text{(M7.2.13)}$$

where

$$x = 2(0.06)(\lambda_T)(SZF)/(r_o - r_i) \; . \qquad \text{(M7.2.14)}$$

A similar expression is obtained for the MULTIREGION case. For optically thin regions such as voids or thin cladding, N is assigned a value of 4 whenever the equation yields a smaller value. N is always defaulted to 1 for an infinite-homogeneous-media calculation.

M7.2.5.7 The Automatic Quadrature Generator

The discrete-ordinates code, XSDRNPM, solves for the angular flux (ψ_m) in a number of discrete directions ($\bar{\Omega}_m = \mu_m\bar{i} + \eta_m\bar{j} + \xi_m\bar{k}$) in each spatial mesh. The scalar flux in each mesh (ϕ) is then computed using a numerical quadrature of the form:

$$\phi = \sum_m W_m \psi_m , \qquad \text{(M7.2.15)}$$

where W_m is the weight associated with direction $\bar{\Omega}_m$.

XSDRNPM automatically calculates the direction cosines and the associated weights for the specified geometry. The number of discrete directions (MM) generated for a quadrature of order ISN is given by

$$MM = ISN + 1 \quad \text{for slab or spherical geometry} \qquad \text{(M7.2.16)}$$

and

$$MM = ISN*(ISN + 4)/4 \quad \text{for cylindrical geometry.} \qquad \text{(M7.2.17)}$$

In spherical geometry, the calculated directions and weights correspond to those of a simple Gaussian quadrature set of order ISN.* In slab geometry, XSDRNPM calculates a Gaussian quadrature set of order ISN/2, compresses it from 180° down to 90° (for symmetry), and uses this compressed quadrature in combination with its mirror image.** (In both slab and spherical geometry, one additional direction having an associated weight of 0.0 is also included.) In cylindrical geometry, the polar angles (θ) correspond to the positive angles of a Gaussian quadrature of order ISN while the azimuthal angles (ϕ) are equally spaced as shown in Fig. M7.2.5.*** This equal spacing of the azimuthal angles corresponds to a Chebyschev quadrature in ϕ. Note that one additional angular direction having an associated weight of 0.0 is also included for each of the polar angles (θ).

The quadrature order (ISN) is an optional control parameter that may be specified by the user. The SCALE criticality safety analysis sequences normally default to ISN = 8. The user may increase or decrease the quadrature order to verify the accuracy of a particular calculation. ISN = 8 has been found to be adequate for most LATTICECELL calculations. In MULTIREGION calculations having a reflector, ISN = 8 will generally be adequate, although the user may wish to compare the resulting k_{eff} and/or scalar fluxes with those of another calculation using ISN = 12. Accurate determination of the scalar fluxes deep in a thick shield may require ISN = 16.

---

*More precisely: $\mu_i = \pm x_j$, where $\{x_j\}$ are the (m/2) positive roots of $P_m(x) = 0.0$, where m = ISN; and $w_i = W_j/2$, where $\{W_j\}$ are the Gaussian weights associated with $\{x_j\}$. The starting direction, $\mu_o = -1$, is assigned a zero weight.

**More precisely: $\mu_i = \pm (1 \pm x_j)/2$, where $\{x_j\}$ are the (m/2) positive roots of $P_m(x) = 0.0$, where m = ISN/2; and $w_i = W_j/4$, where $\{W_j\}$ are the Gaussian weights associated with $\{x_j\}$. The starting direction, $\mu_o = -1$, is assigned a zero weight.

***More precisely: $\eta_i = \cos(\theta_i)$ are the (m/2) positive roots of $P_m(\eta) = 0.0$ where m = ISN; $\mu_{i,j} = \pm \sqrt{1-\eta_i^2}\cos[\pi(j - 0.5)/2i]$ where j = 1, 2, ..., i; and $w_{i,j} = W_i/(2i)$ where $\{W_i\}$ are the Gaussian weights associated with $\{\eta_i\}$. The starting direction, $\mu_{i,o} = -\sqrt{1-\eta_i^2}$, is assigned a zero weight.

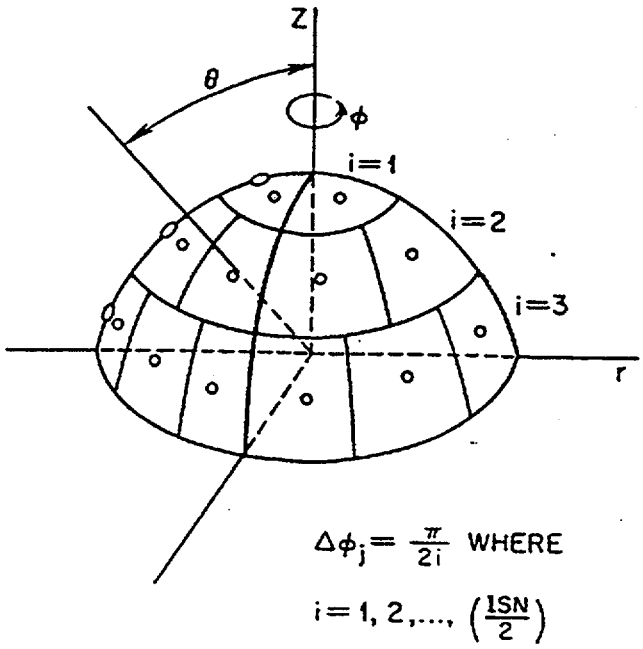

Figure M7.2.5 Angular directions associated with an S_6 Gauss-Chebyschev quadrature set for cylindrical geometry

M7.2.5.8 XSDRNPM Convergence Criteria

The convergence criteria for the XSDRNPM calculation used to create the cell-weighted cross sections are the optional control parameters EPS and PTC in the Material Information Processor input. Terms useful in describing the convergence criteria are defined below:

Q ≡ total fixed source in system

F ≡ total fission neutron source

D ≡ total outscatter = $\sum_i \sum_g \sum_{g' \neq g} \phi_{i,g} \sigma_{g \to g'} V_i$

$\phi_{i,g}$ ≡ scalar flux in group g, interval i

V_i ≡ volume of interval i

$\sigma_{g \to g'}$ ≡ group g to group g′ transfer cross section

IGM ≡ number of energy groups

q_g ≡ fixed source in group g

f_g ≡ fission source in group g

$$\epsilon_p' \equiv \left(\frac{q_g + f_g}{IGM} \right) EPS$$

k ≡ outer iteration number (do not confuse with the multiplication factor)

$$\lambda_k \equiv \frac{Q + F_k}{Q + F_{k-1}} \quad \text{(SOURCE RATIO in output)}$$

$$G_k \equiv \frac{D_k}{Q + F_k}$$

$$\lambda_k' \equiv \frac{G_{k-1}}{G_k} \quad \text{(SCATTER RATIO in output)}$$

$$U_k \equiv \text{total upscatter rate} = \sum_i \sum_g \sum_{g'<g} \phi_{i,g} \sigma_{g \to g'} V_i .$$

An inner iteration consists of sweeping one time through the entire spatial mesh and calculating the flux for all the S_n angles in one energy group. A sweep through all energy groups is called an outer iteration.

When the fluxes for a particular group are being calculated, the inner iterations will continue until (1) the number of inner iterations in this outer exceed IIM (the inner iteration maximum), or (2) until the following criteria are met:

$$(1) \quad \sum_i | (\phi_{i,g}^k - \phi_{i,g}^{k-1}) | \sigma_{g \to g'} V_i \le \epsilon_g'$$

$$(2) \quad \sum_i | (\phi_{i,g}^k - \phi_{i,g}^{k-1}) | (\sigma_t - \sigma_{g \to g'}) V_i \le \epsilon_g'$$

If PTC (the point flux convergence criteria) is greater than zero, XSDRNPM also requires

$$(3) \quad \max_i \left| \frac{\phi_{i,g}^k - \phi_{i,g}^{k-1}}{\phi_{i,g}^k} \right| \le PTC$$

At the end of an outer iteration, the following checks are made:

(4) $|1.0 - \lambda_k| \leq EPS$

(5) $R|1.0 - \lambda'_k| \leq EPS$

(6) $R|1.0 - \frac{U_{k-1}}{U_k}| \leq EPS$

R is a convergence relaxation factor that is automatically set to 0.5 within XSDRNPM. If all the convergence criteria are met or if the maximum allowed number of outer iterations is reached, the XSDRNPM calculation will terminate with full output. Otherwise, another outer iteration will be started.

M7.3 THE LOGICAL PROGRAM FLOW

The general flow of the Material Information Processor is given in this section. An abbreviated representation, rather than a formal flow chart, is used to outline the program flow. A flow chart may show a subroutine or library routine only once, even though it may be called several times. The text usually states when multiple calls are made to a subroutine or library routine. Each flow chart is accompanied by an explanation of the purpose of that segment of the program and text describing the subroutines referenced in the flow chart.

The segment of the program shown in Fig. M7.3.1 activates the Material Information Processor. The Material Information Processor reads data that specify the cross-section library, defines the materials to be used in the problem, and provides data used to apply resonance corrections to the cross sections. The data are read and checked, and calculations are performed to create a mixing table and provide data to the functional modules that are invoked by the control module.

C4DATA - This is the subroutine through which the Material Information Processor is activated. It opens the units that will be used to pass data to the functional modules. Throughout the subroutine, pointers are defined for various types of data, and STOP is called to write a message if the data arrays require more storage than is available. The call to subroutine KNIGHT initiates the reading and preparation of data for use in the functional modules involved in cross-section preparation. All other subroutines called by C4DATA carry out operations to prepare and check data that will be used by the functional modules activated by the sequence.

AXSDRN - This subroutine is used by the SAS4 sequence and is replaced by a dummy for the CSAS sequences.

STOP - This library routine may be called many times from C4DATA. If the computer storage is insufficient to contain the data arrays, it is called to write an error message. Depending on the arguments passed to it, this routine can also do any or all of the following: print a traceback, execute a stop, or return to the calling program.

KNIGHT - This subroutine initiates the preparation of data for use in the functional modules involved in cross-section preparation. It is described in more detail in Sect. M7.3.1.

SMMTBA - This subroutine is called to set the unit number corresponding to the specified master cross-section library.

SHORTX - The purpose of this subroutine is to copy only those nuclides utilized in the standard composition specification data to unit 11 for processing by the functional module BONAMI and to print the Data Information Table. LOGID determines if the composition name from the standard composition library was specified in the standard composition specification data. OPNFIL is used to open the specified cross-section library and unit 11. COPY is used to copy the cross-section data to unit 11.

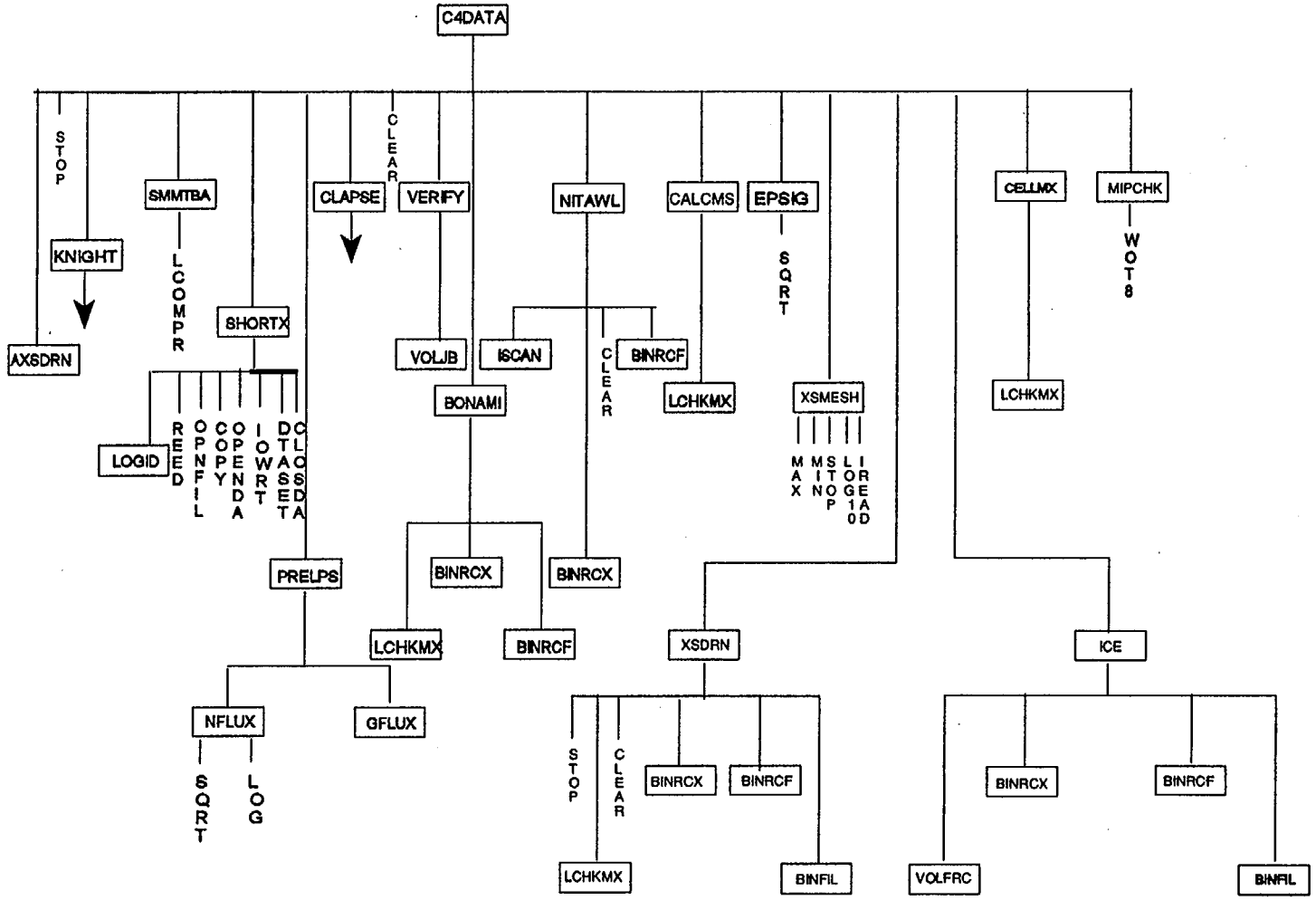

Figure M7.3.1 Flow chart of the Material Information Processor

The library routine OPENDA is called to open the direct-access data set. IOWRT is a library routine that prints the data set name and the volume where the data set resides for the specified unit number. It is called several times to generate and print portions of the Data Library Information Table. The library routine DTASET is called to set the data set name and volume serial number associated with a specified unit number. The library routine CLOSDA is called to close the direct-access data set.

PRELPS - This subroutine defines the collapsed group structure for the shielding analytical sequences. It should not be used in the criticality safety analytical sequences. The call to PRELPS is triggered by entering COLL in MORE DATA. PRELPS calls NFLUX to generate a neutron flux spectrum and GFLUX to generate a gamma flux spectrum.

CLAPSE - This subroutine controls the collapsing of the appropriate AMPX master format library to the new group structure. It is described in more detail in Sect. M7.3.9.

CLEAR - This library routine is called to zero the volume fraction array.

VERIFY - This subroutine checks the mixture-by-zone array. A warning message is written if the same mixture number is specified for more than one zone. It also determines the number of void zones in the 1-D model for use in the BONAMI mixing table.

VOLJB - This function is used in calculating volume fractions. It returns the volume for a sphere, the volume per unit height for a cylinder, and the thickness for a slab.

BONAMI - This subroutine prepares binary input data for the functional module BONAMI-S. The binary data are written on unit 96 by subroutines BINRCX and BINRCF.

LCHKMX - This logical function returns a value of true if a variable is referenced. BONAMI, NITAWL, CALCMS, and CELLMX utilize this function to determine if a mixture is referenced in the mixture-by-zone array.

BINRCX - Each time this subroutine is called, it writes a binary integer data array on a specified data file. This data array is part of the binary input data used by certain functional modules for processing the cross sections. BINRCX is called with six arguments. The first argument is the array identification number for FIDO-type data. The second argument is the starting point of the data to be written in the array defined by the first argument. The third argument is the end point of the data to be written in the array defined by the first argument. The fourth argument is the offset of the first location of the array defined by the first argument, from the beginning of the base array. The fifth argument is the name of the base array that contains the data to be written. The sixth argument is the unit number where the data is to be written. For example, arguments of (13,1,4,0,L,40) writes the first four entries of array L on unit 40 as the first four entries of the 13$$ array. Arguments of (13,1,4,20,L,40) would write entries 21 through 24 of array L on unit 40 as the first four entries in the 13$$ array.

BINRCF - Each time this subroutine is called, it writes a binary floating-point data array on a specified data file. This array is part of the binary data used by certain functional modules for processing the cross sections. BINRCF is called with six arguments that are identical in function to those

for BINRCX. For example, arguments of (13,1,4,0,B,40) write the first four entries of array B on unit 40 as the first four entries of the 13** array. Arguments of (13,1,4,20,B,40) would write entries 21 through 24 of array B on unit 40 as the first four entries in the 13** array.

NITAWL - This subroutine prepares binary input data for the functional module NITAWL-II. Subroutine ISCAN is called to return the nuclide number. The library routine CLEAR is called to zero the data array before loading data. The binary data are written on unit 97 for NITAWL-II by subroutines BINRCX and BINRCF.

CALCMS - This subroutine corrects the mixing table length to account for mixtures that are to be passed through XSDRNPM-S without being cell-weighted. LCHKMX is used to determine whether a mixture occurs in the mixture-by-zone array.

EPSIG - This subroutine is called only if a cell-weighted mixture is to be created. It calculates the total epithermal cross section and the corresponding asymptotic relaxation factor for use in determining the number of spatial mesh intervals. SQRT is used in determining the asymptotic relaxation factor.

XSMESH - This subroutine is called only if a cell-weighted mixture is to be created. It calculates the number of spatial intervals and their corresponding locations for XSDRNPM-S. STOP is called if more storage is required than is available. LOG10 is used in determining the interval boundary locations. MAX and MIN are used to determine the larger of two values and the smaller of two values, respectively.

XSDRN - This subroutine is called only if a cell-weighted mixture is to be created. It prepares binary input data for the functional module XSDRNPM-S. The binary input data are written on unit 98. LCHKMX is used to determine if a mixture is in the mixture-by-zone array, STOP is called if an error is recognized, CLEAR is used to zero arrays, BINRCX is used to write the binary integer data arrays, BINRCF is used to write the binary floating-point data arrays, and BINFIL is used to load an array with a specified number and write it on a specified unit number.

ICE - This subroutine is called only when the control modules CSASI and CSASIX are executed. It prepares binary input data for the functional module ICE-S. VOLFRC returns the volume fraction of a mixture in a cell. BINRCX writes the binary integer data arrays, BINRCF writes the binary floating-point data arrays, and BINFIL is used to fill an array with a number and write it on the specified unit number. The binary input data for ICE-S are written on unit 92.

VOLFRC - This function is used to determine the volume fraction of a mixture in the cell.

CELLMX - This subroutine is used to determine the number of components in a cell-weighted mixture. LCHKMX is used to determine if a mixture is in the mixture-by-zone array.

MIPCHK - This subroutine is activated if PARM=CHECK is specified on the analytical sequence indicator as shown by the following example:

```
=CSAS25    PARM=CHECK
```

MIPCHK prints additional information including the mixing table, resonance data, data for BONAMI-S and NITAWL-II, and all KENO V.a data that are printed prior to creating the initial source distribution. The library routine WOT8 is used to print part of the data.

M7.3.1 READ THE INPUT DATA

Figure M7.3.2 illustrates the beginning of the data reading and processing segment of the program known as the Material Information Processor.

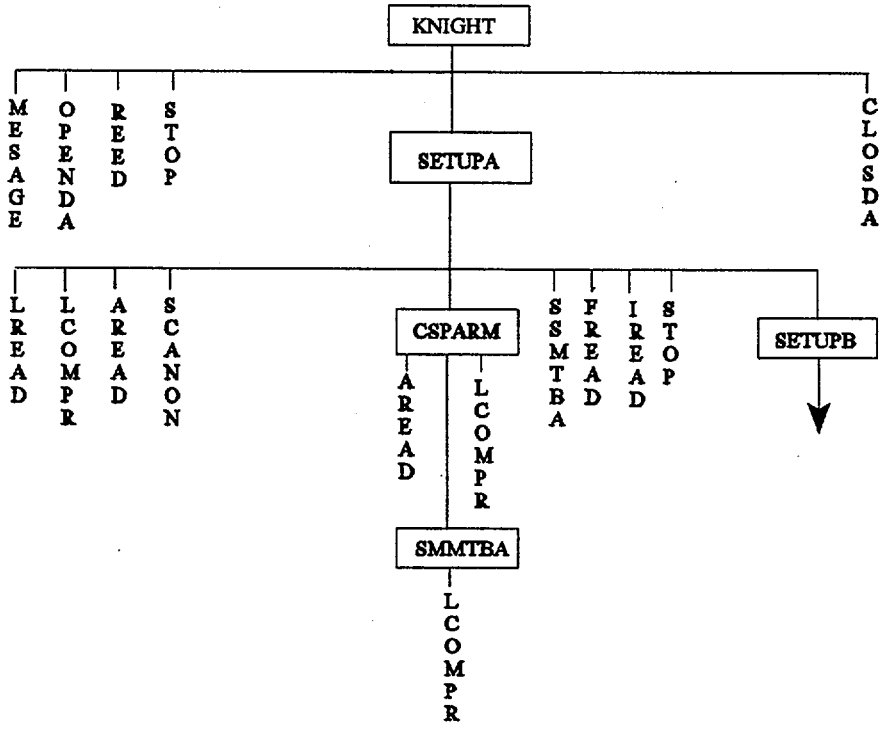

Figure M7.3.2 Read the Material Information Processor input data

KNIGHT - This subroutine initiates the data-reading portion of the Material Information Processor. It defines the output unit for the analytical sequence and sets up storage for various data arrays needed by the Material Information Processor. STOP is called if the available storage is too small to contain the data arrays. Data from the Standard Composition Library (see Sect. M8) are loaded for use by the Material Information Processor. SETUPA is called to control the data reading. CLOSDA is called to close out the standard compositions specification data file when the Material Information Processor is finished.

MESAGE - This library routine is called with two arguments: an eight-character hollerith argument and an output unit. Additional library routines are called from MESAGE to print a header page in block letters and the Program Verification Information Table for quality- assurance purposes.

The header page includes the eight-character hollerith argument defining the analytical sequence being executed, the date and time execution was begun, and the job name. The program verification information table includes the program name, its creation date, the library name, the job name, and the date and time of execution.

OPENDA - This library routine initializes the direct-access files.

REED - This library routine is called to load data from the Standard Composition Library into data arrays.

SETUPA - This subroutine is responsible for reading the standard composition specification data and geometry description data from the input unit and determining the number of mixtures specified in the data, the number of standard composition specifications entered as data, the number of solutions specified in the standard composition specification data, and the number of material zones to be used by XSDRNPM-S. The input unit is rewound so it can be read by subroutine SETUPB. Then the problem parameters are printed, and pointers are established for subsequent information storage. The library routine STOP is called to print a message if more computer storage is required for the problem.

AREAD - This library routine is used to read the standard composition names and other alphanumeric data.

SCANON - This library routine is called to activate the feature that allows scanning for the word END, when reading data.

CSPARM - This subroutine uses the library routine AREAD to read the problem title, cross-section library name, and type of calculation to be performed. It is called twice from SETUPA: once at the beginning, and again before calling SETUPB.

SMMTBA - This subroutine sets the logical cross-section unit number based on the cross-section library specified in the input data.

LCOMPR - This library routine is called from CSPARM to verify that the cross-section library name specified in the data matches one of the available libraries. It is called from SETUPA to determine if infinite homogeneous cell data and/or optional parameter data are to be read.

FREAD - This library routine is called as needed to read floating-point data in the standard composition specification data and geometry description data.

IREAD - This library routine is used to read integer data in the standard composition specification data and geometry description data.

LREAD - This library routine returns a value of "true" if the next character in a free-form reading buffer is a numeric digit. It is called from SETUPA to determine if DEN= or SPG= was entered in the standard composition data.

SETUPB - This subroutine is described in more detail in the following section.

M7.3.2 CONTROL DATA READING AND PROCESSING

Figure M7.3.3 illustrates the control of the data reading and processing for the Material Information Processor.

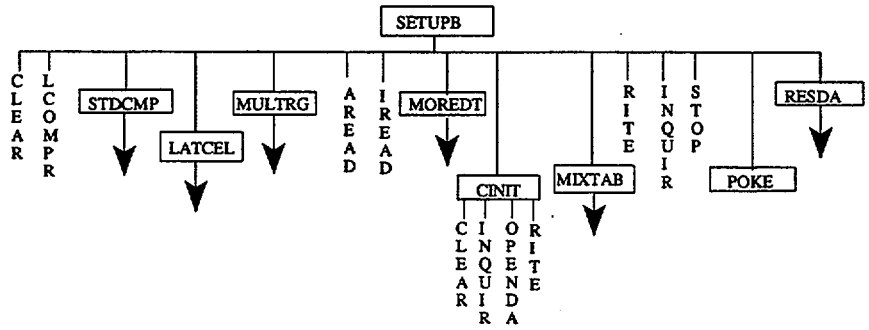

Figure M7.3.3 Control Material Information Processor data reading and processing

SETUPB - This subroutine controls reading the standard composition data, the unit cell specification data, and the optional parameter data. It is responsible for generating the mixing table information and determining the resonance parameters required for NITAWL-S. Various consistency checks are made as the data are read and processed. STOP is called if more storage is needed for the resonance treatment data arrays than is available.

CLEAR - This library routine is called to clear storage arrays.

LCOMPR - This library routine is called many times to compare character strings of input data with the allowed data names specified in the program. It compares as many characters as are supplied in the input data, thus allowing terse input of variable length.

STDCMP - This subroutine is called from SETUPB to read the standard compositions data. See Sect. M7.3.3 for more details.

LATCEL - This subroutine reads the unit cell specification associated with a LATTICECELL problem. See Sect. M7.3.4 for more details.

MULTRG - This subroutine reads the unit cell specification for a MULTIREGION problem. See Sect. M7.3.5 for more details.

AREAD - This library routine is called from SETUPB to read the alphanumeric data used to define the cell mixture for an infinite homogeneous medium problem.

IREAD - This library routine is called from SETUPB to read the mixture number used in the cell mixture definition in an infinite homogeneous medium problem.

MOREDT - This subroutine reads the optional parameter data as described in Sect. M7.3.6.

CINIT - This subroutine is called to clear the offsets into the pointer storage array and set the CSAS and KENO V.a offsets. OPENDA is called to open the random access units or devices, RITE writes the offsets on a random access unit, and INQUIR returns the number of the next random access block.

MIXTAB - This subroutine is called to generate mixing table information. It is described in more detail in Sect. M7.3.7.

STOP - This library routine is called to write error messages.

POKE - This subroutine uses the geometry description data to calculate the outer boundary of each zone. The zone boundary and mixture by zone data are then loaded in the appropriate arrays.

RESDA - This subroutine creates the resonance data required by NITAWL-S. It is described in more detail in Sect. M7.3.8.

M7.3.3 READ THE STANDARD COMPOSITION SPECIFICATION DATA

Figure M7.3.4 illustrates the program flow for reading the standard composition specification data. The data format is discussed in Sect. M7.4.4.

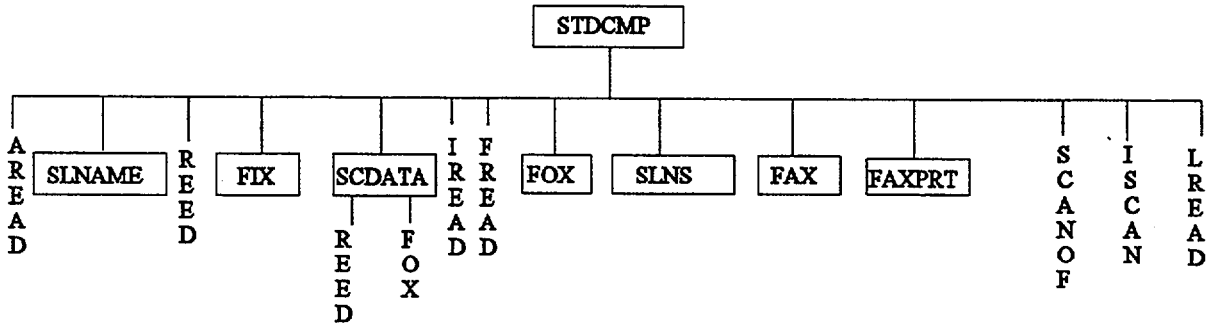

Figure M7.3.4 Flow chart for reading the Standard Compositions Specification data

STDCMP - This subroutine is called from SETUPB to read and process the standard composition specification data for a problem.

AREAD - This library routine is called to read the standard composition names, the END for each standard composition, and the END COMP that terminates the standard composition specification data.

SLNAME - This subroutine returns the standard composition name of the fuel used in a solution.

REED - This library routine is used to load the table of contents from the Standard Composition Library into temporary storage before calling subroutines FIX and FOX.

FIX - This subroutine loads the data for an arbitrary material into the appropriate data arrays.

IREAD - This library routine is used to read integer data encountered in the standard composition specification data and the unit cell specification data.

SCDATA - This subroutine checks the standard composition material for multiple nuclides and sets up temporary storage for the nuclide data.

FREAD - This library routine is used to read floating-point data encountered in the standard composition specification data and unit cell specification data.

LREAD - This library routine is used to determine if the next character is a numeric digit. A value of true is returned if it is a numerical digit. Otherwise, a value of false is returned.

ISCAN - This subroutine is used to determine if a nuclide ID specified in the input data is found on the specified cross-section library. The cross-section library is scanned, and a value of true is returned if a match is found. Otherwise, a value of false is returned.

SCDATA - This subroutine checks the input for multi-isotope nuclides. If multi-isotope nuclides are specified, one of three things occur: (1) if isotopic data are specified in the material that is used, else (2) if it is in the cross-section library that is used, else (3) isotope distributions are read from the standard composition library.

FOX - This subroutine is called to provide the nuclide IDs and corresponding natural abundance in weight percent if the isotopic distribution is not specified in the input data.

SLNS - When a solution is specified in the standard composition specification data, this subroutine is used to calculate the volume fraction corresponding to the water, acid, and heavy metal according to the empirical formula applicable to the specified solution.

FAX - This subroutine is called from SETUPB to read the standard composition information for an arbitrary material. IREAD is used to read the integer data, and FREAD is used to read the floating-point data. Entry FAXPRT prints the standard composition specification data for an arbitrary material.

FAXPRT - This subroutine is responsible for printing the nuclide IDs and either the corresponding abundance in weight percent or the number of atoms in the compound. If multi-isotope nuclides are specified, a list of the isotopes and weight percents is printed for each multi-isotope nuclide.

SCANOF - This library routine is called to disable the ability to scan ahead for the word END.

M7.3.4 READ THE LATTICECELL UNIT CELL SPECIFICATION

Figure M7.3.5 shows the program flow for reading the unit cell specification for a LATTICECELL problem. The input data for this option are described in Sect. M7.4.6.

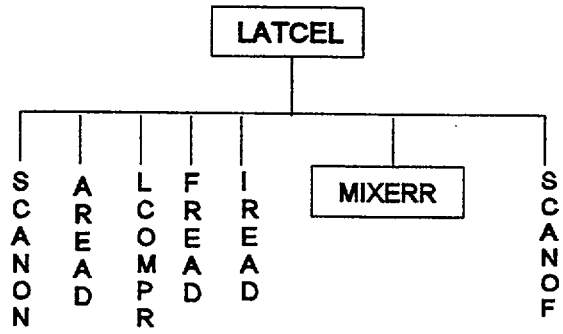

Figure M7.3.5 Flow chart for reading the unit cell specification for LATTICECELL

LATCEL - This subroutine is called from SETUPB to control reading and processing the unit cell specification for a LATTICECELL problem.

SCANON - This library routine is used to activate the feature that allows scanning for the word END while reading data.

AREAD - This library routine is called from LATCEL to read the type of cell to be used in a LATTICECELL problem.

LCOMPR - This library routine is used to compare the type of cell entered in the data with the allowed cell names. It checks as many characters as are entered in the input data. A value of true is returned if a match is found.

FREAD - This library routine is used to read the floating-point data encountered in the unit cell description of a LATTICECELL problem.

IREAD - This library routine is used to read the integer data encountered in the unit cell description of a LATTICECELL problem.

MIXERR - This subroutine is used to verify that mixture numbers utilized in the geometry description data have been defined in the standard composition specification data.

SCANOF - This library routine is called to disable the ability to scan ahead for the word END.

M7.3.5 READ THE MULTIREGION UNIT CELL SPECIFICATION

Figure M7.3.6 shows the program flow for reading the unit cell specification for a MULTIREGION problem. The input data for this option are described in Sect. M7.4.7.

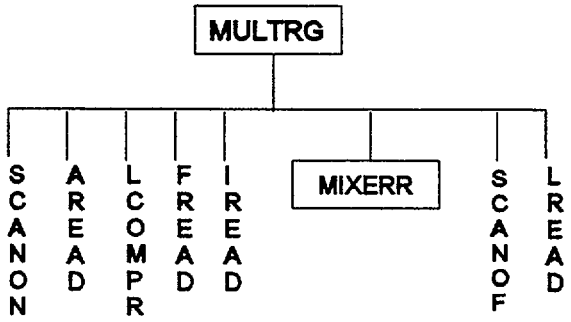

Figure M7.3.6 Flow chart for reading the unit cell specification for MULTIREGION

MULTRG - This subroutine is called from SETUPB to control reading and processing the unit cell specification for a MULTIREGION problem.

SCANON - This library routine is used to activate the feature that allows scanning for the word END while reading data.

AREAD - This library routine is called from MULTRG to read the type of cell to be used in a MULTIREGION problem.

LCOMPR - This library routine is used to compare the type of cell entered in the data with the allowed cell names. It checks as many characters as are entered in the input data. A value of true is returned if a match is found.

FREAD - This library routine is used to read the floating-point data encountered in the unit cell description of a MULTIREGION problem.

IREAD - This library routine is used to read the integer data encountered in the unit cell description of a MULTIREGION problem.

LREAD - This library routine returns a value of true if the next data entry is a numeric digit. It is used to test whether the optional moderator index data are present.

MIXERR - This subroutine is used to verify that mixture numbers utilized in the geometry description data have been defined in the standard compositions specification data.

SCANOF - This library routine is called to disable the ability to scan ahead for the word END.

M7.3.6 READ THE OPTIONAL PARAMETER DATA

The optional parameter data in the CSAS4 family of control modules allow certain parameters to be adjusted as described in Sect. M7.4.8. The program flow for this option is given in Fig. M7.3.7. This portion of the code is entered if the words MORE DATA are encountered after reading all of the other Material Information Processor data.

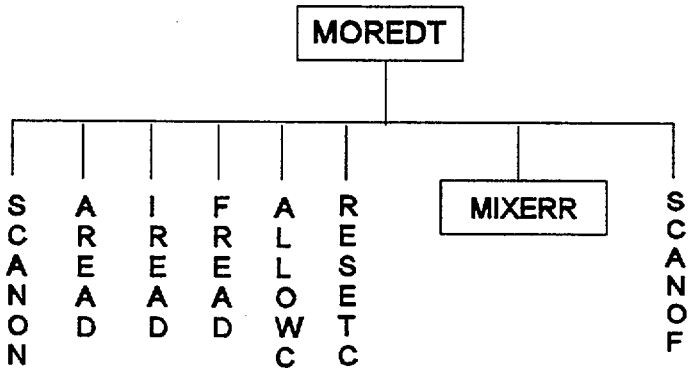

Figure M7.3.7 Flow chart for reading optional parameter data

SCANON - This library routine is used to activate the feature that allows scanning for the word END while reading data.

AREAD - This library routine is used to read the parameter names and other alphanumeric data used in the optional parameter data.

IREAD - This library routine is used to read integer data in the standard composition specification data and geometry description data.

FREAD - This library routine is called as needed to read floating-point data in the standard composition specification data and geometry description data.

ALLOWC - This library routine is called to cause the numeric data reading routines to terminate a number when a non-numerical character is encountered.

RESETC - This library routine is called to reset the numeric data reading routines to cause a number to be terminated only when a blank or a comma is encountered.

MIXERR - This subroutine is used to verify that mixture numbers specified in the resonance and/or Dancoff parameter data have been defined in the standard composition specification data.

SCANOF - This library routine is called to disable the ability to scan ahead for the word END.

M7.3.7 GENERATE THE MIXING TABLE

Figure M7.3.8 shows the subroutines used in generating the mixing table for the Material Information Processor.

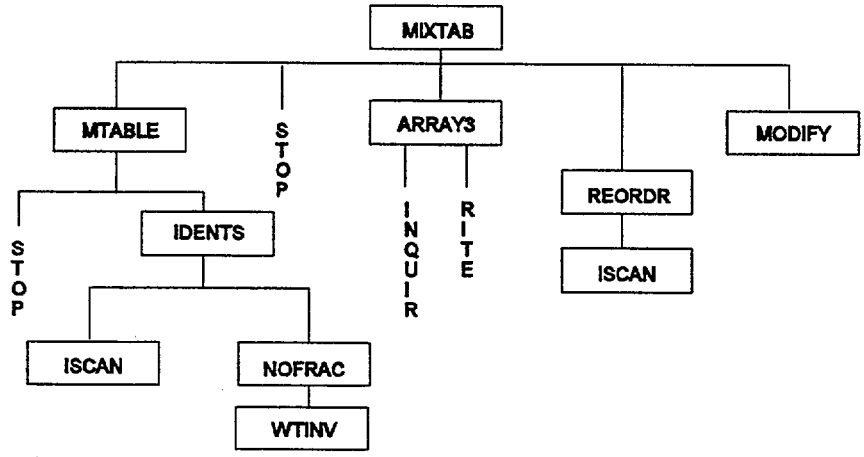

Figure M7.3.8 Flow chart for generating the mixing table

MIXTAB - This subroutine is responsible for generating the mixing table information required for the analytical sequence. It uses information from the Standard Composition Library and standard composition specification data to calculate the number density in atoms/b-cm for each nuclide in each mixture. STOP is called if the code needs more computer storage than is available. The final mixing table consists of a mixture number array, a nuclide ID array, and a number density array.

MTABLE - This subroutine is responsible for generating a mixing table containing a set of data for every isotope in every mixture. Each set of data consists of a mixture number, nuclide ID, and

number density in atoms/b-cm. Some nuclides may occur more than once in a mixture. STOP is called if the code needs more computer storage than is available. IDENTS is called to calculate the number density for each nuclide in each mixture.

IDENTS - This subroutine calculates the number density for each occurrence of each nuclide. ISCAN is used to locate the input nuclide in the Standard Composition Library. NOFRAC calculates the number fraction for each isotope in an element from the weight fraction data and atomic mass.

ISCAN - This function scans a vector to locate a matching component.

NOFRAC - This subroutine is called for compounds containing multiple isotope elements. It uses the weight fractions and atomic masses to determine the number fraction of each isotope in an element. Subroutine WTINV inverts the matrix.

WTINV - This subroutine inverts the weight-fraction matrix using the Gauss-Jordan reduction.

ARRAY3 - This subroutine divides the mixing table into separate arrays for the mixture number array, the nuclide ID array, and the number density array. It also compacts the mixing table, combining the number densities for duplicate nuclide IDs that appear in the same mixture.

INQUIR - Returns the number of the next random access block.

RITE - Writes the offsets on a random access unit.

REORDR - This subroutine reorders the mixing table based on isotope rather than mixture number. Therefore, all entries for a given isotope are loaded consecutively.

ISCAN - This function is used by subroutine REORDR to determine if a nuclide ID occurs in the Standard Composition Library.

MODIFY - This subroutine modifies the nuclide ID array portion of the mixing table to provide unique IDs for each appearance of a resonance nuclide and/or a nuclide for which multiple sets of thermal-scattering data are available.

M7.3.8 GENERATE RESONANCE DATA

Figure M7.3.9 shows the portion of the Material Information Processor that is responsible for generating the resonance data required by the analytical sequence.

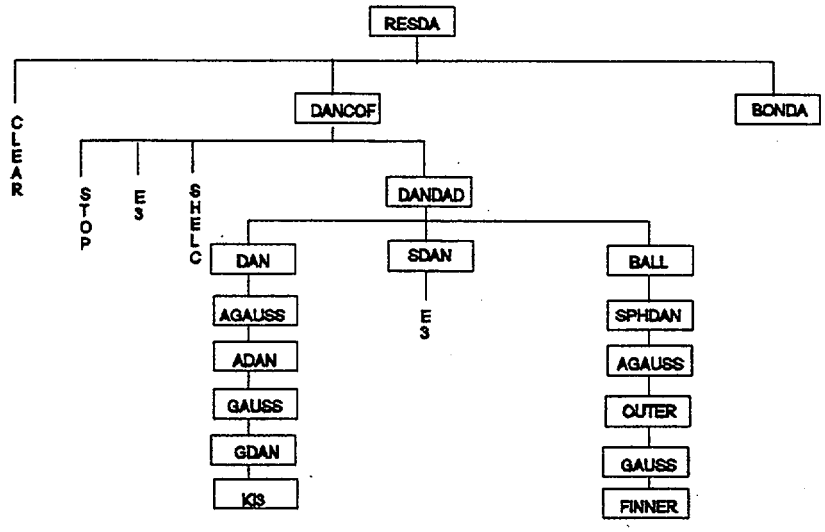

Figure M7.3.9 Flow chart for generating resonance data

RESDA - This subroutine is responsible for determining the resonance data required by NITAWL-II and BONAMI for each nuclide having resonance information in the master cross-section library. CLEAR is called to clear arrays. ALOG is used in calculating the average logarithmic slowing-down decrement for determining the first and second moderator for NITAWL-II. DANCOF is called to provide Dancoff factors[1,8] for resonance materials. BONDA is called to provide a factor to be used in calculating the escape cross section for materials having Bondarenko data.

CLEAR - This library routine is called to clear storage arrays.

DANCOF - This subroutine controls the calculation of the Dancoff factors for the different zones in the cell. It determines the Dancoff factor across the inner surface for a curvilinear coordinate system and calculates the Dancoff factor to an outer curved surface that has a white boundary condition applied to it. E3 is used to determine the Dancoff factor for slabs, and SHELC is used to determine the Dancoff factor across cylindrical shells. DANDAD is called to provide the Dancoff factor for a LATTICECELL problem.

STOP - This library routine is called to write error messages.

E3 - This library routine is a third-order exponential integral function.

SHELC - This library routine evaluates the transmission probabilities for a cylindrical shell.

DANDAD - This subroutine provides Dancoff factors between fuel lumps in a LATTICECELL calculation. DAN provides Dancoff factors for cylindrical geometry; SDAN, for slab geometry; and BALL, for spherical geometry. The Dancoff factors are part of the resonance data required by NITAWL-II and BONAMI to reduce the effective escape probability from the fuel in a heterogeneous lattice. See Sect. M7.2.5.3 for additional information concerning Dancoff factors.

DAN - This subroutine provides the Dancoff factors for the nearest and next-nearest cylinders in an array having a square or triangular pitch. ERRSET is used to trap errors caused by invalid arguments to the arcsine or arccosine routines by invoking subroutine ARCHK. ACOS, SQRT, and COS are used in determining the limits for the outer integration loop to be provided to AGAUSS.

AGAUSS - This subroutine uses a Gaussian quadrature to numerically evaluate the outer integral of the double integral defining the Dancoff factor.

ADAN - This function provides point-by-point values of the outer integral of the Dancoff equation for cylindrical geometry. COS, SQRT, ACOS, SIN, and ASIN are used in evaluating this Dancoff equation. ADAN also provides the limits for the inner integration.

GAUSS - This subroutine uses a Gaussian quadrature to numerically evaluate the inner integral of the double integral defining the Dancoff factor.

GDAN - This subroutine provides point-by-point values of the inner integral of the Dancoff equation for cylindrical geometry. COS, SQRT, ACOS, SIN, and ASIN are used in evaluating the Dancoff equation. The library routine KI3 is used to evaluate the third-order Bickley function, which evaluated the effect of the moderating material between the cylinders.

SDAN - This subroutine determines the Dancoff factor for slab geometry. ALOG and ABS are used in this determination.

BALL - This subroutine computes the Dancoff factor for spherical geometry in an array having a square or triangular pitch.

SPHDAN - This subroutine sets up the double integration required in the evaluation of the Dancoff factor in spherical geometry.

OUTER - This function provides point-by-point values for the outer integral of the Dancoff equation for spherical geometry.

FINNER - This function provides point-by-point values for the inner integral of the Dancoff equation for spherical geometry. COS, SIN, ABS, ACOS, SQRT, and EXP are utilized in this evaluation.

BONDA - This subroutine provides a geometry-dependent factor that is used in calculating the escape cross section for isotopes having Bondarenko data associated with them. ALOG and SQRT are utilized in the calculations.

M7.3.9 COLLAPSE THE ENERGY GROUP STRUCTURE

Figure M7.3.10 illustrates the portion of the Material Information Processor that collapses the master library to the specified group structure for the SAS sequences.

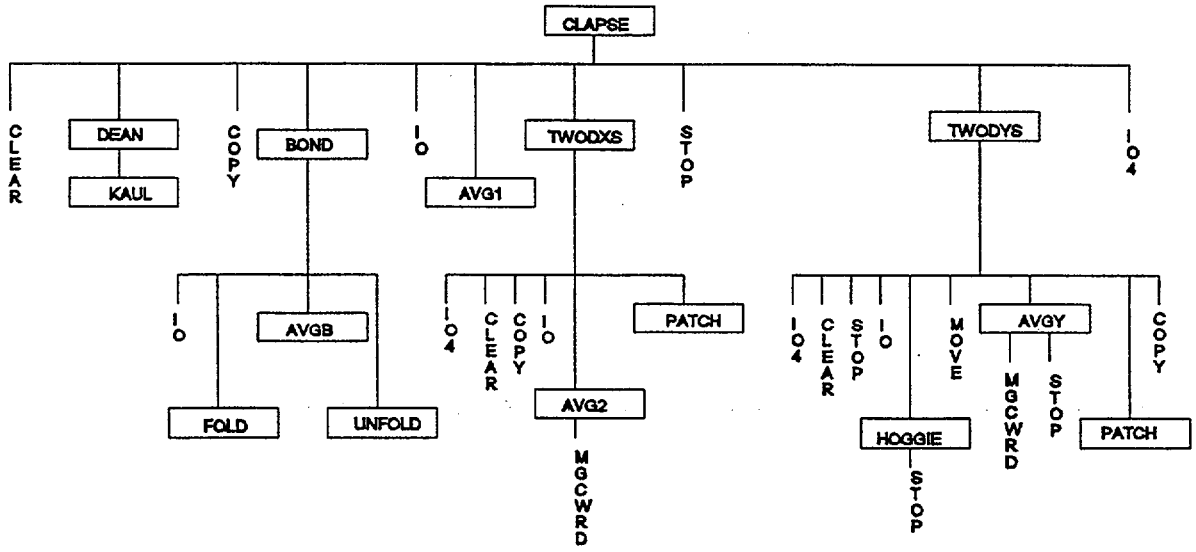

Figure M7.3.10 Flow chart for collapsing the energy group structure for shielding analytical sequences

CLAPSE - This subroutine is responsible for collapsing the master library to the specified group structure for the Shielding Analytical Sequences. It should not be invoked by the Criticality Safety Analytical Sequences. The call to CLAPSE is triggered by entering COLL in MORE DATA. See Sect. M7.4.8 for input data details.

CLEAR - This library routine is used to zero the work space.

DEAN - This subroutine reads the energy group boundaries.

KAUL - This subroutine generates the collapsed energy group boundaries and the collapsed flux spectrum. It is called once to process neutron data and once to process gamma data.

COPY - This library routine is used to copy data from one library to another.

BOND - This subroutine controls processing the Bondarenko data to obtain collapsed Bondarenko data.

IO - This library routine is called several times to read and write data.

FOLD - This subroutine multiplies the Bondarenko factors by the cross sections.

AVGB - This subroutine collapses the folded Bondarenko factors and the cross sections.

UNFOLD - This subroutine divides the collapsed and folded Bondarenko factors by the collapsed cross sections to obtain collapsed Bondarenko factors.

AVG1 - This subroutine collapses the 1-D neutron and gamma cross sections.

TWODXS - This subroutine collapses the 2-D neutron and gamma cross sections. IO4 is used to read and write the 2-D scattering matrix directory. COPY is used several times to copy data from the old library to a scratch file and from the scratch file to the new library. CLEAR is used to zero working arrays. IO is used several times reading and writing data to various units.

AVG2 - This subroutine is used to collapse the 2-D scattering or transfer arrays. The library routine MGCWRD is used to decipher "magic" words that define the contents of subsequent cross-section data strings.

PATCH - This subroutine defines the first group transfer of every empty array to be zero.

TWODYS - This subroutine governs the collapsing of the gamma production arrays. IO4 is used to read and write the production array directory. MOVE is called to move data from one array to another. STOP is called to write error messages. IO is used several times for reading and writing data. CLEAR is used to zero arrays and COPY is used to copy the weighted yield libraries from the scratch unit to the new library.

HOGGIE - This subroutine generates flux integrated fine- and broad-group cross sections for converting the yield arrays to cross-section arrays. STOP is called to write an error message.

AVGY - This subroutine collapses the 2-D gamma production array. The library routine MGCWRD is used to decipher "magic" words within cross-section arrays. These words define the contents of subsequent data strings. STOP is called to write an error message.

M7.4 INPUT DATA GUIDE

This section describes the input data required for the Material Information Processor.

All data are entered in free form, allowing alphanumeric data, floating-point data, and integer data to be entered in an unstructured manner. Eighty columns of data entry are allowed, simulating a card of data. Data can usually start or end in any column. Each data entry must be followed by one or more blanks to terminate the data entry. For numeric data, either a comma or a blank can be used to terminate each data entry. Integers may be entered for floating values. For example, 10 will be interpreted as 10.0. Imbedded blanks are not allowed within a data entry unless an E precedes a single blank as in an unsigned exponent in a floating-point number. For example, 1.0E 4 would be correctly interpreted as 1.0×10^4.

The word "END" is a special data item. An "END" may have a name or label associated with it. The name or label associated with an "END" is separated from the "END" by a single blank and is a maximum of 12 characters long. *At least 2 blanks MUST follow every labeled and unlabeled "END." It is the user's responsibility to assure compliance with this restriction. Failure to observe this restriction can result in the use of incorrect or incomplete data without the benefit of warning or error messages.*

Multiple entries of the same data value can be achieved by specifying the number of times the data value is to be entered, followed by either R, *, or $, followed by the data value to be repeated. Imbedded blanks are not allowed between the number of repeats and the repeat flag. For example, 5R12, 5*12, 5$12, or 5R 12, etc., will enter five successive 12's in the input data. Multiple zeros can be specified as nZ where n is the number of zeroes to be entered. The SCALE free-form reading routines are described in more detail in Sect. M3.

The major function of the Material Information Processor is to create binary input data files for BONAMI, NITAWL, and XSDRNPM and/or ICE. Table M7.4.1 lists the I/O units for the cross-section libraries, Standard Composition Library, temporary files, and the binary input data files. Optional files that can be defined include (1) the unit from which XSDRNPM may read fluxes, (2) the unit on which XSDRNPM may write fluxes, (3) unit 7, where ICE may write a card-image ANISN library, and (4) the unit on which ICE may write a binary ANISN library (see Sect. M7.4.8 on optional parameter data).

Table M7.4.1 Description of I/O units utilized by the Material Information Processor

Unit No.	Type of data	Type of file
5	Input	Sequential
11	Short master xsec library	Sequential
70	User-supplied xsecs	AMPX Master Format Library
81	16-group xsecs	AMPX Master Format Library
82	27-group xsecs	AMPX Master Format Library
83	44-group xsecs	AMPX Master Format Library
84	238-group xsecs	AMPX Master Format Library
85	22 neutron-18 gamma xsecs	AMPX Master Format Library
86	18 gamma xsecs	AMPX Master Format Library
87	27-group xsecs for burnup	AMPX Master Format Library
88	27 neutron-18 gamma xsecs	AMPX Master Format Library
89	Standard Composition Library	Direct or random access data file
90	Scratch file	Direct or random access
92	ICE input data	Sequential
96	BONAMI input data	Sequential
97	NITAWL input data	Sequential
98	XSDRNPM input data	Sequential
99	Printed output	Sequentials

M7.4.1 INPUT DATA SUMMARY FOR EXPERIENCED USERS

Section M7.4.1 is provided for the convenience of experienced users. Other users should skip to Sect. M7.4.2, p. M7.4.8.

All the input data for the Material Information Processor are summarized in Table M7.4.2 and presented in more detail in Table M7.4.3. Each component table of Table M7.4.3 is repeated and discussed in detail in Sects. M7.4.3 through M7.4.8.

The Material Information Processor allows terse data input for all data except the standard composition names and the keyword entries in the optional parameter data (MORE DATA). Terse data entry requires the user to enter only as many characters as are necessary to uniquely define the data entry. However, as many characters as are specified by the user must match the name allowed by the code. For example, refer to Table M7.4.2, **Outline of Material Information Processor data**, data position 3. The available choices for the type of calculation are: INFHOMMEDIUM, LATTICECELL, and MULTIREGION. Therefore, I would be sufficient to specify an infinite homogeneous medium, L would be sufficient for LATTICECELL, and M would specify MULTIREGION. If it is desirable to use more characters, the user is free to do so. However, as many characters as are entered must match the name allowed by the code. For example, if INFHOMMEDIUM is to be specified, INFH is correct, but INFI is not.

WARNING: If several choices begin with the same letters, sufficient characters should be entered to uniquely define the name. For example, ASPHSQUAREP and ASPHTRIANGP are identical through the first four characters. If only ASPH is entered, the code will accept the first name whose first four characters are ASPH. This may not be the one the user intended to use.

Table M7.4.2 Outline of Material Information Processor data (see Sect. M7.4.3 for details)

Data position	Type of data	Data entry	Comments
1	TITLE	Enter a title	80 characters
2	Cross-section library name	HANSEN-ROACH 27GROUPNDF4 44GROUPNDF5 238GROUPNDF5 27BURNUPLIB etc.	The currently available libraries are listed in Table M4.1.1.
3	Type of calculation	INFHOMMEDIUM LATTICECELL MULTIREGION	These are the available options. See the explanation in Sect. M7.4.3.
4	Standard Composition specification data	Enter the appropriate data	Terminate this data block with END COMP. See Sect. M7.4.4.
5	Unit cell geometry specification	Enter the appropriate data (optional for INFHOMMEDIUM)	Optional for INFHOMMEDIUM. See Sect. M7.4.5 for INFHOMMEDIUM. See Sect. M7.4.6 for LATTICECELL. See Sect. M7.4.7 for MULTIREGION.
6	Optional parameter data	Enter the desired data	Precede this data block by MORE DATA if more parameter data are to be entered. Otherwise, omit these data entirely. See Sect. M7.4.8.

Table M7.4.3 Tables of Material Information Processor data requirements

Outline of standard compositions specification data (see Sect. M7.4.4 for details)

Entry No.	Variable name	Type of data	Entry requirement	Comments
1	SC	Standard composition component name	Always	Enter once for each standard composition. Enter the alphanumeric description from Sect. M8.2. Additional allowed names include those beginning with ARBM for arbitrary materials, and SOLN for solutions.
A1	ROTH	Theoretical density of material (g/cc)	ARBM	Enter once for each arbitrary material.
A2	NEL	Number of elements or nuclides in the material	ARBM	Enter once for each arbitrary material.
A3	IVIS	No longer used but must still be entered	ARBM	Enter once for each arbitrary material. Enter 0 or 1.
A4	ICP	Compound indicator	ARBM	Enter once for each arbitrary material. Enter 1 for a chemical compound, 0 for alloys, mixtures, etc.
A5	IRS	No longer used but must still be entered	ARBM	Enter once for each standard composition component that is an arbitrary material. Enter 0 or 1.
A6	NCZA	ID number (from far right column of Table M8.2.1 or M8.2.2)	ARBM	Repeat the sequences A6 and A7 for each element in the arbitrary material before entering entry number 2. Enter the number from the far right column of Table M8.2.1 or M8.2.2. (Premixed standard compositions cannot be used in an arbitrary material definition.)
A7	ATPM	Number of atoms of this element per molecule of arbitrary material or Weight percent of this element in this arbitrary material	ARBM & ICP = 1 or ARBM & ICP = 0	Repeat the sequence A6 and A7 for each element in the arbitrary material before entering entry number 2. Do not enter a value unless ICP = 1. or Repeat the sequence A6 and A7 for each element in the arbitrary material before entering entry number 2. Do not enter a value unless ICP = 0.

Table M7.4.3 (continued)

Outline of standard compositions specification data (continued)

Entry No.	Variable name	Type of data	Entry requirement	Comments
2	MX	Mixture ID number	Always	Enter once for each standard composition component.
S1	FD	Fuel density (grams of U or Pu per liter of solution)	SOLN	Enter once for a solution.
S2	AML	Acid molarity of the solution	SOLN	Enter once for a solution. AML = 0 if there is no acid in the solution.
O1	SPGR or ROTH	Specific gravity of the solution or Density of the basic standard composition	Optional	If the specific gravity (SPGR) of the solution is known, it should be entered as SPG = SPGR. or If the density of a basic standard composition (ROTH) is to be entered, use DEN = ROTH.
3	VF	Density multiplier	See comment column	Enter the density multiplier (density fraction, volume fraction, or a combination). Default value is 1. This item can be omitted if entries 4, 5, 6a, and 6b are also omitted. VF = 0 is not allowed for SOLN or ARBM.
4	ADEN	Number density (atoms/b-cm) for the nuclide	VF = 0	Enter only if VF = 0.0.
5	TEMP	Temperature, in degrees K	See comment column	Default value is 293 K. This entry can be omitted if entries 6a and 6b are also omitted.
6a	IZA	Isotope's ZA number	VF ≠ 0	Enter for each isotope in a multiple isotope nuclide. Omit if VF = 0. Entries 6a and 6b are entered in pairs until each isotope in the nuclide is defined.
6b	WTP	Weight percent of the isotope	VF ≠ 0	Enter for each isotope in a multiple isotope nuclide. Omit if VF = 0.0. Entries 6a and 6b are entered in pairs until each isotope in the nuclide is defined.
7	END	Terminate a standard composition	Always	Enter once for each standard composition component. This terminates the data for a standard composition component. Enter END to terminate the component. Repeat entries 1 through 7 until all the mixtures have been defined. At least two blanks must separate entry 7 from the next entry.
	END COMP	Terminate the data block	Terminus	Enter once for a problem. Enter the words END COMP when all the standard composition components have been described. At least two blanks must follow the END COMP.

NOTE: Entry 7 should not begin in column 1 unless a name is associated with it.
At least two blanks should separate the last entry 7 from the END COMP.

Table M7.4.3 (continued)

Optional unit cell specifications for INFHOMMEDIUM problems (see Sect. M7.4.5 for details)

Entry number	Variable name	Type of data	Data entry	Comments
1	NAME	Keyword	CELLMIX	Initiate reading cell data for INFHOMMEDIUM.
2	MFUEL	Mixture number in the cell	Mixture number	Specifies the mixture number to be used in the cell. Defaults to the smallest mixture number entered in the Standard Composition Data.

NOTE: Unit cell data are necessary for INFHOMMEDIUM only if a mixture number other than the smallest mixture number is to be used in the cell and a control sequence that executes XSDRNPM has been specified. If mixtures 1, 2, and 3 are specified and mixture 3 is to be used in the cell, enter CELLMIX 3.

Unit cell specification for LATTICECELL problems (see Sect. C4.4.6 for details)

Entry No.	Variable name	Type of data	Entry requirement	Data entry	Comments
1	CTP	Type of lattice	Always		Describes the type of lattice or array configuration.
				SQUAREPITCH	Use for cylindrical rods in a square pitch.
				ASQUAREPITCH	Use for annular cylindrical rods in a square pitch.
				ASQP	Use for annular cylindrical rods in a square pitch.
				TRIANGPITCH	Use for cylindrical rods in a triangular pitch.
				ATRIANGPITCH	Use for annular cylindrical rods in a triangular pitch.
				ATRP	Use for annular cylindrical rods in a triangular pitch.
				SPHSQUAREP	Use for spherical pellets in a cubic lattice.
				ASPHSQUAREP	Use for annular spherical pellets in a cubic lattice.
				ASSP	Use for annular spherical pellets in a cubic lattice.
				SPHTRIANGP	Use for spherical pellets in a bi-centered or face centered hexagonal close-packed lattice.
				ASPHTRIANGP	Use for spherical pellets in a bi-centered or face centered hexagonal close-packed lattice.
				ASTP	Use for spherical pellets in a bi-centered or face centered hexagonal close-packed lattice.
				SYMMSLABCELL	Use for a symmetric array of slabs.
				ASYMSLABCELL	Use for a periodic, but asymmetric array of slabs.
2	PITCH	Array pitch (cm)	Always	Appropriate dimension	The center-to-center spacing (cm) between fuel lumps. For asymmetric slab cell, enter the distance from the center of one moderator to the center of the other moderator (cm).

Table M7.4.3 (continued)

Unit cell specification for LATTICECELL problems (see Sect. C4.4.6 for details) (continued)

Entry No.	Variable name	Type of data	Entry requirement	Data entry	Comments
3	FUELOD	Outside dimension of fuel (cm)	Always	Appropriate dimension	Outside diameter of fuel (cm), or the thickness of the fuel in a slab.
4	MFUEL	Fuel mixture number	Always	Mixture number	Mixture number representing the fuel.
5	MMOD	Moderator mixture number	Always	Mixture number	Mixture number representing the moderator
6	MMOD2	2nd moderator mixture number	Annular cell	Mixture number	Mixture number representing the second moderator.
7	TKMOD2	2nd moderator thickness or 2nd moderator diameter (cm)	ASYMSLABCELL or annular cell	Thickness or Diameter	Thickness of the second moderator (cm) for ASYMSLABCELL. or Diameter of inner moderator (cm) for other annular cells.
8	CLADOD	Outside diameter of clad (cm)	If clad	Clad OD	OMIT IF NO CLAD. For a slab, CLADOD is the sum of thickness of the fuel, gap, and clad.
9	MCLAD	Clad mixture number	If clad	Mixture number	OMIT IF NO CLAD. Mixture number representing the clad.
10	CLADID	Inside diameter of clad (cm)	If gap	Clad ID	OMIT IF NO GAP between the fuel and clad.
11	MGAP	Gap mixture number	If gap	Mixture number	OMIT IF NO GAP between the fuel and clad A mixture number of zero is often used.
12	END	Terminate LATTICECELL data	Always	END	Terminate the LATTICECELL input data by entering the word END. Do not start in column 1. At least two blanks must follow entry No. 12.

Table M7.4.3 (continued)

Unit cell specification for MULTIREGION problems (see Sect. C4.4.7 for details)

Entry No.	Variable name	Type of data	Entry requirement	Data entry	Comments
1	CS	Type of geometry	Always		Describes the type of geometry. The options are listed below.
				SLAB	Use for slab geometry.
				CYLINDRICAL	Use for cylindrical geometry.
				SPHERICAL	Use for spherical geometry.
				BUCKLEDSLAB	Use for slab geometry with a buckling correction for the two transverse directions.
				BUCKLEDCYL	Use for cylindrical geometry with a buckling correction in the axial direction.
2	BR	Right boundary condition	Required for BUCKLEDSLAB & BUCKLEDCYL Optional for other geometries		Default is VACUUM. Describes the right/outside boundary condition.
				VACUUM	This provides a non-return condition at the boundary.
				REFLECTED	Do not use for cylindrical or spherical.
				PERIODIC	Do not use for cylindrical or spherical.
				WHITE	This provides isotopic return at the boundary.
3	BL	Left boundary condition	Required for BUCKLEDSLAB & BUCKLEDCYL Optional for other geometries		Default is REFLECTED. Describes the left boundary condition.
				VACUUM	This provides a non-return condition at the boundary.
				REFLECTED	Recommended for cylindrical or spherical.
				PERIODIC	Do not use for cylindrical or spherical.
				WHITE	This provides isotropic return at the boundary.
4	ORGN	Location of left boundary on the x-axis (cm)	BUCKLEDSLAB & BUCKLEDCYL Optional for other geometries	Appropriate dimension	Default is 0.0. Should not be changed for cylindrical or spherical geometry. A value must be entered if subsequent data are to be entered.
5	DY	Buckling height (cm)	BUCKLEDSLAB & BUCKLEDCYL	Appropriate dimension	OMIT FOR SLAB, CYLINDRICAL, and SPHERICAL. This corresponds to one of the transverse dimensions of an actual 3-D slab assembly or to the length of a finite cylinder.
6	DZ	Buckling depth (cm)	BUCKLEDSLAB	Appropriate dimension	OMIT UNLESS BUCKLEDSLAB WAS SPECIFIED. This is the buckling depth corresponding to the second transverse dimension of a 3-D slab assembly.
7	END	End geometry parameters	Always	END	Enter the word END. Do not start in column 1. At least two blanks must separate entry 7 from the first entry 8.
8	MXZ	Mixture number in the zone	Always	Mixture number	Repeat entry numbers 8-10 until all zones are defined. Enter the mixture number for this zone.

Table M7.4.3 (continued)

Unit cell specification for MULTIREGION problems (see Sect. C4.4.7 for details)

Entry No.	Variable name	Type of data	Entry requirement	Data entry	Comments
9	RZ	Outside radius of the zone (cm)	Always	Appropriate dimension	Repeat entry numbers 8-10 until all zones are defined. Enter the outside dimension of the zone (cm).
10	XMOD	External moderator index	Optional		Repeat entry numbers 8-10 until all zones are defined. Entry 10 is optional and can be omitted. If it is omitted, repeat entry numbers 8 and 9 until all zones are defined.
				NOEXTERMOD	No moderating materials in the adjacent zones.
				ONEEXTERMOD	A moderating material is present in one adjacent zone.
				TWOEXTERMOD	Moderating materials are present in two adjacent zones.
	END ZONE	Terminate zone data		END ZONE	Enter when all zones have been defined by repeating entry numbers 8 through 10 for each zone. At least two blanks must follow this entry.

Table M7.4.3 (continued)
Summary of available optional parameter data (see Sect. C4.4.8)

Entry No.	Keyword name	Type of data	Applicable module	Comments
1	MORE DATA	Input flag		This signals that optional parameter data will be entered. Enter only those parameters you wish to change.
2	ISN=	Order of angular quadrature	XSDRNPM	The default value is 8. This allows using another value.
3	SZF=	Spatial mesh size factor	XSDRNPM	The default value is 1.0. 0<SZF<1.0 gives a finer mesh. SZF>1.0 gives a coarser mesh. SZF ≤0 user specifies the number of mesh intervals in each zone.
4	IIM=	Max. number of inner iterations	XSDRNPM	The default value is 20. This allows using another value.
5	ICM=	Max. number of outer iterations	XSDRNPM	The default value is 25. This allows using another value.
6	EPS=	Overall convergence criteria	XSDRNPM	The default value is 0.0001. This allows using another value.
7	PTC=	Point convergence criteria	XSDRNPM	The default value is 0.0001. This allows using another value.
8	BKL=	Buckling factor	XSDRNPM	The default value is 1.420892. Use ONLY for a MULTIREGION problem that specifies BUCKLEDSLAB or BUCKLEDCYL.
9	IUS=	Upscatter scaling factor	XSDRNPM	The default value is zero. IUS=0 doesn't utilize upscatter scaling. IUS=1 uses upscatter scaling to accelerate the solution and/or speed convergence.
10	RES=	Resonance data	BONAMI NITAWL	Enter the mixture number, geometry type (SLAB, CYLINDER, SPHERE) and the thickness of the slab or radius of the sphere or cylinder, in cm. Optionally enter the inner radius (cm) to specify an annular cylinder or sphere.
11	DAN(mm)=	Dancoff factor for the specified mixture	BONAMI NITAWL	Enter the mixture number, mm, to which the Dancoff factor applies inside the parentheses; enter the Dancoff factor after the equal sign. **Repeat entry numbers 10 and 11 for all resonance mixtures used in the problem that are not treated in the LATTICECELL or MULTIREGION description.**
12	BAL=	Key to print balance tables	XSDRNPM	The default value is FINE. BAL=NONE suppresses printing the balance table. BAL=ALL prints all balance tables. BAL=FINE prints only the fine-group balance tables.
13	DY=	First transverse dimension	XSDRNPM	The first transverse dimension, in cm, used in a buckling correction to calculate leakage normal to the principal calculation direction (i.e., the height of a slab or a cylinder).
14	DZ=	Second transverse dimension	XSDRNPM	The second transverse dimension in centimeters used for a buckling correction (i.e., the width of a slab).
15	COF=	Diffusion coefficient option for transverse leakage corrections	XSDRNPM	The default is 0. See Sect. F3.5, 3$ array, variable IPN.
16	FRD=	Unit from which fluxes will be read	XSDRNPM	Enter the unit number from which the flux guess for XSDRNPM will be read.

Table M7.4.3 (continued)

Summary of available optional parameter data (see Sect. C4.4.8)

Entry No.	Keyword name	Type of data	Applicable module	Comments
17	FWR=	Unit on which fluxes will be written	XSDRNPM	Enter the unit number where the binary fluxes from XSDRNPM will be written.
18	ADJ=	Adjoint mode flag	XSDRNPM	Enter a 1 to cause XSDRNPM to solve the problem in adjoint mode
19	NBU=	Unit on which balance tables will be written	XSDRNPM	Enter the unit number where the balance tables from XSDRNPM will be written
20	WGT=	Cross-section weighting flag	XSDRNPM	Enter a 0 to suppress doing the cross-section weighting in XSDRNPM
21	ZMD(iz)=	Zone width modifier for the specified zone	XSDRNPM	Enter the zone number for which the modifier applies inside the parentheses; enter the zone width modifier after the equal sign. **Repeat number 20 to specify all zones to be modified in a search.**
22	INT(iz)=	Number of intervals for the specified zone	XSDRNPM	Enter the zone number inside the parentheses; enter the number of intervals after the equal sign. Repeat number 22 to specify all needed zones.
23	KEF=	Value of k_{eff} to be searched for	XSDRNPM	Enter the value of k_{eff} that it is desired to search for. The default is 1.0.
24	KFM=	Value of the eigenvalue modifier	XSDRNPM	Enter the value of the eigenvalue modifier (i.e., the relative change for the first guess of a search). The default is -0.1.
25	DAB=	Number of direct access data blocks	MIP[a]	The default is 200. Number of blocks allocated for direct access unit 90.
26	AXS=	Unit on which a mixed ANISN library will be written	ICE	Enter the unit number where ICE is to write a mixed ANISN library.
27	MSH=	Maximum number of mesh points/resonance	NITAWL	The default value is 2001. This allows using another value.
28	MLV=	Highest resonance ℓ-value for self-shielding	NITAWL	The default value is 2. This allows using another value.
29	ID1=	Print control for scalar fluxes	XSDRNPM	The default value is -1. See Sect. F3.5, 2$ array, variable ID1.
30	COLL	Key to activate collapse of thermal groups	MIP[a]	Enter COLL to collapse all thermal groups into one group for the shielding sequences.
31	END	Terminus		Terminate the optional parameter data. Do not start in column 1. At least two blanks must follow this entry.

[a]MIP is the Material Information Processor.

M7.4.2 PARAMETERS FOR DATA CHECKING AND SPACE ALLOCATION

To check the Material Information Processor input data, run CSASN and specify PARM=CHECK or PARM=CHK starting after column 10 of the analytical sequence specification as shown below.

```
=CSASN    PARM=CHK
or
#CSASN    PARM=CHK
```

The data are checked, the problem description is printed, appropriate error and warning messages are printed, and a table of additional data is printed. These data include the mixing table, resonance data, NITAWL data, CSAS(XSDRN) data, and BONAMI data. An example of this output is given in Sect. M7.6. The region size for a problem can be specified by the user by entering PARM=SIZE=nnnn starting after column 10 of the analytical sequence specification. The region size, nnnn, is specified in words. The following examples run CSASN and set the region size to 120,000 words.

```
=CSASN    PARM=SIZE=120000
#CSASN    PARM=SIZE=120000
```

To run CSASN and utilize data checking with the region size set to 120,000 words, enter an analytical sequence specification as shown below. PARM should start after column 10.

```
=CSASN    PARM=(CHECK,SIZE=120000)
=CSASN    PARM=(SIZE=120000,CHECK)
=CSASN    PARM='CHECK,SIZE=120000'
=CSASN    PARM='SIZE=120000,CHECK'
```

M7.4.3 MATERIAL INFORMATION PROCESSOR DATA

The Material Information Processor reads the standard composition specification data and the unit cell geometry specifications. It then produces the mixing table and unit cell information necessary for processing the cross sections. Table M7.4.4 outlines the input data for the Material Information Processor.

The input data for the Material Information Processor are identical to the input for CSAS1 of SCALE 3.1 and older versions of SCALE with the following exceptions:

- The analytical sequence card is considered to be part of the overall data input.
- Items 2, 3, 4, 6, and 7 from Sect. C1.6 of SCALE 3.1 and older versions of SCALE are omitted from the parameter card.
- The words END COMP are entered to signal the completion of the standard composition specification data.
- The MULTIREGION zone description data are terminated by the words END ZONE.
- If optional control parameters are entered, the words MORE DATA must precede the first optional parameter data entry.

Table M7.4.4 Outline of Material Information Processor data

Outline of Material Information Processor Data (see Sect. C4.4.3 for details)

Data position	Type of data	Data entry	Comments
1	TITLE	Enter a title	80 characters
2	Cross-section library name	HANSEN-ROACH 27GROUPNDF4 44GROUPNDF5 238GROUPNDF5 27BURNUPLIB etc.	The currently available libraries are listed in Table M4.1.1.
3	Type of calculation	INFHOMMEDIUM LATTICECELL MULTIREGION	These are the available options. See the explanation in Sect. M7.4.3.
4	Standard Composition specification data	Enter the appropriate data	Terminate this data block with END COMP. See Sect. M7.4.4.
5	Unit cell geometry specification	Enter the appropriate data (optional for INFHOMMEDIUM)	Optional for INFHOMMEDIUM. See Sect. M7.4.5 for INFHOMMEDIUM. See Sect. M7.4.6 for LATTICECELL. See Section M7.4.7 for MULTIREGION.
6	Optional parameter data	Enter the desired data	Precede this data block by MORE DATA if more parameter data are to be entered. Otherwise, omit these data entirely. See Sect. M7.4.8.

Note that the CSAS1 program is not included in SCALE beginning with the SCALE-4 release.

The Material Information Processor allows terse data input for all data except the standard composition names and the keyword entries in the optional parameter data (MORE DATA). Terse data entry requires the user to enter only as many characters as are necessary to uniquely define the data entry. However, as many characters as are specified by the user must match the name allowed by the code. For example, refer to Table M7.4.4, **Outline of Material Information Processor data**, data position 3. The available choices for the type of calculation are: INFHOMMEDIUM, LATTICECELL, and MULTIREGION. Therefore, it would be sufficient to specify I for an infinite homogeneous medium, L for LATTICECELL, and M for MULTIREGION. If it is desirable to use more characters, the user is free to do so. However, as many characters as are entered must match the name allowed by the code. For example, if INFHOMMEDIUM is to be specified, INFH is correct, but INFI is not.

WARNING: If several choices begin with the same letters, sufficient characters should be entered to uniquely define the name. For example, ASPHSQUAREP and ASPHTRIANGP are identical through the first four characters. If only ASPH is entered, the code will accept the first name whose first four characters are ASPH. This may not be the one the user intended to use.

The types of data required for the Material Information Processor are given in Table M7.4.4. The individual entries are explained in the text following the table.

1. TITLE...An 80-character title is required. The title is the first 80 characters of the Material Information Processor data.

2. CROSS-SECTION LIBRARY NAME...This item specifies the cross-section library that is to be used in the calculation. See Sect. M4, Table M4.1.1, for a discussion of the available libraries.

3. TYPE OF CALCULATION...The options are INFHOMMEDIUM, LATTICECELL, and MULTIREGION.

   INFHOMMEDIUM is used for an infinite homogeneous medium. It provides cross sections to represent large homogeneous pieces. The cross sections are treated as if each mixture is infinite. Thus, the self-shielding calculations will not account for any geometrical effects. By default, the smallest mixture number will be used in the cell. A different mixture can be specified as described in Sect. M7.4.5 and Table M7.4.6.

   LATTICECELL is used when the geometry can be described as a lattice. It is especially suited for arrays of cylindrical rods or spherical pellets. The use of LATTICECELL requires the entry of additional geometry information (unit cell specification), which is described in Sect. M7.4.6 and Table M7.4.7. When the problem consists of an array of fuel bundles or similar geometry, the cross sections are corrected for resonance self-shielding, including geometry effects. If cell-weighted cross sections are desired, an appropriate control sequence must be used (CSAS2X, for example). A flux disadvantage factor is then applied to the cross sections of the materials that are used in the unit cell.

   MULTIREGION may be used to define a geometric configuration that is more complicated than that allowed by LATTICECELL. It can also be used for a system involving large geometric regions where geometry effects may be minimal. The cross sections utilized in the unit cell are corrected for resonance self-shielding, and an appropriate Dancoff factor is applied (see Sect. M7.2.4.3). If a cell-weighted mixture is generated, it is derived from homogenizing the entire MULTIREGION unit cell. The additional geometry information (Unit Cell Specification) required for a MULTIREGION problem is described in Sect. M7.4.7 and Table M7.4.8.

4. STANDARD COMPOSITIONS...These data are used to define the mixtures that will be used in the problem. See Sect. M7.4.4 and Table M7.4.5 for a description of the standard composition specification data. These data are required for every problem.

5. CELL GEOMETRY SPECIFICATION...See Sect. M7.4.5, and Table M7.4.6 for an explanation of the optional unit cell data associated with an INFHOMMEDIUM problem. See Sect. M7.4.6 and Table M7.4.7 for an explanation of the data associated with LATTICECELL problems. Section M7.4.7 and Table M7.4.8 explain the data required for a MULTIREGION problem.

6. OPTIONAL PARAMETER DATA...This option allows certain defaulted parameters to be respecified by the user. Omit these data unless they are needed. If data are to be entered, see Sect. M7.4.8 and Table M7.4.9 for assistance.

M7.4.4 STANDARD COMPOSITION SPECIFICATION DATA

The standard composition specification data are used to define mixtures that are to be utilized in the problem. These data can be considered to be a mixing table that defines mixtures in terms of standard composition specification data (available from Sect. M8.2, Table M8.2.1). The required input for the standard composition specification data varies, depending on the standard composition component name. However, every standard composition specification must include the following:

1. a standard composition component name (SC),

2. the mixture that contains this component (MX), and

3. a terminator for the standard composition specification data (enter the word END).

Enter as many standard composition specifications as necessary to define all the mixtures needed for the problem. When all the necessary mixtures have been described, enter the words END COMP to signal the completion of this type of data.

The data required to define a standard composition specification are contained in Table M7.4.5. In the column entitled "Entry Requirement," "ARBM" is used to denote entries required only for arbitrary materials, and "SOLN" is used for entries required only for solutions.

The input data for standard composition specifications are arranged with entry numbers 1 through 7 that apply to all standard composition data. Entries A1 through A7 apply only to arbitrary materials. Entries S1 and S2 apply only to solutions. Entry O1 is optional information that applies to both basic standard composition and solutions. The individual entries specified in Table M7.4.5 are explained in more detail in the text following the table.

1. SC STANDARD COMPOSITION COMPONENT NAME...The names of the standard composition components (the alphanumeric identifiers) may be (1) chosen from Sect. M8.2, which contains the list of elements, compounds, and alloys found in the Standard Composition Library; (2) chosen from the table of available solutions, Sect. M8.3; or (3) designated as an arbitrary material (ARBM). An error message will be printed if the user enters an invalid standard composition component name as if the composition does not exist in the specified library.

   For standard compositions taken from Sect. M8.2 of the Standard Composition Library (basic standard composition), certain data such as the volume fraction or theoretical density and other engineering-type data may need to be entered. For standard compositions containing more than one isotope of an element (such as UO_2), the user is free to specify the weight percent for each isotope, such that they total 100%. See Sect. M7.5.5.1 for examples of basic standard compositions.

Table M7.4.5 Outline of standard composition specification data

Outline of standard compositions specification data (see Sect. C4.4.4 for details)

Entry number	Variable name	Type of data	Entry requirement	Comments
1	SC	Standard composition component name	Always	Enter once for each standard composition. Enter the alphanumeric description from Sect. M8.2. Additional allowed names include those beginning with ARBM for arbitrary materials and SOLN for solutions
A1	ROTH	Theoretical density of material (g/cc)	ARBM	Enter once for each standard composition component that is an arbitrary material
A2	NEL	Number of elements in the material	ARBM	Enter once for each standard composition component that is an arbitrary material
A3	IVIS	No longer used but must still be entered	ARBM	Enter once for each standard composition component that is an arbitrary material. Enter 0 or 1
A4	ICP	Compound indicator	ARBM	Enter once for each standard composition component that is an arbitrary material. Enter 1 for a compound, 0 for alloys, mixtures, etc.
A5	IRS	No longer used but must still be entered	ARBM	Enter once for each standard composition component that is an arbitrary material. Enter 0 or 1
A6	NCZA	ID number (from far right column of Table M8.2.1)	ARBM	Repeat the sequences A6 and A7 for each element or isotope in the arbitrary material before entering entry number 2. Enter the number from the far right column of Table M8.2.1 or M8.2.2. (Premixed standard compositions cannot be used in an arbitrary material definition)
A7	ATPM	Number of atoms of this element per molecule of arbitrary material	ARBM & ICP=1	Repeat the sequence A6 and A7 for each element in the arbitrary material before entering entry number 2. Do not enter a value unless ICP=1
		or	or	or
		Weight percent of this element in this arbitrary material	ARBM & ICP=0	Repeat the sequence A6 and A7 for each element in the arbitrary material before entering entry number 2. Do not enter a value unless ICP=0

Table M7.4.5 (continued)

Outline of standard compositions specification data (continued)

Entry number	Variable name	Type of data	Entry requirement	Comments
2	MX	Mixture ID number	Always	Enter once for each standard composition component
S1	FD	Fuel density (grams of U or Pu per liter of solution)	SOLN	Enter once for a solution
S2	AML	Acid molarity of the solution	SOLN	Enter once for a solution. AML=0 if there is no acid in the solution
O1	SPGR	Specific gravity of the solution	Optional	If the specific gravity (SPGR) of the solution is known, it should be entered as SPG=SPGR
	or	or		or
	ROTH	Density of the basic standard composition		if the density of a basic standard composition (ROTH) is to be entered, use DEN=ROTH
3	VF	Density multiplier	See comment column	Enter the density multiplier (density fraction, volume fraction, or a combination). Default value is 1. This item can be omitted if entries 4, 5, 6a, and 6b are also omitted. VF=0 is not allowed for SOLN or ARBM
4	ADEN	Number density (atoms/b-cm) for the nuclide	VF=0	Enter only if VF=0.0
5	TEMP	Temperature, in K	See comment column	Default value is 293 K. This entry can be omitted if entries 6a and 6b are also omitted
6a	IZA	Isotope's ZA number	VF≠0	Enter for each isotope in the standard composition component. Omit if VF=0. Entries 6a and 6b are entered in pairs until each isotope in the component is defined
6b	WTP	Weight percent of the isotope	VF≠0	Enter for each isotope in the standard composition component. Omit if VF=0.0. Entries 6a and 6b are entered in pairs until each isotope in the component is defined
7[a]	END	Terminate a standard composition	Always	Enter once for each standard composition component. This terminates the data for a standard composition component. Enter END to terminate the component. Repeat entries 1 through 7 until all the mixtures have been defined. At least two blanks must separate entry 7 from the next entry
	END COMP	Terminate the data block	Terminus	Enter once for a problem. Enter the words END COMP when all the standard composition components have been described. At least two blanks must follow the END COMP

[a]NOTE: Entry 7 should not begin in column 1 unless a name is associated with it.
At least two blanks should separate the last entry 7 from the END COMP.

Solutions require the specification of the density of the heavy metal in the solution and the acid molarity of the solution. The alphanumeric specification of a solution starts with the four characters "SOLN." Some common fissile solutions are SOLNUO2(NO3)2, SOLNPU(NO3)4, and SOLNUO2F2. See Sect. M8.3 for a complete listing of the available solutions. Sections M7.5.5.3 and M7.5.9 contain examples of the input data for solutions.

Arbitrary materials require the user to provide all the information normally found in the Standard Composition Library. The arbitrary material option allows specifying a compound or alloy not available in the Standard Composition Library by utilizing the standard composition available in the library.

An arbitrary material name must start with the four characters "ARBM." A maximum of twelve characters is allowed for the standard composition component name. Imbedded blanks are not allowed in a standard composition component name. Section M7.5.5.2 contains input data for arbitrary materials.

An additional example of an arbitrary material specification is given below:

Consider a mixture of boral having 35 wt % B_4C, 65 wt % Al and an overall density of 2.64 g/cc. If neither BORAL nor B4C were available in the Standard Composition Library, the components BORON, C, and AL could be used as basic standard compositions to describe the boral. The necessary volume fractions would have to be determined as shown in Sect. M7.5.5.4, examples 3 and 4. By utilizing the arbitrary material option, both B_4C and Al can be described as a component of the same mixture (assume it is desired to be mixture 3), both have a density of 2.64 g/cc and the volume fractions are 0.35 for the B_4C and 0.65 for the Al. The resulting standard composition specification data do not require any calculations (see example 1, Sect. M7.5.5.5 for a similar situation) and could be entered as:

```
ARBMTL-B4C  2.64 2 1 1 0 5000 4 6012 1 3 0.35 END
ARBMTL-AL   2.64 1 0 0 0 13027 100.0 3 0.65 END
```

A1. ROTH — THEORETICAL DENSITY OF MATERIAL...Enter ONLY for arbitrary materials. The density of the arbitrary material is entered in units of g/cc.
NOTE: ROTH can be entered for a basic standard composition as shown by entry O1.

A2. NEL — NUMBER OF ELEMENTS IN THE MATERIAL...Enter ONLY for arbitrary materials. Enter the number of components from the Standard Composition Library that are to be used to define this arbitrary material. In the above example, the ARBMTL-B4C contains two components, the B and the C. Therefore, NEL is 2 for the B_4C arbitrary material. The ARBMTL-AL contains only one component, so NEL is 1 for it.

A3. IVIS — UNUSED VARIABLE...Enter ONLY for an arbitrary material. Enter 0 or 1. Previously used to indicate multiple-isotope nuclide. These data are now automatically obtained from the standard composition library. An arbitrary material may contain more than one multiple-isotope indicator.

A4. ICP — COMPOUND INDICATOR...Enter ONLY for arbitrary materials. A compound is a substance containing more than one constituent element and having properties different from those which their constituents had as elementary substances. The composition of a pure compound is perfectly definite and is always the same, regardless of the method of formation. Examples of compounds are: H_2O, B_4C, CO_2, $Ca(OH)_2$, C_2H_6, Fe_2S_3, Cr_2O_3, etc. ICP is 1 for a compound. ICP is 0 for alloys (stainless steel, Monel, etc.), and conglomerates or mixtures such as concrete.

In the B_4C arbitrary material example, ICP is 1; in the aluminum arbitrary material example, ICP is 0. These examples are given in the explanation of entry number 1, SC.

A5. IRS — UNUSED VARIABLE...Enter ONLY for arbitrary materials. Enter 0 or 1. Previously used to indicate a resonance nuclide. These data are now automatically obtained from the cross-section library. An arbitrary material may contain more than one resonance nuclide.

A6. NCZA — ID NUMBER... Enter ONLY for arbitrary materials. This is the "ZA" ID number for the element or isotope. Usually, NCZA=A+1000*Z, where A is the atomic mass or weight of the nuclide, and Z is the atomic number.

REPEAT THE SEQUENCE NCZA and ATPM (A6 and A7) FOR EVERY ELEMENT IN THE ARBITRARY MATERIAL.

A7. ATPM — Enter ONLY for arbitrary materials. Repeat the sequence A6 and A7 for every element in the arbitrary material before going on to entry 2.

If ICP is 1 (entry A4) enter the NUMBER OF ATOMS PER MOLECULE. If the arbitrary material is a compound (entry A4, ICP is 1), enter the number of atoms of this element per molecule of arbitrary material.

If ICP is 0 (entry A4) enter the WEIGHT PERCENT OF THIS ELEMENT IN THE ARBITRARY MATERIAL. If the arbitrary material is not a compound (entry A4, ICP is 0), enter the weight percent of this element in the arbitrary material. If ICP is 0, the sum of all the weight percents for the arbitrary material MUST be 100.0.

2. MX — MIXTURE ID NUMBER...A mixture number is required on every standard composition specification. It defines the mixture that contains the material defined by the standard composition specification data. The mixture numbers are utilized in the Unit Cell Specification for INFHOMMEDIUM, LATTICECELL, or MULTIREGION problems and the KENO V.a geometry data.

S1. FD — FUEL DENSITY...Enter ONLY for a solution. The standard composition component name for a solution starts with the four characters "SOLN." The available solution names are listed in Sect. M8.3. Enter the fuel density in units of grams of heavy metal (fissile material) per liter of solution.

S2. AML — ACID MOLARITY...Enter ONLY for a solution. If there is no acid in the solution, enter zero. If acid is present in the solution, enter the molarity of the solution.

O1. SPGR or ROTH — OPTIONAL DATA...Does NOT apply to ARBITRARY MATERIALS. These optional data can be entered for a solution or for a basic standard composition using a keyword in the form: SPG=SPGR, DEN=SPGR,DEN=ROTH, or SPG=ROTH. The keywords SPG= and DEN= are interchangeable. SPGR is the specific gravity of the fuel solution. If the standard composition name begins with SOLN and the specific gravity of the solution is known, it should be entered. Otherwise the code has to interpolate in a table to obtain a specific gravity to use in the calculation. ROTH is the specified density of the standard composition in g/cc and can be entered if desired. It should always be entered for materials that contain enriched multi-isotopic nuclides. The interaction between ROTH, the density of the standard composition, and VF (entry 3) is demonstrated in Sect. M7.5.5.

3. VF — VOLUME FRACTION...The default value of the volume fraction is 1.0. It can be omitted if entries 4, 5, 6a, and 6b are also omitted. The volume fraction can be interpreted as:

a. the volume fraction of this standard composition component in the mixture,

b. the density of the standard composition component in this application, divided by the theoretical density listed in the Standard Composition Library (Sect. M8.2), or

c. the product of (a) and (b).

Section M7.5.5 discusses the interaction between ROTH and VF. For example, assume a homogenized mixture representing the water moderator and Zircaloy cladding around a fuel pin is to be described. If the volume of the clad is 5.32 cc and the volume of the water moderator is 44.68 cc, the mixture can be described using H_2O with a volume fraction of 0.8936 [i.e., 44.68/(44.68+5.32)] and ZIRCALOY with a volume fraction of 0.1064 [i.e., 5.32/(44.68+5.32)].

For UO_2 fuel at 95% theoretical density, the volume fraction is 0.95. For the coolant water in an operating PWR, the volume fraction might typically be 0.71.

To describe a mixed-oxide fuel pin with a density of 10.5 g/cc, that is 17.8 wt % PuO_2 and 82.2 wt % UO_2, two standard composition specifications must be entered: one for the PuO_2 component and one for the UO_2 component. From the Standard Composition Library, Table M8.2.1, the theoretical density of the PuO_2 is 11.46 g/cc, and that of the UO_2 is 10.96 g/cc. Therefore, the volume fraction for the PuO_2 is 0.1631 (i.e.,

0.178*10.50/11.46), and the volume fraction for the UO_2 is 0.7875 (i.e., 0.822*10.50/10.96).

Occasionally, a special mixture will be desired for which the determination of the component volume fractions will not be so straightforward. Consider a mixture of boral having 35 wt % B_4C, 65 wt % Al, and an overall density of 2.64 g/cc. Assume that neither BORAL nor B_4C is in the Standard Composition Library. The volume fractions corresponding to BORON, C, and AL may be computed as illustrated in Sect. M7.5.5.4, examples 3 and 4. Note that the calculation is complicated by the fact that B_4C is a compound and boron has two isotopes. It might be simpler to enter B_4C and Al as arbitrary materials as illustrated in example 1 of Sect. M7.5.5.5. Examples 1 and 2 of Sect. M7.5.5.4 illustrate the use of B_4C and aluminum to describe a boral mixture. If the volume fraction is set to 0.0, the user can enter the number density for the nuclide (in atoms per barn-cm) for entry 4. Number densities cannot be entered for standard compositions that represent multiple nuclides.

4. ADEN — NUMBER DENSITY...Enter a value for the number density ONLY if the volume fraction (VF, entry 3) was entered as zero. The number density is entered in units of atoms per barn-cm.

5. TEMP — TEMPERATURE...The default value of the temperature is 293 K. The temperature can be omitted if entries 6a and 6b are also omitted.

The temperature is used for Doppler broadening and/or the selection of the proper set of thermal scattering data.

The resonance self-shielding calculation performed by NITAWL uses the Nordheim Integral Method and can account for Doppler broadening of the resonances at any specified temperature. If this material is known to contain a resonance nuclide, the user should enter the temperature of the material.

For each of the light nuclides ($A \leq 20$ a.m.u.), the master cross-section library may contain one or more sets of thermal-scattering data, each set corresponding to a different temperature. Section M4.2 lists the available sets of data for the SCALE cross-section libraries. Scattering matrices for nuclides in media at elevated temperatures are generally fuller than those at lower temperatures. If multiple sets of thermal-scattering data are available, the user should enter the temperature of the material.

6a. IZA — ISOTOPE ZA NUMBER...Enter a value for each isotope in the standard composition component, entry 1. Do not enter a value if the volume fraction, VF, is zero (entry 3).

The ZA number of the isotope is entered if the user wishes to specify the isotopic distribution. This is done by entering 6a and 6b for each isotope until all the desired isotopes have been described. The "ZA" ID number is (A+1000*Z), where A is the atomic mass or weight of the isotope, and Z is the atomic number.

Entries 6a and 6b can be skipped if the default values listed in the isotopic distribution, Sect. M8.2, are acceptable.

6b. WTP — WEIGHT PERCENT OF THE ISOTOPE...Do not enter a value if the volume fraction, VF, entry 3, is zero. If entry 6a is entered, a value must also be entered for 6b. The weight percent of the isotope is the percent of this isotope in the element.

The user need not input entries 6a and 6b for each isotope listed for the element in Sect. M8.2. The only requirement is that the sum of entries 6b for the element must sum to 100.0. Thus, uranium could be specified as 92235 3.2 92238 96.8 to represent 3.2% enriched uranium and ignore the 234 and 236 isotopes. However, 92235 3.0 and 92238 96.8 would not be correct because the 3.0 and 96.8 do not sum to 100.0. 92235 3.0 92234 0.2 92238 96.8 would be correct.

REPEAT THE SEQUENCE 6a and 6b until all the isotopes of the element have been defined as desired.

7. END — The word END is entered to terminate the input data for a standard composition component. This END can have a label associated with it that can be as long as 12 characters. The label is optional, and if entered must be preceded from the END by a single blank. At least two blanks must separate item 7 from the next data entry.

END COMP — The words END COMP are entered only once for a problem. Their purpose is to signal the end of all the standard composition specification data that will be used in the problem. At least two blanks should separate entry 7 from the END COMP. Note that COMP is a label associated with this END. This label can be as long as 12 characters, but the first four characters must be COMP.

M7.4.5 OPTIONAL UNIT CELL SPECIFICATION FOR INFINITE HOMOGENEOUS PROBLEMS

This section describes the unit cell data that can be entered for an INFHOMMEDIUM problem (data position 3 of Table M7.4.4). By default, the smallest mixture number is the mixture that will be used for the cell in XSDRNPM. In order to calculate the eigenvalue of the system, the mixture should contain fissionable material. Unit cell data are required for an infinite homogeneous medium problem ONLY if XSDRNPM is utilized by the control sequence and a mixture number other than the smallest mixture number is to be used in the cell. Control sequences that end in X, (CSAS1X, etc.) utilize XSDRNPM. Additional information is available in Sect. M7.5.12.

The data required to specify the unit cell for an INFHOMMEDIUM problem are given in Table M7.4.6. The individual entries are explained in the text following the table.

Table M7.4.6 Optional unit cell specification for INFHOMMEDIUM problems

Entry No.	Variable name	Type of data	Data entry	Comments
1	NAME	Keyword	CELLMIX	Initiates reading cell data for INFHOMMEDIUM.
2	MFUEL	Mixture number in the cell	Mixture number	Specifies the mixture number to be used in the cell. Defaults to the smallest mixture number entered in the Standard Composition Data.

1. NAME — KEYWORD...The keyword CELLMIX is entered to indicate that unit cell data will be entered. If this entry is entered, entry 2 must also be entered. These data can be entered ONLY if entry 3, the Type of Calculation from Table M7.4.4, is entered as INFHOMMEDIUM.

2. MFUEL — MIXTURE NUMBER...The mixture number that defines the mixture to be used in the cell. The default value is the smallest mixture number specified in the standard composition specification data. If either item 1 or 2 is entered, the other must also be entered.

To enter the above data, enter the keyword CELLMIX, one or more blanks, and the desired mixture number, MFUEL, as shown below.

```
CELLMIX MFUEL
```

To specify mixture 5 to be used in the cell, enter the following data.

```
CELLMIX 5
```

WARNING: If unit cell data are to be entered for an infinite homogeneous problem, the word CELLMIX must be spelled correctly. If it is misspelled, the code will not give an error message and will attempt to use the smallest mixture number. The input data will get out of phase for CSAS and SAS sequences that expect to read data after the unit cell specification.

M7.4.6 UNIT CELL SPECIFICATION FOR LATTICECELL PROBLEMS

This section describes the unit cell data that must be entered for a LATTICECELL problem (data position 3 of Table M7.4.4). Additional information is available in Sects. M7.5.4, M7.5.4.2, M7.5.6.2, and M7.5.8.2. The LATTICECELL description is especially suited to large arrays of identical cells. The code is limited to a single unit cell description for each problem. The unit cell data are used to provide the lump shape and dimensions for resonance cross-section processing, to provide lattice corrections for cross-section processing, and to provide data used by XSDRNPM to create cell-weighted cross sections. Thus the unit cell specification plays a major role in providing problem-dependent cross sections. The configuration of the unit

cell is determined by the specified "type of lattice." The unit cells are limited to infinitely long cylindrical rods in a square or triangular lattice, spheres in a cubic or triangular lattice, a symmetric array of slabs, or an asymmetric array of slabs. Two distinct types of cells ("Regular" and "Annular") are available to be used in a LATTICECELL problem. "Regular" cells allow a concentric spherical, cylindrical, or symmetric slab configuration constrained to a central fuel region surrounded by an optional gap, an optional clad, and an external moderator. The outer boundary of the cell is limited to provide an array having a square or triangular pitch. "Annular" cells allow a concentric spherical, cylindrical, or asymmetric slab configuration constrained to a central (second) moderator region surrounded by a fuel region having an optional gap and optional clad on each side of the fuel. The gap, if present, is identical on both sides of the fuel. The clad, if present, is identical in dimension and composition on both sides of the fuel. The outer region of the cell is filled with an external (first) moderator. The outer boundary of the cell is limited to provide an array having a square or triangular pitch.

Regular cells are: SQUAREPITCH, TRIANGPITCH, SPHSQUAREP, SPHTRIANGP, and SYMMSLABCELL.

Annular cells are: ASQUAREPITCH, ASQP, ATRIANGPITCH, ATRP, ASPHSQUAREP, ASSP, ASPHTRIANGP, ASTP, and ASYMSLABCELL

The unit cell data are utilized by the code to define the geometric and resonance self-shielding corrections that will be applied to the cross sections. Cell-weighted cross sections are created only if XSDRNPM is invoked by executing a control sequence ending in X, (CSAS1X, CSAS2X, etc.). The cell-weighted cross sections have a flux disadvantage factor applied to them. Because this weighting is applied to each mixture used in the cell, these cell-weighted mixtures should not be used in the geometry description of a subsequent module. However, the cell-weighted mixture that is created is always assigned a mixture number of 500 and can be used in a subsequent module.

The unit cell geometry data required to specify a LATTICECELL problem are given in Table M7.4.7. The individual entries are explained in the text accompanying the table.

1. CTP TYPE OF LATTICE...This defines the type of lattice or array configuration. Any one of the following alphanumeric descriptions may be used. Note that the alphanumeric description must be separated from subsequent data entries by one or more blanks. Figures M7.4.1 through M7.4.6 are used to illustrate the type of lattice configurations available in a LATTICECELL problem. The fuel region is labeled F; the gap, G; the clad, C; and the moderator, M. If two moderators are present, M1 is the first moderator, and M2 is the second moderator. Both "regular" and "annular" unit cells are available. The arrangement of the materials in the unit cell is strictly constrained. Regular cells are limited to a minimum of two regions and a maximum of four regions. The innermost region must be fuel, which is surrounded by an optional gap and/or optional clad. The outer region is moderator. Annular cells are limited to a minimum of three regions. The innermost region must be the second moderator. The annular fuel region is outside the second moderator. If a clad is present, it must be identical in thickness and composition on both sides of the fuel. If a gap is present, it is the same thickness on both sides of the fuel. If the first and second moderators are the same material at the same density and temperature, and do not contain resonance nuclides, the same mixture number can be used

for both moderators. Otherwise, different mixture numbers must be used for the two moderators.

Regular and annular cell configurations are specified as shown below.

Regular Cells

SQUAREPITCH is used for an array of cylinders arranged in a square lattice, as shown in Fig. M7.4.1. The clad and/or gap can be omitted.

TRIANGPITCH is used for an array of cylinders arranged in a triangular-pitch lattice as shown in Fig. M7.4.2. The clad and/or gap can be omitted.

SPHSQUAREP is used for an array of spheres arranged in a square-pitch lattice. A cross-section view through a cell is represented by Fig. M7.4.1. The clad and/or gap can be omitted.

SPHTRIANGP is used for an array of spheres arranged in a triangular-pitch (dodecahedral) lattice. A cross-section view through a cell is represented by Fig. M7.4.2. The clad and/or gap can be omitted.

SYMMSLABCELL is used for an infinite array of symmetric slab cells, as shown in Fig. M7.4.3. The clad and/or gap can be omitted.

Annular Cells

ASQUAREPITCH or ASQP is used for annular cylindrical rods in a square-pitch lattice as shown in Fig. M7.4.4. The gap on both sides of the fuel must be identical, as must the clad. The clad and/or gap can be omitted.

ATRIANGPITCH or ATRP is used for annular cylindrical rods in a triangular-pitch lattice as shown in Fig. M7.4.5. The gap on both sides of the fuel must be identical, as must the clad. The clad and/or gap can be omitted.

ASPHSQUAREP or ASSP is used for spherical shells in a square-pitch lattice as shown in Fig. M7.4.4. The gap on both sides of the fuel must be identical, as must the clad. The clad and/or gap can be omitted.

ASPHTRIANGP or ASTP is used for spherical shells in a triangular-pitch (dodecahedral) lattice as shown in Fig. M7.4.5. The gap on both sides of the fuel must be identical, as must the clad. The clad and/or gap can be omitted.

ASYMSLABCELL is used for a periodic, but asymmetric, array of slabs as shown in Fig. M7.4.6. The gap on both sides of the fuel must be identical, as must the clad. The clad and/or gap can be omitted.

Table M7.4.7 Unit cell specification for LATTICECELL problems

Entry No.	Variable name	Type of data	Entry requirement	Data entry	Comments
1	CTP	Type of lattice	Always		Describes the type of lattice or array configuration.
				SQUAREPITCH	Use for cylindrical rods in a square pitch.
				ASQUAREPITCH	Use for annular cylindrical rods in a square pitch.
				ASQP	Use for annular cylindrical rods in a square pitch.
				TRIANGPITCH	Use for cylindrical rods in a triangular pitch.
				ATRIANGPITCH	Use for annular cylindrical rods in a triangular pitch.
				ATRP	Use for annular cylindrical rods in a triangular pitch.
				SPHSQUAREP	Use for spherical pellets in a cubic lattice.
				ASPHSQUAREP	Use for annular spherical pellets in a cubic lattice.
				ASSP	Use for annular spherical pellets in a cubic lattice.
				SPHTRIANGP	Use for spherical pellets in a bi-centered or face centered hexagonal close-packed lattice.
				ASPHTRIANGP	Use for spherical pellets in a bi-centered or face centered hexagonal close-packed lattice.
				ASTP	Use for spherical pellets in a bi-centered or face centered hexagonal close-packed lattice.
				SYMMSLABCELL	Use for a symmetric array of slabs.
				ASYMSLABCELL	Use for a periodic, but asymmetric array of slabs.
2	PITCH	Array pitch (cm)	Always	Appropriate dimension	The center-to-center spacing (cm) between fuel lumps. For asymmetric slab cell, enter the distance from the center of one moderator to the center of the other moderator (cm).
3	FUELOD	Outside dimension of fuel (cm)	Always	Appropriate dimension	Outside diameter of fuel (cm), or the thickness of the fuel in a slab.
4	MFUEL	Fuel mixture number	Always	Mixture number	Mixture number representing the fuel.
5	MMOD	Moderator mixture number	Always	Mixture number	Mixture number representing the moderator
6	MMOD2	2nd moderator mixture number	Annular cell	Mixture number	Mixture number representing the second moderator.
7	TKMOD2	2nd moderator thickness	ASYMSLABCELL	Thickness	Thickness of the second moderator (cm) for ASYMSLABCELL.
		or	or	or	or
		2nd moderator diameter (cm)	annular cell	Diameter	Diameter of inner moderator (cm) for other annular cells.
8	CLADOD	Outside diameter of clad (cm)	If clad	Clad OD	OMIT IF NO CLAD. For a slab, CLADOD is the sum of thickness of the fuel, gap, and clad.
9	MCLAD	Clad mixture number	If clad	Mixture number	OMIT IF NO CLAD. Mixture number representing the clad.
10	CLADID	Inside diameter of clad (cm)	If gap	Clad ID	OMIT IF NO GAP between the fuel and clad.
11	MGAP	Gap mixture number	If gap	Mixture number	OMIT IF NO GAP between the fuel and clad. A mixture number of zero is often used.
12	END	Terminate LATTICECELL data	Always	END	Terminate the LATTICECELL input data by entering the word END. Do not start in column 1. At least two blanks must follow entry number 12.

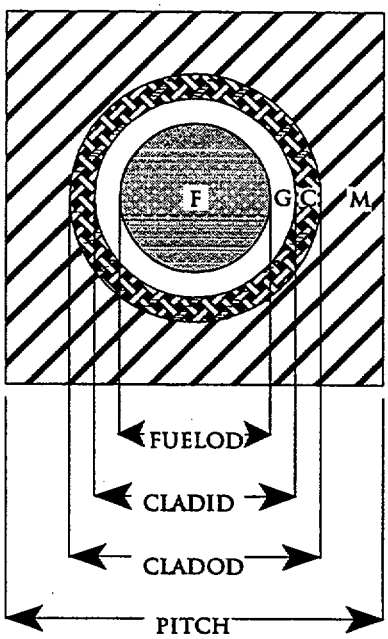

Figure M7.4.1 Arrangement of materials in a SQUAREPITCH and SPHSQUAREP unit cell

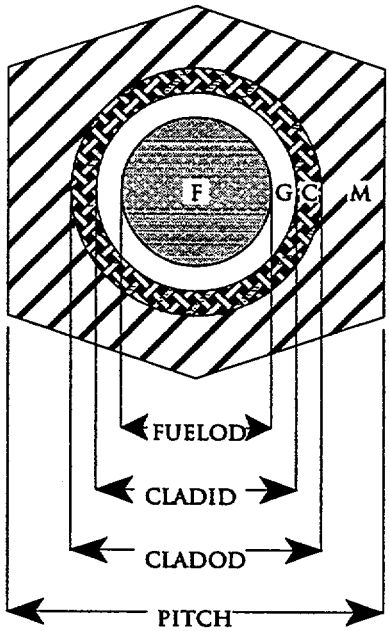

Figure M7.4.2 Arrangement of materials in a TRIANGPITCH and SPHTRIANGP unit cell

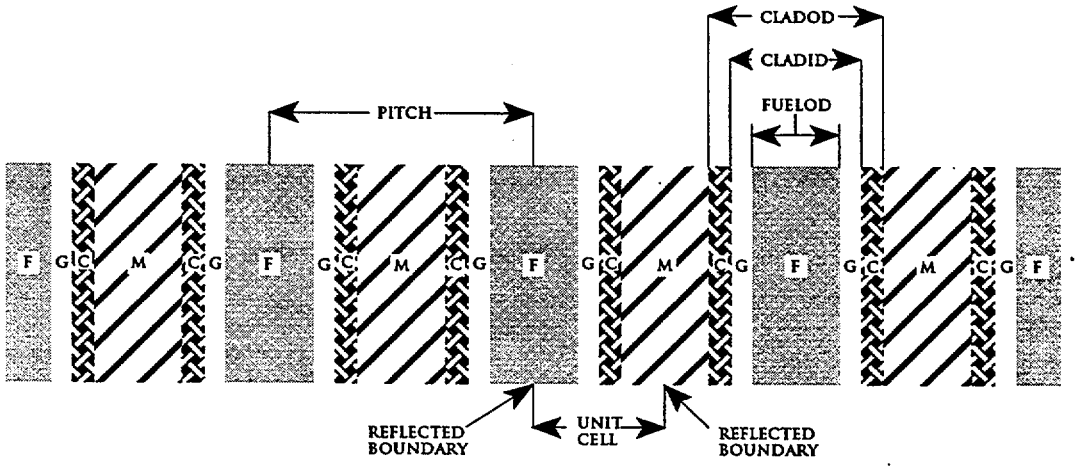

Figure M7.4.3 Arrangement of materials in a SYMMSLABCELL unit cell having reflected left and right boundary conditions

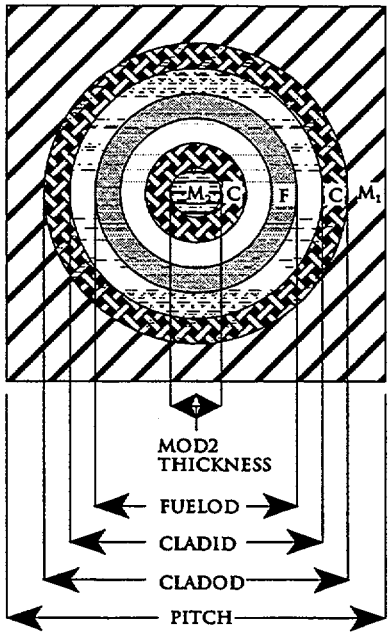

Figure M7.4.4 Arrangement of materials in an ASQUAREPITCH and ASPHSQUAREP unit cell

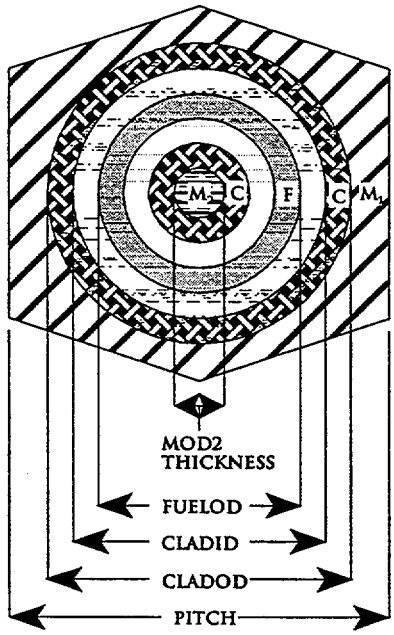

Figure M7.4.5 Arrangement of materials in an ATRIANGPITCH or ASPHTRIANGP unit cell

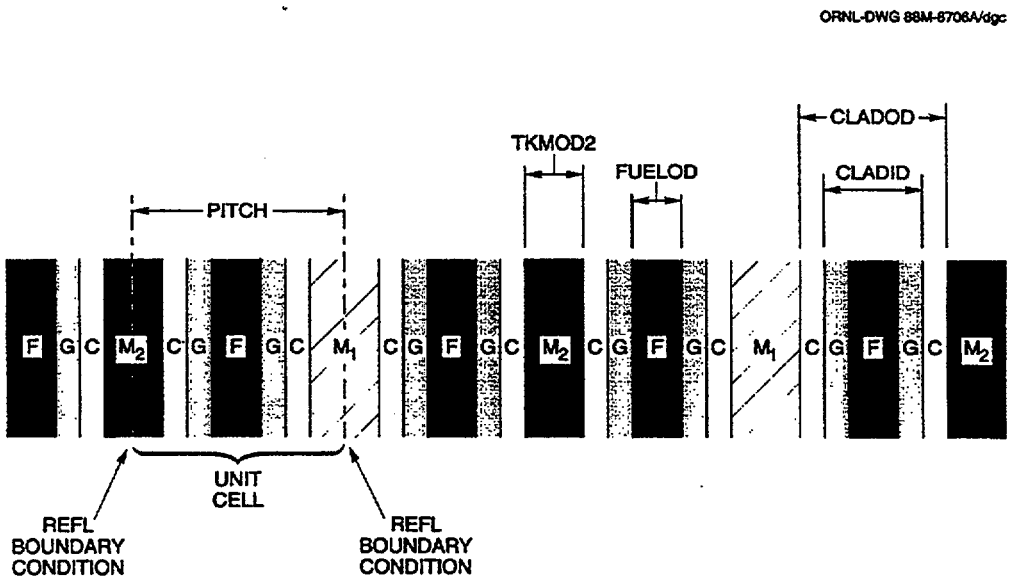

Figure M7.4.6 Arrangement of materials in an ASYMSLABCELL unit cell

2. PITCH — ARRAY PITCH...This is the center-to-center spacing between the fuel lumps (rods, pellets, or slabs) in cm, as shown in Figs. M7.4.1 through M7.4.6. For an ASYMSLABCELL, enter the distance from the center of one moderator to the center of the other moderator. (See Fig. M7.4.6.)

3. FUELOD — OUTSIDE DIMENSION OF FUEL...This is the outside diameter of the fuel in cm, as shown in Figs. M7.4.1 through M7.4.6. In slab geometry, enter the thickness of the fuel (see Figs. M7.4.1 through M7.4.6).

4. MFUEL — FUEL MIXTURE NUMBER...This is the mixture number representing the fuel (F in Figs. M7.4.1 through M7.4.6).

5. MMOD — MODERATOR MIXTURE NUMBER...This is the mixture number representing the moderator (M or M1 in Figs. M7.4.1 through M7.4.6).

6. MMOD2 — SECOND MODERATOR MIXTURE NUMBER...Enter ONLY for annular cells. This is the mixture number representing the second moderator (M2 in Figs. M7.4.4 through M7.4.6).

7. TKMOD2 — SECOND MODERATOR THICKNESS...Enter ONLY for annular cells. This is the thickness or diameter of the second moderator in cm (see Figs. M7.4.4 through M7.4.6).

8. CLADOD — OUTSIDE DIAMETER OF CLAD...Enter ONLY if a clad is present. Enter the diameter of the clad in cm. For a slab, CLADOD is the sum of the fuel thickness, twice the gap thickness, and twice the clad thickness. See Figs. M7.4.1 through M7.4.6.

9. MCLAD — CLAD MIXTURE NUMBER...Enter ONLY if a clad is present. Enter the mixture number that represents the clad (C in Figs. M7.4.1 through M7.4.6).

10. CLADID — INSIDE DIAMETER OF CLAD...Enter ONLY if a gap is present between the fuel and the clad. Omit if there is no gap. If a gap is present, enter the inside diameter of the clad in cm. This corresponds to the outside diameter of the gap. In slab geometry, CLADID is the sum of the fuel thickness and twice the gap thickness. See Figs. M7.4.1 through M7.4.6.

11. MGAP — GAP MIXTURE NUMBER...Enter ONLY if a gap is present between the fuel and the clad. Omit if there is no gap. Enter the mixture number representing the gap (G in Figs. M7.4.1 through M7.4.6). Zero is often used to represent a void.

12. END — The word END is entered to terminate the LATTICECELL data. An optional label can be associated with this END. The label can be as many as 12 characters long and is separated from the END by a single blank. At least two blanks must follow entry number 12.

M7.4.7 UNIT CELL SPECIFICATION FOR MULTIREGION PROBLEMS

These data are entered only if the problem is defined as a MULTIREGION problem. They describe the additional geometry data that are required for a MULTIREGION problem (data position 3 of Table M7.4.4). A MULTIREGION problem can be used to define a geometric arrangement that is more complicated than is allowed by a LATTICECELL. It can also be used for large geometric regions where the geometry effects for the cross sections are minimal. Additional information is available in Sects. M7.5.4, M7.5.4.3, M7.5.6.3, and M7.5.8.3. BE FULLY AWARE THAT CROSS SECTIONS GENERATED USING MULTIREGION IGNORE THE LATTICE GEOMETRY EFFECTS IN PROCESSING THE RESONANCE CORRECTIONS.

The additional data required for a MULTIREGION problem are given in Table M7.4.8 and explained in the text following the table.

1. CS TYPE OF GEOMETRY...The type of geometry must always be specified for a MULTIREGION problem. The cross-section corrections do not account for lattice effects. The available geometry options are listed below.

   SLAB...This is used to describe a slab geometry.

   CYLINDRICAL...This is used to describe cylindrical geometry.

   SPHERICAL...This is used to describe spherical geometry.

   BUCKLEDSLAB...This is used for slab geometry with a buckling correction for the two transverse directions.

   BUCKLEDCYL...This is used for cylindrical geometry with a buckling correction in the axial direction.

2. BR RIGHT BOUNDARY CONDITION...This is defaulted to vacuum. A value for BR MUST be entered for BUCKLEDSLAB and BUCKLEDCYL, but is optional for SLAB, CYLINDRICAL, or SPHERICAL. The available options and their qualifications are listed below:

   VACUUM...This imposes a vacuum at the boundary of the system.

   REFLECTED...This imposes mirror image reflection at the boundary. Do not use for CYLINDRICAL or SPHERICAL.

   PERIODIC...This imposes periodic reflection at the boundary. Do not use for CYLINDRICAL or SPHERICAL.

   WHITE...This imposes isotropic return at the boundary.

Table M7.4.8 Geometry specification for MULTIREGION problems

Entry No.	Variable name	Type of data	Entry requirement	Data entry	Comments
1	CS	Type of geometry	Always		Describes the type of geometry. The options are listed below.
				SLAB	Use for slab geometry.
				CYLINDRICAL	Use for cylindrical geometry.
				SPHERICAL	Use for spherical geometry.
				BUCKLEDSLAB	Use for slab geometry with a buckling correction for the two transverse directions.
				BUCKLEDCYL	Use for cylindrical geometry with a buckling correction in the axial direction.
2	BR	Right/outside boundary condition	Required for BUCKLEDSLAB & BUCKLEDCYL Optional for other geometries	VACUUM REFLECTED PERIODIC WHITE	This provides a nonreturn condition at the boundary. Do not use for cylindrical or spherical. Do not use for cylindrical or spherical. This provides isotopic return at the boundary. Default is VACUUM.
3	BL	Left/inside boundary condition	Required for BUCKLEDSLAB & BUCKLEDCYL Optional for other geometries	VACUUM REFLECTED PERIODIC WHITE	This provides a non-return condition at the boundary. Recommended for cylindrical or spherical. Do not use for cylindrical or spherical. This provides isotropic return at the boundary. Default is REFLECTED.
4	ORGN	Location of left boundary on the x-axis (cm)	BUCKLEDSLAB & BUCKLEDCYL Optional for other geometries	Appropriate dimension	Default is 0.0. Should not be changed for cylindrical or spherical geometry. A value must be entered if subsequent data are to be entered.
5	DY	Buckling height (cm)	BUCKLEDSLAB & BUCKLEDCYL	Appropriate dimension	OMIT FOR SLAB, CYLINDRICAL, and SPHERICAL. This corresponds to one of the transverse dimensions of an actual 3-D slab assembly or to the length of a finite cylinder.
6	DZ	Buckling depth (cm)	BUCKLEDSLAB	Appropriate dimension	OMIT UNLESS BUCKLEDSLAB WAS SPECIFIED. This is the buckling depth corresponding to the second transverse dimension of a 3-D slab assembly.
7	END	End geometry parameters	Always	END	Enter the word END. Do not start in column 1. At least two blanks must separate entry 7 from the first entry 8.
8	MXZ	Mixture number in the zone	Always	Mixture number	Repeat entry numbers 8-10 until all zones are defined. Enter the mixture number for this zone.
9	RZ	Outside radius of the zone (cm)	Always	Appropriate dimension	Repeat entry numbers 8-10 until all zones are defined. Enter the outside dimension of the zone (cm).
10	XMOD	External moderator index	Optional		Repeat entry numbers 8-10 until all zones are defined. Entry 10 is optional and can be omitted. If it is omitted, repeat entry numbers 8 and 9 until all zones are defined.
				NOEXTERMOD	No moderating materials in the adjacent zones.
				ONEEXTERMOD	A moderating material is present in one adjacent zone.
				TWOEXTERMOD	Moderating materials are present in two adjacent zones.
	END ZONE	Terminate zone data		END ZONE	Enter when all zones have been defined by repeating entry numbers 8 through 10 for each zone. At least two blanks must follow this entry.

3. BL LEFT BOUNDARY CONDITION...This is defaulted to reflected. A value for BL MUST be entered for BUCKLEDSLAB, but is optional for SLAB, CYLINDRICAL, or SPHERICAL. The available options and their qualifications are listed below:

VACUUM...This imposes a vacuum at the boundary of the system.

REFLECTED...This imposes mirror image reflection at the boundary. For CYLINDRICAL or SPHERICAL, this is the only valid boundary condition because the left boundary corresponds to the centerline.

PERIODIC...This imposes periodic reflection at the boundary.

WHITE...This imposes isotropic return at the boundary.

4. ORGN LOCATION OF LEFT BOUNDARY ON THE ORIGIN...The default value of ORGN is 0.0. This is the only value allowed for CYLINDRICAL or SPHERICAL geometry. Enter the location of the left boundary on the x-axis perpendicular to the slab (in cm).

5. DY BUCKLING HEIGHT...Enter ONLY for BUCKLEDSLAB or BUCKLEDCYL. This is the buckling height in cm. It corresponds to one of the transverse dimensions of an actual 3-D slab assembly or the length of a finite cylinder.

6. DZ BUCKLING DEPTH...Enter ONLY for BUCKLEDSLAB. This is the buckling width in cm. It corresponds to the second transverse dimension of an actual 3-D slab assembly.

7. END The word END is entered to terminate these data before entering the zone description data. It must not be entered in columns 1 through 3 and at least two blanks must separate it from the zone description. A label can be associated with this END. The label can be a maximum of 12 characters and is separated from the END by a single blank. At least two blanks must follow entry number 7.

The zone description data are entered at this point. Entries 8, 9, and 10 are entered for each zone, and the sequence is repeated until all the desired zones have been described. To terminate the data, enter the words END ZONE.

8. MXZ MIXTURE NUMBER IN THE ZONE...Enter the mixture number of the material that is present in the zone. Enter a zero for a void. Repeat the sequence of entries 8 through 10 for each zone.

9. RZ OUTSIDE RADIUS OF THE ZONE...Enter the outside dimension of the zone in cm. In slab geometry, RZ is the location of the zone's right boundary on the x-axis. Repeat the sequence of entries 8 through 10 for each zone.

10. XMOD Optional EXTERNAL MODERATOR INDEX...This optional entry describes the conditions existing in the zones adjacent to the present zone. Appropriate conditions are provided by default. The available options are listed below:

NOEXTERMOD...This means there are no moderating materials between this zone and either boundary.

ONEEXTERMOD...This means one of the zones between this zone and one of the boundaries contains a material.

TWOEXTERMOD...This indicates that at least one zone on either side of this zone contains a material.

CAUTION: User-provided entries do not always supersede the default values.
(1) For SLAB geometry, user-supplied values will be used everywhere except zone 1. If the left boundary is reflected, the default value of ONEEXTERMOD will be used unless NOEXTERMOD is specified.
(2) For SPHERICAL and CYLINDRICAL geometry, default values will be used for all zones unless NOEXTERMOD is specified. NOEXTERMOD allows the user to "turn off" geometric corrections.

Repeat the sequence of entries 8 and 9 or 8 through 10 for each zone. When all the zones have been described, enter the words END ZONE.

END ZONE is used to terminate the MULTIREGION zone data. Enter the words END ZONE when all the zones have been described. Note that ZONE is a label associated with this END. This label can be as long as 12 characters, but the first four characters must be ZONE. At least two blanks must follow this entry.

M7.4.8 OPTIONAL PARAMETER DATA

Most of the parameter data for the Material Information Processor are determined by the code and cannot be adjusted. However, certain parameters can be altered. If the default parameters are acceptable, this section of input data should be omitted in its entirety. Nondefault values for one or more of the parameters can be specified by entering the words MORE DATA followed by the desired keyworded parameters and their associated values. One or more of the parameters can be entered in any order. Default values are used for parameters that are not entered. Each parameter is entered by spelling its name, followed immediately by an equal sign and the value to be entered. There should not be a blank between the parameter name and the equal sign. Each parameter specification must be separated from the rest by at least one blank. For example:

MORE DATA ISN=16 EPS=0.00008 END

would result in using an S16 angular quadrature set and tightening the convergence criteria to 0.00008 in the XSDRNPM calculation.

Table M7.4.9 describes the optional parameters that can be entered as data and the code or codes where the parameters apply. A description of each entry is given.

1. MORE DATA...These words, followed by one or more blanks, are entered ONLY if optional parameter data are to be entered. They must precede all other optional parameter data. Entries 2 through 28 can be entered in any order.

2. ISN — ORDER OF ANGULAR QUADRATURE FOR XSDRNPM...Quadrature sets are geometry-dependent quantities that are defaulted to order 8 by the Material Information Processor. See Sects. M7.2.5.7 and M7.5.7 for a more detailed explanation.

3. SZF — SPATIAL MESH SIZE FACTOR FOR XSDRNPM...The size of the largest mesh interval can be adjusted by entering a value for SZF. The default value is 1.0. A value between zero and 1.0 yields a finer mesh; a value greater than 1.0 yields a coarser mesh. See Sects. M7.2.5.6 and M7.5.7 for more details. If SZF $\leq$0, the user specifies the number of mesh intervals in each zone immediately following the MORE DATA block. If SZF = 0, the interval spacing is generated as described in M7.2.5.6, while if SZF <0 the intervals are equally spaced intervals in each zone.

4. IIM — MAXIMUM NUMBER OF INNER ITERATIONS FOR XSDRNPM...This is the maximum number of inner iterations to be used in the XSDRNPM calculation. The default value is 20. See Sect. M7.5.7 for a more detailed explanation.

5. ICM — MAXIMUM NUMBER OF OUTER ITERATIONS FOR XSDRNPM...This is the maximum number of outer iterations to be used in the XSDRNPM calculation. The default value is 25. If the calculation reaches the outer iteration limit, a larger value should be used. See Sect. M7.5.7 for a more detailed explanation.

6. EPS — OVERALL CONVERGENCE CRITERIA FOR XSDRNPM...This is used by XSDRNPM after each outer iteration to determine if the problem has converged. The default value of EPS is 0.0001. A value less than 0.0001 tightens the convergence criteria; a larger value loosens the convergence criteria. See Sects. M7.2.5.8 and M7.5.7 for additional information.

7. PTC — POINTWISE CONVERGENCE CRITERIA FOR XSDRNPM...This is the point flux convergence criteria used by XSDRNPM to determine if convergence has been achieved after an inner iteration. The default value is 0.00001. A smaller value tightens convergence; a larger value loosens it. See Sects. M7.2.5.8 and M7.5.7 for a more detailed explanation.

8. BKL — BUCKLING FACTOR FOR XSDRNPM...A buckling factor should be used ONLY for a MULTIREGION BUCKLEDSLAB or BUCKLEDCYL problem. Because cylinders are assumed to be infinitely long and slabs are assumed to be infinite in both transverse directions, the analytic sequence may tend to overestimate the total flux for a finite system. A buckling correction can be used to approximate the leakage from the system in the transverse direction(s). The extrapolation distance factor, BKL, is defaulted to 1.420892. See Sects. M7.2.5.4 and M7.5.7 for additional details.

Table M7.4.9 Optional parameter data

Entry No.	Keyword name	Type of data	Applicable module	Comments
1	MORE DATA	Input flag		This signals that optional parameter data will be entered. Enter only those parameters you wish to change.
2	ISN=	Order of angular quadrature	XSDRNPM	The default value is 8. This allows using another value.
3	SZF=	Spatial mesh size factor	XSDRNPM	The default value is 1.0. 0<SZF<1.0 gives a finer mesh. SZF>1.0 gives a coarser mesh. SZF ≤ user specifies the number of mesh intervals in each zone.
4	IIM=	Max. number of inner iterations	XSDRNPM	The default value is 20. This allows using another value.
5	ICM=	Max. number of outer iterations	XSDRNPM	The default value is 25. This allows using another value.
6	EPS=	Overall convergence criteria	XSDRNPM	The default value is 0.0001. This allows using another value.
7	PTC=	Point convergence criteria	XSDRNPM	The default value is 0.00001. This allows using another value.
8	BKL=	Buckling factor	XSDRNPM	The default value is 1.420892. Use ONLY for a MULTIREGION problem that specifies BUCKLEDSLAB or BUCKLEDCYL.
9	IUS=	Upscatter scaling factor	XSDRNPM	The default value is zero. IUS=0 doesn't utilize upscatter scaling. IUS=1 uses upscatter scaling to accelerate the solution and/or speed convergence.
10	RES=	Resonance data	BONAMI NITAWL	Enter the mixture number, geometry type (SLAB, CYLINDER, SPHERE) and the thickness of the slab or radius of the sphere or cylinder, in cm. Optionally enter the inner radius (cm) to specify an annular cylinder or sphere.
11	DAN(mm)=	Dancoff factor for the specified mixture	BONAMI NITAWL	Enter the mixture number, to which the Dancoff factor applies, mm, inside the parentheses; enter the Dancoff factor after the equal sign. Repeat entries 10 and 11 for all resonance mixtures used in the problem that are not treated in the LATTICECELL or MULTIREGION description.
12	BAL=	Key to print balance tables	XSDRNPM	The default value is FINE. BAL=NONE suppresses printing the balance table. BAL=ALL prints all balance tables. BAL=FINE prints only the fine-group balance tables.

Table M7.4.9 (continued)

Entry No.	Keyword name	Type of data	Applicable module	Comments
13	DY=	First transverse dimension	XSDRNPM	The first transverse dimension, in cm, used in a buckling correction to calculate leakage normal to the principal calculation direction (i.e., the height of a slab or a cylinder).
14	DZ=	Second transverse dimension	XSDRNPM	The second transverse dimension, in cm, used for a buckling correction (i.e., the width of a slab).
15	COF=	Diffusion coefficient option for transverse leakage correction	XSDRNPM	The default is 0. See Sect. F3.5, 3$ array, variable IPN.
16	FRD=	Unit from which fluxes will be read	XSDRNPM	Enter the unit number from which the flux guess for XSDRNPM will be read.
17	FWR=	Unit on which fluxes will be written	XSDRNPM	Enter the unit number where the binary fluxes from XSDRNPM will be written.
18	ADJ=	Adjoint mode flag	XSDRNPM	Enter a 1 to cause XSDRNPM to solve the problem in adjoint mode
19	NBU=	Unit on which balance tables will be written	XSDRNPM	Enter the unit number where the balance tables from XSDRNPM will be written
20	WGT=	Cross-section weighting flag	XSDRNPM	Enter a 0 to suppress doing the cross-section weighting in XSDRNPM
21	ZMD(iz)=	Zone width modifier for the specified zone	XSDRNPM	Enter the zone number for which the modifier applies inside the parentheses; enter the zone width modifier after the equal sign. **Repeat number 21 to specify all zones to be modified in a search**
22	INT(iz)	Number of intervals in the specified zone	XSDRNPM	Enter the zone number inside the parenthesis; enter the number of intervals after the equal sign. Repeat number 22 to specify all needed zones.
23	KEF=	Value of k_{eff} to be searched for	XSDRNPM	Enter the value of k_{eff} that it is desired to search for
24	KFM=	Value of the eigenvalue modifier	XSDRNPM	Enter the value of the eigenvalue modifier (i.e., the relative change for the first guess of a search)
25	DAB=	Number of direct access data blocks	MIP[a]	The default is 200. Number of blocks allocated for direct access unit 90.
26	AXS=	Unit on which a mixed ANISN library will be written	ICE	Enter the unit number where ICE is to write a mixed ANISN library.
27	MSH=	Maximum number of mesh points/resonance	NITAWL	The default value is 2001. This allows using another value.

Table M7.4.9 (continued)

Entry No.	Keyword name	Type of data	Applicable module	Comments
28	MLV=	Highest resonance ℓ-value for self-shielding	NITAWL	The default value is 2. This allows using another value.
29	ID1=	Print control for scalar fluxes	XSDRNPM	The default value is -1. See Sect. F3.5, 2$ array, variable ID1.
30	COLL	Key to activate collapse of thermal groups	MIP[a]	Enter COLL to collapse all thermal groups into one group for the shielding sequences.
31	END	Terminus		Terminate the optional parameter data. Do not start in column 1. At least two blanks must follow this entry.

[a]MIP is the Material Information Processor.

9. IUS — UPSCATTER SCALING FLAG FOR XSDRNPM...This option allows the use of upscatter scaling to accelerate the solution or force convergence. The default value is zero, in which case upscatter scaling is not used. IUS=1 facilitates upscatter scaling. Guidelines are not available to indicate when upscatter scaling is needed. Some problems will not converge with it, and some will not converge without it. See Sect. M7.5.7 for a more detailed explanation.

10. RES — RESONANCE DATA FOR BONAMI AND NITAWL...This parameter allows overriding the default resonance data for materials that are not used in the unit cell. The default resonance data are infinite homogeneous media, which may not accurately represent the geometry (for example, an additional fuel mixture, a thin clad, or a container region). The resonance data are entered in the form:

RES= mixture number geometry type thickness [inner radius]

The mixture number is the material for which the resonance data apply. The geometry type can be a sphere, slab, or cylinder, and defines the third entry of the 3* array in NITAWL. The thickness is the thickness of a slab or the radius of a sphere or cylinder in cm and defines the fourth entry of the 3* array in NITAWL. An inner radius, in cm, may optionally be entered to treat a cylinder or sphere as an annular geometry. It defines the sixth entry in the 3* array in NITAWL. This entire data sequence should be entered for each material for which the default data are inadequate. See Sect. M7.5.7 for additional details. WARNING: If this parameter is used to enter resonance data for a mixture that is used in the unit cell specification, it will NOT be used. Information provided in the unit cell data will be used instead.

11. DAN(mm)= DANCOFF FACTOR for the specified mixtures. This allows entering a Dancoff factor to be used in the resonance correction for the specified mixture. The Dancoff data are entered in the form:

DAN(mm) = Dancoff factor

Note that the parentheses must be entered as part of the data. The mixture number, mm, to which the Dancoff factor applies, must be enclosed in the parentheses. The Dancoff factor to be used is entered after the equal sign. See Sect. M7.5.7 for additional details.

Items 10 and 11 should be entered for each resonance mixture that is not specified in the LATTICECELL or MULTIREGION unit cell specification data. See Sect. M7.5.10.

12. BAL BALANCE TABLE PRINT FLAG FOR XSDRNPM...This allows control of the balance table print from XSDRNPM. The default value is FINE. BAL=NONE suppresses the balance table print. BAL=ALL prints all of the balance tables. BAL=FINE prints only the fine-group balance tables. See Sect. M7.5.7 for additional details.

13. DY= FIRST TRANSVERSE DIMENSION FOR XSDRNPM...This is the first transverse dimension, in centimeters, used in a buckling correction to calculate the leakage normal to the principal calculation direction (the height of a slab or cylinder). It should only be entered if XSDRNPM is to create cell-weighted cross sections and/or calculate the eigenvalue of a cylinder or slab system of finite height for a LATTICECELL problem. DY= is defaulted to an infinite height, or is set to DY for a buckled MULTIREGION cell description. See Sects. M7.2.5.4 and M7.5.7 for additional details. A value entered here overrides any buckling height value entered in the MULTIREGION data.

14. DZ= SECOND TRANSVERSE DIMENSION FOR XSDRNPM...This is the second transverse dimension, in centimeters, used for a buckling correction for a slab of finite width. It should only be entered if XSDRNPM is to create cell-weighted cross sections and/or calculate the eigenvalue of a LATTICECELL slab of finite width. DZ= is defaulted to an infinite width, or is set to DZ for a buckled MULTIREGION slab cell of finite width.

See Sects. M7.2.5.4 and M7.5.7 for additional details. A value entered here overrides any buckling depth value entered in the MULTIREGION data.

15. COF= DIFFUSION COEFFICIENT FOR TRANSVERSE LEAKAGE CORRECTIONS IN XSDRNPM...The default value is 0. The available options are:

COF=0 sets a transport-corrected cross section for each zone

COF=1 use a spatially averaged diffusion coefficient for each zone

COF=2 use a diffusion coefficient for all zones that is one-third the diffusion coefficient determined from the spatially averaged transport cross section for all zones

COF=3 use a flux and volume weighting across all zones

See Sect. M7.5.7 or Sect. F3.5, 3$ array, variable IPN for more details.

16. FRD= UNIT FROM WHICH FLUXES ARE READ FOR XSDRNPM. If fluxes are to be used for the initial flux guess, enter the unit number from which they are to be read. The user is responsible for supplying job control language data that are necessary for reading the flux data set. See Sect. M7.5.7 for more details.

17. FWR= UNIT ON WHICH FLUXES WILL BE WRITTEN FOR XSDRNPM. If binary fluxes are to be saved from this XSDRNPM calculation, enter the unit number where they will be written. The user is responsible for supplying job control language data that are necessary for creating and saving the flux data set. See Sect. M7.5.7 for more details.

18. ADJ= Adjoint mode flag for XSDRNPM. Set to 1 to cause XSDRNPM to solve the adjoint problem.

19. NBU= Unit on which the balance tables will be written from XSDRNPM. If the balance tables file is to be saved, enter the unit number where they are to be written. The user is responsible for supplying job control data necessary to create and save the balance table dataset.

20. WGT= Cross-section weighting flag for XSDRNPM. The default is to do cross-section weighting. If a user needs to not do cross-section weighting, then a value of 0 should be entered.

21. ZMD(iz)= Zone width modifiers for an XSDRNPM search problem. This allows entering a zone width modifier for zone iz in the XSDRNPM problem description. The zone width data are entered in the form:
ZMD(iz)=modifier
Note that the parentheses must be entered as part of the keyword. The zone number iz, to which the modifier is applied must be enclosed in the parentheses. The modifier is entered after the equal sign. See Sect. F3.2.8 for more information.

22. INT(iz)= Number of mesh intervals for zone iz in XSDRNPM. The default is 0, which causes the number to be calculated. The data are entered in the form:
INT(iz)=number
Note that the parentheses must be entered as part of the keyword. The zone number iz, for which the number of intervals is specified, must be enclosed in the parenthesis. The number of intervals is entered after the equal sign.

23. KEF= The desired value of k_{eff} for an XSDRNPM zone width search. The default value is 1.0. If it is desired to search for some other value, such as 0.9, then input it here.

24. KFM= The first eigenvalue modifier used in an XSDRNPM search. This value is used to make the first change in the XSDRNPM search. The default value is -0.1. A user may sometimes need to change this to make the search converge.

25. DAB= NUMBER OF DIRECT-ACCESS DATA BLOCKS FOR THE MATERIAL INFORMATION PROCESSOR. These are the number of blocks allocated for direct access on unit 90. The default is 200. See Sect. M7.5.7 for additional details. If the job fails in the Material Information Processor with an LMP005 DA ERROR, then DAB must be used to enter a larger value. See Sect. M7.7.3 for additional details.

26. AXS= LOGICAL UNIT NUMBER FOR ICE. Write a mixed ANISN library on this unit. The default is zero (no library). If the unit number is input as 7, the ANISN library will be in free-form card image. For any other unit number, the library will be binary. The user is responsible for supplying job control language data that are necessary for creating and saving the ANISN cross-section library. An ANISN cross section can only be created by the control sequences CSASI, CSASIX, and SAS3. See Sect. M7.5.7 for additional details.

27. MSH= THE MAXIMUM NUMBER OF MESH POINTS PER RESONANCE. The default value is 2001. This is the maximum number of mesh points allowed for the Simpson's rule integration in NITAWL. This should be an odd number. See Sect. M7.5.7 for additional details.

28. MLV= HIGHEST RESONANCE ℓ-VALUE FOR SELF-SHIELDING. The default value is 2. This is the highest resonance ℓ-value for which a self-shielding calculation will be performed in NITAWL. See Sect. M7.5.7 for additional details.

29. ID1= SCALAR FLUX PRINT CONTROL. The default value is -1, which suppresses printing the scalar fluxes in XSDRNPM. See Sect. F3.5, 2$ array, variable ID1 for allowed values and corresponding actions.

30. COLL ACTIVATE COLLAPSE OF THERMAL GROUPS. This parameter should only be used with the shielding analysis sequences (SAS1, etc.). It causes the Material Information Processor to instruct XSDRNPM to collapse all thermal groups into one group. See Sect. M7.5.7 for additional details.

31. END The word END is entered to terminate the optional parameter data. A label can be associated with this END. The label can be as long as 12 characters, but must be preceded by a single blank. If this END is entered without a label, it must not begin in column 1. At least two blanks must follow this entry.

M7.5 NOTES ABOUT THE MATERIAL INFORMATION PROCESSOR

This section provides tips about the use of the Material Information Processor utilized by many of the SCALE modules. To assist in locating specific data in this section, see Table M7.5.1.

M7.5.1 USE OF THE MATERIAL INFORMATION PROCESSOR

The Material Information Processor performs the functions of (1) reading user-specified input data about material specifications and unit cell geometry pertinent to cross-section processing and (2) accessing information from the Standard Composition Library to determine nuclide atom densities and resonance data.

M7.5.2 MATERIAL INFORMATION PROCESSOR TITLE

The first information required by the Material Information Processor is a title. The title is a maximum of 80 characters and is the first entry after the Analytical Sequence Indicator record. The Analytical Sequence Indicator begins in column 1. The title also begins in column 1. An example is

```
=CSASN
THIS IS THE TITLE
```

M7.5.3 CROSS-SECTION LIBRARY NAME

There are several cross-section libraries available for use with SCALE. They are in the AMPX master library format and are specified as the first data following the Material Information Processor title. The libraries that are available in SCALE are discussed in Sect. M4. The available libraries include:

HANSEN-ROACH
27GROUPNDF4
44GROUPNDF5
218GROUPNDF4
18GROUPGAMMA
27BURNUPLIB
27N-18COUPLE
22N-18COUPLE
238GROUPNDF5

The first five libraries listed above are criticality safety libraries, and the last three are shielding libraries. The 27BURNUPLIB library is used for depletion analyses or criticality safety analyses where higher-order actinides or fission products are needed. Terse input is accepted for the cross-section library name, so only the number of characters necessary to uniquely define the library need be entered. However, the entered name must be an exact match for the number of characters that are entered. Thus, 27G is sufficient to define the 27GROUPNDF4 library. Entering 27GRP is incorrect because the fifth character does not match, but 27GR or 27GRO are correct.

Table M7.5.1 Organization of notes about the Material Information Processor

Table M7.5.1 (continued)

Table M7.5.1 (continued)

M7.5.4 TYPE OF CALCULATION

The type of calculation specifies the basic geometry description that is used for cross-section processing. The type of calculation is very important because it can substantially affect the calculated results. The available options are:

INFHOMMEDIUM
LATTICECELL
MULTIREGION

Terse input is accepted so only the number of characters necessary to uniquely define the type of calculation need be entered. However, the entered name must be an exact match for the number of characters that are entered. Thus, I is sufficient to specify an infinite homogeneous medium treatment. However, it may be more informative to use names such as INF, LAT or MULT.

M7.5.4.1 INFHOMMEDIUM

The choice of infinite homogeneous medium means that the cross sections are treated as if each mixture is an infinite lump. Thus the self-shielding calculations do not account for any geometrical effects. Because the geometric effect to the cross-section resonance correction is a surface effect, infinite homogeneous medium is an appropriate choice if the volume of the material is very large. The fraction of the fuel that is within a mean-free path of the surface is the governing consideration. If the fraction is large, the geometric effect is very important. If the fraction is very small, the geometric effect is unimportant. Therefore, infinite homogeneous medium is a good choice if the size of the material is large relative to the mean-free path in the material. Infinite homogeneous medium is a very poor choice for large arrays of small lumps or fuel pins where the geometric correction for each fuel pin is extremely important. The unit cell specification is optional in an infinite homogeneous medium problem. If it is to be entered, it follows the standard compositions specification data. Examples of **INFHOMMEDIUM** unit cell specifications are given in Sect. M7.5.6.1. Examples of problems using the infinite homogeneous medium treatment are given in Sect. M7.5.8.1.

M7.5.4.2 LATTICECELL

The choice of **LATTICECELL** is used when the geometry can be described as a lattice. The **LATTICECELL** treatment assumes an infinite array of identical cells. It is especially suited for large arrays of cylindrical rods or spherical pellets. The use of **LATTICECELL** requires a unit cell specification following the last entry of the standard composition specification data. The use of **LATTICECELL** assures that the cross sections are corrected for both geometric and resonance self-shielding. The geometric correction for a LATTICECELL specification utilizes the Dancoff correction factor in order to approximate the effects of a lattice of fuel lumps. NOTE THAT ONLY ONE UNIT CELL SPECIFICATION IS ALLOWED IN A PROBLEM. Thus if a problem utilizes more than one kind of fuel pin (different dimensions, different enrichments, etc.) special procedures must be invoked to assure adequate cross-section treatment as described in Sect. M7.5.10. The unit cell specification associated with the choice of **LATTICECELL** is used to provide information used in processing the cross sections. Only those mixtures used in the unit cell specification have geometric corrections applied to their cross sections. ALL OTHER MIXTURES SPECIFIED IN THE PROBLEM ARE TREATED AS INFINITE HOMOGENEOUS MEDIA unless otherwise specified as described in Sect. M7.5.7 using the parameter keywords RES= and DAN(_)=. Section M7.5.10 demonstrates this procedure. The unit cell configurations available as a LATTICECELL specification are described in Sect. M7.5.6.2.

M7.5.4.3 MULTIREGION

MULTIREGION can be used for a system of geometric regions where the geometry effects may be important but infinite homogeneous media treatment or LATTICECELL treatment are inappropriate. It can also be used to define a geometric configuration that is more complicated than that allowed by the **LATTICECELL**. The **MULTIREGION** treatment assumes a single cell and does not allow a true lattice geometry. Therefore, the cross sections are corrected for resonance self-shielding and the geometric size and shape, but the Dancoff factor is an approximation. The use of **MULTIREGION** requires a unit cell specification following the standard composition specification data. Only one unit cell specification is allowed in a problem. Examples of MULTIREGION geometries are given in Sect. M7.5.6.3.

M7.5.5 STANDARD COMPOSITION SPECIFICATION DATA

The standard composition specification data are used to define mixtures using standardized engineering data entered in a free-form format. The Material Information Processor uses the standard composition specification data and information from the Standard Composition Library to provide number densities for each nuclide of every defined mixture according to Eq. (M7.5.1):

$$NO = \frac{RHO \times AVN \times C}{AWT}, \qquad \text{(M7.5.1)}$$

where

NO is the number density of the nuclide in atoms/b-cm,,

RHO is the actual density of the nuclide in g/cm^3,

AVN is Avogadro's number in atoms/mol,

C is a constant, 10^{-24} cm^2/b,

AWT is the atomic or molecular weight of the nuclide in g/mol.

The actual density, RHO, is defined by

$$RHO = ROTH \times VF \times WGTF, \qquad \text{(M7.5.2)}$$

where

RHO is the actual density of the standard composition in g/cm^3,

ROTH is either the specified density of the standard composition or the theoretical density of the standard composition in g/cm^3,

VF is a density multiplier compatible with ROTH as defined by Eq. (M7.5.3),

WGTF is the weight fraction of the nuclide in the standard composition. This value is automatically obtained by the code from the Standard Composition Library. WGTF is 1.0 for a single nuclide standard composition.

$$VF = DFRAC \times VFRAC, \qquad \text{(M7.5.3)}$$

where

VF is the density multiplier,

DFRAC is the density multiplier,

VFRAC is the volume fraction.

To illustrate the interaction between ROTH and VF, consider an Inconel having a density of 8.5 g/cm^3. It is 7.0% by weight iron, 15.5% chromium, and 77.5% nickel. The Inconel occupies a volume of 4 cm^3.

Method 1: To describe the iron, enter 8.5 for ROTH and 0.07 for VF.
To describe the chromium, enter 8.5 for ROTH and 0.155 for VF.
To describe the nickel, enter 8.5 for ROTH and 0.775 for VF.

Method 2: Do not enter the density, and by default the theoretical density of each component will be used for ROTH. DFRAC will be the ratio of the specified density to the theoretical density. The specified density of each component is the density of the Inconel × the weight fraction of that component. Thus, the density of the iron is $8.5 \times 0.07 = 0.595$ g/cm^3
chromium is $8.5 \times 0.155 = 1.318$ g/cm^3
nickel is $8.5 \times 0.775 = 6.588$ g/cm^3

To calculate DFRAC, the theoretical density of each material must be obtained from Table M8.2.3. These values are
7.86 g/cm^3 for iron
8.90 g/cm^3 for nickel
7.20 g/cm^3 for chromium

The DFRAC entered for the iron is 0.595/7.86 = 0.0757
for the nickel is 1.318/8.90 = 0.1481
for the chromium is 6.588/7.20 = 0.9163

Since there are no volumetric corrections, VFRAC is 1.0 and the values of DFRAC are entered for VF.

Method 3: Assume the Inconel, which occupies 4 cm^3, is to be spread over a volume of 5 cm^3. Then the volume fraction, VFRAC, is 4 cm^3/5 cm^3 = 0.8 and can be combined with the density fraction, DFRAC, to obtain the density multiplier, VF, according to Eq. (M7.5.3).

To describe the iron, enter 8.5 for ROTH and $0.07 \times 0.8 = 0.056$ for VF
or chromium, enter 8.5 for ROTH and $0.155 \times 0.8 = 0.124$ for VF
for nickel, enter 8.5 for ROTH and $0.775 \times 0.8 = 0.620$ for VF

Alternatively, the volume fraction can be applied to the density before it is entered. Then the ROTH can be entered as 8.5 g/cm^3 × 0.8 = 6.8 g/cm^3, and DFRAC is entered for the density multiplier, VF.
To describe the iron, enter 6.8 for ROTH and 0.07 for VF
for chromium, enter 6.8 for ROTH and 0.155 for VF
for nickel, enter 6.8 for ROTH and 0.775 for VF

Method 4: Assume the Inconel, which occupies 4 cm^3, is to be spread over a volume of 5 cm^3. Then the volume fraction, VFRAC, is 4 cm^3/5 cm^3 = 0.8. Do not enter the density, and by default the theoretical density of each component will be used for ROTH.

VF is then entered as the product of VFRAC and DFRAC according to Eq. (M7.5.3).
The specified density of each component is the density of the Inconel × the weight fraction of that component.

Thus, the density of the iron is 8.5 × 0.07 = 0.595 g/cm^3
chromium is 8.5 × 0.155 = 1.318 g/cm^3
nickel is 8.5 × 0.775 = 6.588 g/cm^3

To calculate DFRAC, the theoretical density of each material must be obtained from Table M8.2.3. These values are
7.86 g/cm^3 for iron
8.90 g/cm^3 for nickel
7.20 g/cm^3 for chromium

Then DFRAC for the iron is 0.595/7.86 = 0.0756
for nickel is 1.318/8.90 = 0.1481
for chromium is 6.588/7.20 = 0.9150

Then VF is DFRAC × VFRAC
VF for the iron is 0.0757 × 0.8 = 0.0606
for nickel is 0.1481 × 0.8 = 0.1185
for chromium is 0.9150 × 0.8 = 0.7320

The number densities calculated by the Material Information Processor are used in processing the problem-specific working format cross-section libraries created for use by many of the SCALE functional modules. Three types of input data are allowed for the standard composition specification data: basic, arbitrary materials, and solutions. Each standard composition is terminated by entering the word END. The code continues to read standard composition data until the words END COMP are encountered. The basic data are described in Sect. M7.5.5.1, the arbitrary materials are described in Sect. M7.5.5.2, and the solutions are described in Sect. M7.5.5.3. Many mixtures can be described using only basic, arbitrary, or solution specifications. However, the description of some mixtures can be greatly simplified by using a combination of those specifications as shown in Sects. M7.5.5.4 through M7.5.5.9.

M7.5.5.1 Basic Standard Composition Specifications

Basic standard compositions are those whose standard composition name is found in the Standard Composition Library. The input data for basic standard compositions are discussed in more detail in Sect. M7.4.4. Examples of basic standard compositions are given below.

GENERIC EXAMPLE

Input data for the basic standard compositions are entered as follows:

SC MX DEN=ROTH VF ADEN TEMP (IZA_i WTP_i) END

or

SC MX SPG=ROTH VF ADEN TEMP (IZA_i WTP_i) END

where

SC is the standard composition component name (see Sect. M8.2).

MX is the mixture number (defined by the user).

ROTH is the density of the material. THESE DATA ARE OPTIONAL AND ARE ENTERED USING THE KEYWORD SPG= or DEN=.

VF is the density multiplier for this standard composition (enter 0 if the number density is to be entered for this standard composition).

ADEN is the number density (atoms/b-cm). Enter only if VF = 0.

TEMP is the temperature in Kelvin.

IZA is the isotope ID number (see Sect. M8.2).

WTP is the weight percent of the isotope in the material. WTP must be between 0 and 100.

Repeat the sequence IZA WTP until the sum of the WTPs sum to 100. IZA and WTP are used to specify the isotopic abundance of a standard composition that has multiple isotopes. IZA identifies the isotope, and WTP specifies its abundance in weight percent. The sequence IZA WTP is repeated until all of the desired isotopes have been specified.

EXAMPLE 1. Material name is given.
Create a mixture 3 that is Plexiglas. Since no other information is given, the information on the Standard Composition Library can be assumed to be adequate. Therefore, the only data to be entered are the standard composition name and the mixture number. The minimum generic input specification for the Plexiglas follows:

```
SC   MX   END
```

where

SC is the standard composition component name (PLEXIGLAS; see Table M8.2.4).

MX is the mixture number (enter a 3). The input data for the Plexiglas are given below.

```
PLEXIGLAS   3   END
```

EXAMPLE 2. Material name and density (g/cm^3) are given.
Create a mixture 3 that is Plexiglas at a density of 1.15 g/cm^3. Since no other data are specified, the defaults from the Standard Composition Library will be used. Therefore, the only data to be entered are the standard composition name, the mixture number, and the density. The minimum generic input specification for the Plexiglas is given below:

```
SC   MX   DEN=ROTH   END
```

where

SC is the standard composition component name (PLEXIGLAS; see Table M8.2.4).

MX is the mixture number (enter a 3).

ROTH is the density of the material (enter DEN=1.15).

The input data for the Plexiglas are given below.

```
PLEXIGLAS   3   DEN=1.15   END
```

EXAMPLE 3. Material name and number density (atoms/b-cm) are given.
Create a mixture 2 that is aluminum having a number density of 0.060244.

The generic standard composition specification is

```
SC   MX   VF   ADEN   END
```

where

SC is the standard composition component name (AL; see Table M8.2.2).

MX is the mixture number (2).

VF is the density multiplier (enter 0 because the number density is to be used).

ADEN is the number density of the standard composition (0.060244).

The input data for the aluminum are given below:

```
AL  2  0  .060244  END
```

EXAMPLE 4. Material name, density (g/cm^3) and isotopic abundance are given.
Create a mixture 1 that is uranium metal at 18.76 g/cm^3 whose isotopic composition is 93.2 wt % ^{235}U, 5.6 wt % ^{238}U, and 1.0 wt % ^{234}U, and 0.2 wt % ^{236}U. This example uses the DEN= keyword to enter the density and define the standard composition. Example 5 demonstrates another method of defining the standard composition.

The generic standard composition specification is

```
SC  MX  DEN=ROTH  VF  TEMP  (IZA_i WTP_i)  END
```

where

SC is the standard composition component name (URANIUM; see Table M8.2.3).

MX is the mixture number (enter a 1).

ROTH is the density of the material (enter DEN = 18.76).

VF is the density multiplier (enter 1 because the density was entered using DEN=).

TEMP is the temperature in Kelvin (293).

IZA is the isotope ID number (92235 for ^{235}U, 92238 for ^{238}U, 92234 for ^{234}U, and 92236 for ^{236}U).

WTP is the weight percent of the isotope in the material (93.2 for ^{235}U, 5.6 for ^{238}U, 1.0 for ^{234}U, and 0.2 for ^{236}U). Repeat the sequence IZA WTP until the sum of the WTPs sum to 100.

The input data for the uranium metal follow:

```
URANIUM  1  DEN=18.76  1  293  92235  93.2  92238  5.6  92234  1.0  92236  0.2
END
```

EXAMPLE 5. Material name, density (g/cm^3) and isotopic abundance are given.
Create a mixture 1 that is uranium metal at 18.76 g/cm^3 whose isotopic composition is 93.2 wt % ^{235}U, 5.6 wt % ^{238}U, and 1.0 wt % ^{234}U, and 0.2 wt % ^{236}U. This method illustrates the standard composition specification without using the DEN= option.

The generic standard composition specification is

SC MX VF TEMP (IZA$_i$ WTP$_i$) END

where

SC is the standard composition component name (URANIUM; see Table M8.2.3).

MX is the mixture number (enter a 1).

VF is the density multiplier (the density multiplier is the ratio of actual to theoretical density (18.76/19.05 = 0.985). The theoretical density (19.05 g/cm^3) is obtained from Table M8.2.3.

TEMP is the temperature in Kelvin (293).

IZA is the isotope ID number (92235 for ^{235}U, 92238 for ^{238}U, 92234 for ^{234}U, and 92236 for ^{236}U).

WTP is the weight percent of the isotope in the material (93.2 for ^{235}U, 5.6 for ^{238}U, 1.0 for ^{234}U, and 0.2 for ^{236}U). Repeat the sequence IZA WTP until the sum of the WTPs sum to 100.

The input data for the uranium metal follow:

```
URANIUM   1  0.985  293  92235  93.2  92238  5.6  92234  1.0  92236  0.2  END
```

EXAMPLE 6. Material name, density (g/cm^3) and isotopic abundance are given.
Create a mixture 7 defining B_4C with a density of 2.45 g/cm^3. The boron is 40 wt % ^{10}B and 60 wt % ^{11}B. This example utilizes the DEN= keyword. Example 7 illustrates an alternative description. The minimum generic input specification for this standard composition is

SC MX DEN=ROTH VF TEMP (IZA$_i$ WTP$_i$) END

where

SC is the standard composition component name (B4C; Table M8.2.4).

MX is the mixture number (7).

ROTH is the density of the material (enter DEN=2.45).

VF is the density multiplier (enter 1.0 because the density was entered).

TEMP is the temperature in Kelvin (293).

IZA is the isotope ID number (5010 for ^{10}B and 5011 for ^{11}B).

WTP is the weight percent of the isotope in the material (40 for ^{10}B and 60 for ^{11}B). Repeat the sequence IZA WTP until the sum of the WTPs sum to 100.

The input data for the B_4C are given below.

```
B4C 7  DEN=2.45  1.0  293  5010  40.0  5011  60.0  END
```

EXAMPLE 7. Material name, density (g/cm^3) and isotopic abundance are given.
Create a mixture 7 defining B_4C with a density of 2.45 g/cm^3. The boron is 40 wt % ^{10}B and 60 wt % ^{11}B. This example incorporates the known density into the density multiplier, VF, rather than using the DEN= keyword. The minimum generic input specification for this standard composition is

```
SC  MX  VF  TEMP  (IZA_i  WTP_i)  END
```

where

SC is the standard composition component name (B4C; Table M8.2.4).

MX is the mixture number (7).

VF is the density multiplier (the density multiplier is the ratio of actual to theoretical density (2.45/2.52 = 0.9722). The theoretical density (2.52 g/cm^3) is obtained from Table M8.2.1.

TEMP is the temperature in Kelvin (293).

IZA is the isotope ID number (5010 for ^{10}B and 5011 for ^{11}B).

WTP is the weight percent of the isotope in the material (40 for ^{10}B and 60 for ^{11}B). Repeat the sequence IZA WTP until the sum of the WTPs sum to 100.

The input data for the B_4C are given below.

```
B4C  7  0.9722  293  5010  40.0  5011  60.0  END
```

Note in the above examples, that the actual density is input for materials containing enriched multi-isotope nuclides (uranium in examples 4 and 5 and boron in examples 6 and 7). The default density should never be used for enriched materials, especially low atomic mass neutron absorbers such as boron and lithium. The default density is a fixed value for nominal conditions and naturally occurring distributions of isotopes. Use of the default density for enriched materials will likely result in incorrect number densities.

M7.5.5.2 Arbitrary Material Specifications

The arbitrary material option allows the user to specify materials that are not found in the Standard Composition Library. To define an arbitrary material, the first four characters of the standard composition component name must be ARBM. The remaining characters of the standard composition component name are chosen by the user. The maximum length of the standard composition name is 16 characters. All the information that would normally be found in the Standard Composition Library must be entered in the arbitrary material specification. Section M7.4.5 contains data input details for arbitrary materials.

GENERIC EXAMPLE

The generic input data for arbitrary materials are entered as follows:

SC ROTH NEL IVIS ICP IRS ($NCZA_i$ $ATPM_i$) MX VF TEMP (IZA_j WTP_j) END

where

SC is the standard composition component name (maximum length is 16 characters, the first four characters must be ARBM, the remaining characters are determined by the user).

ROTH is the density of the compound in g/cm^3.

NEL is the number of elements or nuclides in the material.

IVIS is an unused variable. Enter 0 or 1.

ICP is the compound indicator (enter a 1 for a compound represented by a chemical formula; a 0 for an alloy or mixture).

IRS is an unused variable. Enter 0 or 1.

NCZA is the isotope ID number (see Sect. M8.2 to determine the isotope ID number). For example, aluminum has a standard composition component of AL and an isotope ID number of 13027 so 13027 would be entered for aluminum. If a multiple-isotope nuclide is to be used, enter Z*1000 where Z is the atomic number. For example, 92000 would be entered for uranium or 5000 would be entered for boron.

ATPM is the weight percent of the isotope (NCZA) in this material.

Repeat the sequence NCZA ATPM until the NEL elements in the arbitrary material have been specified.

MX is the mixture number (chosen by the user).

VF is the fraction of this arbitrary material in the mixture. (The relationship between VF and ROTH is given in Sect. M7.5.5.)

TEMP is the temperature in Kelvin.

IZA is the isotope ID number. ENTER ONLY IF MULTIPLE-ISOTOPE NUCLIDE(s) HAVE BEEN SPECIFIED, in which case one or more of the NCZAs was a multiple-isotope nuclide. Then IZA and WTP are used to specify the isotopic abundance of the multiple-isotope nuclide.

WTP is the weight percent of the isotope (NCZA) in the multiple-isotope nuclide.

Repeat the sequence IZA WTP until the sum of the WTPs sum to 100. IZA and WTP are used to specify the isotopic abundance of the multiple-isotope nuclide. IZA identifies the isotope, and WTP specifies its abundance in weight percent. The sequence IZA WTP is repeated until all of the desired isotopes have been specified.

EXAMPLE 1. Density and weight percents are given.

Create a mixture 5 that defines a borated aluminum that is 2.5 wt % natural boron. The density of the borated aluminum is 2.65 g/cm^3. The minimum generic input specification for this arbitrary material is

```
SC  ROTH  NEL  IVIS  ICP  IRS  (NCZA_i  ATPM_i)  MX  END
```

where

SC is the standard composition component name. (ARBMBAL is used as the standard composition name in this example. The first 4 characters **MUST** be ARBM. The remaining characters are chosen by the user.)

ROTH is the density of the compound in g/cm^3 (enter 2.65).

NEL is the number of elements in the material (enter a 2; aluminum and boron).

IVIS is an unused variable. A value must be entered, and 1 was chosen because it is correct for older versions of SCALE.

ICP is the compound indicator (enter 0 because this material is not defined by a chemical formula).

IRS is an unused variable. A value must be entered, and 0 was chosen because it is correct for older versions of SCALE.

NCZA is the isotope ID number [enter 5000 for the boron (1000*Z is entered for multiple-isotope nuclides)]. (Enter 13027 for the aluminum.)

ATPM is the weight percent of the isotope in the material (enter 2.5 for the boron and 97.5 for the aluminum). Repeat the sequence NCZA ATPM until the NEL elements in the arbitrary material have been specified.

MX is the mixture number (enter 5).

Because natural boron was specified in the problem, no further data need be specified. EXAMPLE 2 illustrates the situation where the isotopic abundance of boron must be specified.

The input data for this arbitrary material are given below.

```
ARBMBAL  2.65  2  1  0  0  5000  2.5  13027  97.5  5  END
```

EXAMPLE 2. Density, weight percents, and isotopic abundance are given.

Create a mixture 5 that defines a borated aluminum that is 2.5 wt % boron. The boron is 90 wt % ^{10}B and 10 wt % ^{11}B. The density of the borated aluminum is 2.65 g/cm^3. The minimum generic input specification for this arbitrary material is

```
SC  ROTH  NEL  IVIS  ICP  IRS  (NCZA_i  ATPM_i)  MX  VF  TEMP  (IZA_j  WTP_j)  END
```

where

SC is the standard composition component name. The first 4 characters **MUST** be ARBM (enter ARBMBAL).

ROTH is the density of the compound in g/cm^3 (enter 2.65).

NEL is the number of elements in the material (enter 2).

IVIS is an unused variable. A value must be entered, and 1 was chosen because it is correct for older versions of SCALE.

ICP is the compound indicator. (Enter 0 because this material is not defined by a chemical formula.)

IRS is an unused variable. A value must be entered, and 0 was chosen because it is correct for older versions of SCALE.

NCZA is the isotope ID number [Enter 5000 for the boron (1000*Z is entered for multiple-isotope nuclides). Enter 13027 for the aluminum.]

ATPM is the weight percent of the isotope in the material. (Enter 2.5 for the boron and 97.5 for the aluminum.)

Repeat the sequence NCZA ATPM until the NEL elements in the arbitrary material have been specified.

MX is the mixture number (enter 5).

VF is the density multiplier (use 1 or 1.0 since the density of the material was entered as the theoretical density, ROTH).

TEMP is the temperature in Kelvin. (Enter 293. The temperature must be entered because the isotopic abundance of boron must be specified.)

IZA is the isotope ID number for the isotopes in the multiple-isotope nuclide (enter 5010 for ^{10}B and 5011 for ^{11}B).

WTP is the weight percent of the isotope in the multiple-isotope nuclide (enter 90 for ^{10}B and 10 for ^{11}B).

Repeat the sequence IZA WTP until the sum of the WTPs sum to 100 and all of the isotopes present in the multiple-isotope nuclide have been entered.

The input data for this arbitrary material are given below.

```
ARBMBAL  2.65  2  1  0  0  5000  2.5  13027  97.5  5  1  293  5010  90.  5011  10.  END
```

EXAMPLE 3. Density and chemical equation are given.

Create a mixture 3 that is a hydraulic fluid, C_2H_6SiO, with a density of 0.97 g/cm^3. The minimum generic input specification for this arbitrary material is

```
SC  ROTH  NEL  IVIS  ICP  IRS  (NCZA_i  ATPM_i)  MX  END
```

where

SC is the standard composition component name. The first 4 characters **MUST** be ARBM (enter ARBMC2H6SIO).

ROTH is the theoretical density of the compound in g/cm^3 (0.97).

NEL is the number of elements in the material (there are 4 elements in this material, C, H, Si, and O).

IVIS is an unused variable. A value must be entered, and 0 was chosen because it is correct for older versions of SCALE.

ICP is the compound indicator (enter a 1 because this material is defined by a chemical formula).

IRS is an unused variable. A value must be entered, and 0 was chosen because it is correct for older versions of SCALE.

NCZA is the element ID number. (Tables M8.2.2 and M8.2.3 list the element ID numbers. Enter 6012 for carbon, 1001 for hydrogen, 14000 for silicon and 8016 for oxygen.)

ATPM is the number of atoms of this element per molecule of arbitrary material. (Enter 2 for carbon, 6 for hydrogen, 1 for silicon and 1 for oxygen.)

Repeat the NCZA ATPM sequence until the chemical formula of a molecule has been defined.

MX is the mixture number (3).

The input data for this arbitrary material are given below:

```
ARBMC2H6SIO  0.97  4  0  1  0  6012  2  1001  6  14000  1  8016  1  3  END
```

EXAMPLE 4. Density and chemical equation are given.

Create a mixture 7, TBP, also known as phosphoric acid tributyl ester or tributylphosphate, $(C_4H_9O)_3PO$, having a density of 0.973 g/cm^3.

```
SC  ROTH  NEL  IVIS  ICP  IRS  (NCZA_i  ATPM_i)  MX  END
```

where

SC is the standard composition component name. The first 4 characters **MUST** be ARBM (enter ARBMTBP).

ROTH is the theoretical density of the compound in g/cm^3 (0.973).

NEL is the number of elements in the material. (There are 4 elements in TBP, C, H, O, and P.)

IVIS is an unused variable. A value must be entered, and 0 was chosen because it is correct for older versions of SCALE.

ICP is the compound indicator. (Enter a 1 because TBP is defined by a chemical formula.)

IRS is an unused variable. A value must be entered, and 0 was chosen because it is correct for older versions of SCALE.

NCZA is the nuclide/isotope ID number. (Section M8.2 lists the nuclide/isotope ID numbers. Use 1001 for hydrogen, 6012 for carbon, 8016 for oxygen and 15031 for phosphorus.)

ATPM is the number of atoms of each element in the arbitrary material. (Enter 27 for hydrogen, 12 for carbon, 4 for oxygen, and 1 for phosphorus.)

Repeat the NCZA ATPM sequence until the NEL elements have been described.

MX is the mixture number (7).

The input data for the TBP are given below:

```
ARBMTBP  0.973  4  0  1  0  1001  27  6012  12  8016  4  15031  1  7  END
```

M7.5.5.3 Solution Specifications

Solutions of fissile materials are available in the Material Information Processor. A list of the available solutions are given in Table M8.3.1. When the Material Information Processor processes a solution, it breaks the solution up into its component parts (basic standard composition specifications) and uses the specific gravity to calculate the volume fractions. If the specific gravity is not explicitly entered in the solution specification, the Material Information Processor uses a fitted equation to determine the specific gravity. The specific gravity should be entered if it is known. Section M7.4.4 contains data input details for solutions. See Sect. M7.5.9 for a comparison of three different methods of specifying a uranyl nitrate solution.

GENERIC EXAMPLE

The generic input data for solutions are entered as follows:

SC MX FD AML SPG=SPGR VF TEMP (IZA_i WTP_i) END

or

SC MX FD AML DEN=SPGR VF TEMP (IZA_i WTP_i) END

or

SC MX FD AML VF TEMP (IZA_i WTP_i) END

where

SC is the standard composition component name.

MX is the mixture number.

FD is the fuel density in grams of U or Pu per liter of solution.

AML is the acid molarity of the solution.

SPGR is the specific gravity of the solution. THESE DATA ARE OPTIONAL AND ARE ENTERED USING THE KEYWORD SPG= or DEN=.

VF is the density multiplier (ratio of actual to theoretical density of the solution).

TEMP is the temperature in Kelvin.

IZA is the isotope ID number.

WTP is the weight percent of the isotope in the material.

Repeat the sequence IZA WTP until the sum of the WTPs sum to 100.

Examples of solution specifications follow:

EXAMPLE 1. Fuel density, specific gravity, excess acid and isotopic abundance are given.

Create a mixture 2 that is highly enriched uranyl nitrate solution at 415 g/L, a specific gravity of 1.555 and 0.39 mg of excess nitrate per gram of solution. The uranium isotopic content is 92.6 wt % ^{235}U, 5.9 wt % ^{238}U, 1.0 wt % ^{234}U, and 0.5 wt % ^{236}U.

A generic input specification for this solution is

```
SC   MX   FD   AML   SPG=SPGR   VF   TEMP   (IZA_i   WTP_i)   END
```

where

SC is the standard composition component name from Table M8.3.1 of Sect. M8.3 (enter SOLNUO2(NO3)2).

MX is the mixture number (enter 2).

FD is the fuel density in grams of U or Pu per liter of solution (enter 415).

AML is the acid molarity of the solution. The molecular weight of the NO_3 is 61.9895. The molarity is (0.39 mg nitrate/g soln) × (1000 cm^3 soln/L soln) × (1 g/1000 mg) × (1.555 g soln/cm^3 soln) = 0.60645 g excess nitrate/L soln. (0.60645 g nitrate/L soln)/(61.9895 g nitrate/mol nitrate) = 9.783×10^{-3} mols nitrate/L soln. The mols of nitrate per liter is identical to mols of acid per liter, which is identical to molarity.

SPGR is the specific gravity of the solution. The specific gravity is optional data and is entered using the keyword SPG=SPGR or DEN=SPGR. (Enter SPG=1.555 or DEN=1.555.)

VF is the density multiplier of the solution in the mixture. (Enter a 1 because this mixture is composed entirely of this solution.)

TEMP is the temperature in Kelvin (293).

IZA is the isotope ID number. (Enter 92235 for ^{235}U, 92238 for ^{238}U, 92234 for ^{234}U, and 92236 for ^{236}U.)

WTP is the weight percent of the isotope in the material. (Enter 92.6 for ^{235}U, 5.9 for ^{238}U, 1.0 for ^{234}U, and 0.5 for ^{236}U.)

Repeat the sequence IZA WTP until the sum of the WTPs sum to 100.

The input data for the uranyl nitrate solution are

```
   SOLNUO2(NO3)2 2 415 9.783-3 SPG=1.555 1.0 293 92235 92.6 92238 5.9
92234 1.0 92236 0.5 END
```

M7.5.5.4 Combinations of Basic Standard Compositions to Define a Mixture

Frequently more than one standard composition is required to define a mixture. This section contains such examples.

EXAMPLE 1. Boral from B_4C and Aluminum.

Create a mixture 6 that is boral, 15 wt % B_4C and 85 wt % Al, having a density of 2.64 g/cm^3. Natural boron is used in the B_4C. Boral can be described in several ways. Example 1 of Sect. M7.5.5.5 illustrates how to describe boral using arbitrary materials. Because both B_4C and Al are available in the Standard Composition Library, it is not necessary to use arbitrary materials. Using basic standard compositions is much easier as shown by this example. Example 2 demonstrates the use of the keyword DEN= to enter the density of the mixture and avoid having to look up the theoretical density from Table M8.2.1 and calculate the density multiplier (VF). The generic specification for this example is

```
SC   MX   VF   END
```

where

SC is the standard composition component name (enter B4C for B_4C and AL for aluminum).

MX is the mixture number (enter 6).

VF is the density multiplier. (The density multiplier is the ratio of actual to theoretical density. For B_4C, the density multiplier is (0.15 x 2.64)/2.52, and for the aluminum the density multiplier is (0.85 x 2.64)/2.6989. The theoretical density (2.52 g/cm^3 for B_4C and 2.6989 g/cm^3 for aluminum) is obtained from Table M8.2.1.

The standard compositions input data for the boral are given below.

```
B4C   6   0.1571   END
AL    6   0.8314   END
```

EXAMPLE 2. Boral from B_4C and Aluminum.

This is the same problem as example 1 using a different method of specifying the input data. Create a mixture 6 that is boral, 15 wt % B_4C and 85 wt % Al, having a density of 2.64 g/cm^3. Natural boron is used in the B_4C. Boral can be described in several ways. Example 1 of Sect. M7.5.5.5 illustrates how to describe boral using arbitrary materials. Because both B_4C and Al are available in the Standard Composition Library, it is not necessary to use arbitrary materials. Using standard compositions is much easier as shown by this example. The generic specification for this problem is

```
SC   MX   DEN=ROTH   VF   END
```

where

SC is the standard composition component name (enter B4C for B_4C and AL for aluminum).

MX is the mixture number (enter 6).

ROTH is the density of the material. (Enter DEN=2.64 for both B_4C and Al).

VF is the weight fraction of the mixture that is this standard composition. (Enter 0.15 for B_4C and 0.85 for Al.)

The standard composition input data for the boral are given below:

```
B4C   6   DEN=2.64   0.15   END
AL    6   DEN=2.64   0.85   END
```

EXAMPLE 3. Boral from Boron, Carbon, and Aluminum

If neither boral nor B_4C were available in the Standard Composition Library, boral could be described as follows:

Create a mixture 2 that is boral composed of 35 wt % B_4C and 65 wt % aluminum with an overall density of 2.64 g/cm^3. The boron is natural boron. The generic specification for this problem is

```
SC   MX   VF   END
```

where

SC is the standard composition name (enter BORON for boron, C for carbon, and AL for aluminum).

MX is the mixture number (2 for each standard composition).

VF is the density multiplier. (The density multiplier is the ratio of actual to theoretical density. From the Standard Composition Library, Table M8.2.1, the theoretical density of aluminum is 2.6989 g/cm^3; boron is 2.373 g/cm^3; and carbon is 2.30 g/cm^3. The density multiplier, VF, for Al is (0.65)(2.64)/2.6989 = 0.63581. From Table M8.4.1 of Sect. M8.4, the natural boron is 18.3022 wt % ^{10}B at 10.0129 amu and 81.6978 wt % ^{11}B at 11.0096 amu. C is 12.000 amu.

Convert the weight percents to atom percents for the natural boron where w denotes weight fraction, a denotes atom fraction, and M denotes atomic mass:

$$w_{^{10}B} = 0.183022 = \frac{a_{^{10}B} M_{^{10}B}}{a_{^{10}B} M_{^{10}B} + a_{^{11}B} M_{^{11}B}} =$$

$$\frac{a_{^{10}B}(10.0129)}{a_{^{10}B}(10.0129) + (1 - a_{^{10}B})(11.0096)}$$

$$a_{^{10}B}\left[\left(\frac{10.0129}{0.183022}\right) - 10.0129 + 11.0096\right] = 11.0096$$

$$a_{^{10}B} = 0.19764 = 19.764 \text{ atom } \% \ .$$

Similarly,

$$a_{^{11}B} = 80.236 \text{ atom \%}.$$

The mass of the B_4C molecule is
$[(0.19764 \times 4 \times 10.0129) + (0.80236 \times 4 \times 11.0096) + (12.000)] = 55.25045$ amu.
The mass of the boron is $(55.25045 - 12.000) = 43.25045$ amu.

The VF of boron would be $\left(\frac{43.25045}{55.25045}\right)\left[\frac{(0.35)(2.64)}{2.373}\right] = 0.30481$.

The VF of C would be $\left(\frac{12.000}{55.25045}\right)\left[\frac{(0.35)(2.64)}{2.30}\right] = 0.08725$.

The standard composition input data for the boral follow:

```
AL          2     0.63581        END
BORON       2     0.30481        END
C           2     0.08725        END
```

EXAMPLE 4. Boral from ^{10}B, ^{11}B, Carbon, and Aluminum

Create a mixture 2 that is boral composed of 35 wt % B_4C and 65 wt % aluminum. The boral density is 2.64 g/cm^3. The boron is natural boron. The generic specification for this problem is

```
SC   MX   VF   END
```

where

SC is the standard composition name (enter B-10 for ^{10}B, B-11 for ^{11}B, C for carbon, and AL for aluminum).

MX is the mixture number (2 for each standard composition).

VF is the density multiplier. Enter 0.63581 for AL and 0.08725 for C as explained in Example 3 above. From the Standard Composition Library, Table M8.2.1, the theoretical density of ^{10}B is 1.00 g/cm^3 and ^{11}B is 1.00 g/cm^3. As computed in Example 3, the mass of the B_4C molecule is 55.25045 amu, and the boron is 19.764 atom % ^{10}B and 80.236 atom % ^{11}B. The mass of ^{10}B is 10.0129 amu and the ^{11}B is 11.0096. Thus, the VF of ^{10}B is

$$\left[\frac{(4)(0.19764)(10.0129)}{55.25045}\right]\left[\frac{(0.35)(2.64)}{1.00}\right] = 0.13238 .$$

The VF of ^{11}B is

$$\left[\frac{(4)(0.80236)(11.0096)}{55.25045}\right]\left[\frac{(0.35)(2.64)}{1.00}\right] = 0.59092 .$$

The standard composition input data for the boral are given as

```
AL     2      0.63581     END
B-10   2      0.13238     END
B-11   2      0.59092     END
C      2      0.08725     END
```

EXAMPLE 5. Specify all of the number densities in a mixture.

Create a mixture 1 that is vermiculite, defined as

hydrogen	at a number density of 6.8614-4 atoms/b-cm
oxygen	at a number density of 2.0566-3 atoms/b-cm
magnesium	at a number density of 3.5780-4 atoms/b-cm
aluminum	at a number density of 1.9816-4 atoms/b-cm
silicon	at a number density of 4.4580-4 atoms/b-cm
potassium	at a number density of 1.0207-4 atoms/b-cm
iron	at a number density of 7.7416-5 atoms/b-cm

The generic standard composition specification is

```
SC   MX   VF   ADEN   END
```

where

SC is the standard composition component name.

MX is the mixture number.

VF is the density multiplier (enter 0 because number densities are to be used).

ADEN is the number density of the standard composition.

The standard composition input data for the vermiculite are given below:

```
H          1   0   6.8614-4   END
O          1   0   2.0566-3   END
MN         1   0   3.5780-4   END
AL         1   0   1.9806-4   END
SI         1   0   4.4580-4   END
K          1   0   1.0207-4   END
FE         1   0   7.7406-5   END
```

M7.5.5.5 Combinations of Arbitrary Materials to Define a Mixture

Mixtures can usually be created using only basic standard composition specifications. Occasionally, it is convenient to create two or more arbitrary materials for a given mixture. This procedure is demonstrated in the following example.

EXAMPLE 1. Specify boral using two arbitrary materials.

Create a mixture 6 that is boral, 15 wt % B_4C and 85 wt % Al, having a density of 2.64 g/cm^3. Natural boron is used in the B_4C. Boral can be described in several ways. For demonstration purposes, it will be described as an arbitrary material. This is not necessary, because both B_4C and Al are available as standard compositions. A method of describing the boral without using arbitrary materials is given in Examples 1 and 2 of Sect. M7.5.5.4. The minimum generic input specification for this arbitrary material is

```
SC  ROTH  NEL  IVIS  ICP  IRS  (NCZA_i  ATPM_i)  MX  VF  END
```

where

SC is the standard composition component name. The first four characters must be ARBM (enter ARBM-B4C for B_4C and ARBM-AL for aluminum).

ROTH is the theoretical density of the compound (2.64 g/cm^3).

NEL is the number of elements in the material (there are two elements in B_4C, B & C; there is one element in aluminum).

IVIS is an unused variable. A value must be entered, and 1 was chosen for B4C because it is correct for older versions of SCALE, while 0 was correct for AL.

ICP is the compound indicator (enter a 1 for the B_4C because it is defined by a chemical formula; enter a 0 for the aluminum because it is not defined by a chemical formula).

IRS is an unused variable. A value must be entered, and 0 was chosen because it is correct for older versions of SCALE.

NCZA is the isotope ID number (Table M8.2.1 lists the isotope ID numbers) (enter 5000 for boron, 6012 for carbon, and 13027 for aluminum).

ATPM is the number of atoms of each element in the arbitrary material. For the B_4C enter 4 for the boron and 1 for the carbon. For the aluminum, ATPM is the weight percent of the element in the arbitrary material. Repeat the NCZA ATPM sequence until the chemical formula of B_4C has been defined. Repeat the NCZA ATPM sequence until the weight percents sum to 100.

MX is the mixture number (enter 6).

VF is the density multiplier. (Use 0.15 for the B_4C and 0.85 for the Al because the density of the boral, 2.64 g/cm^3, was entered as the theoretical density, ROTH.)

The input data for the boral are given below:

```
ARBM-B4C  2.64  2  1  1  0  5000  4  6012  1  6  0.15  END
ARBM-AL   2.64  1  0  0  0  13027  100.0  6  0.85  END
```

M7.5.5.6 Combinations of Solutions to Define a Mixture

This section demonstrates the use of more than one solution definition to describe a single mixture. The assumptions used in processing the cross sections are likely to be inadequate for solutions of mixed oxides of uranium and plutonium (see Sect. M7.2.5.2). Therefore, this section is given purely for demonstration purposes. The use of this method is not recommended and should be carefully evaluated for each specific application. The input data for a solution are entered as follows:

```
SC  MX  FD  AML  SPG=SPGR  VF  TEMP  (IZA_i  WTP_i)  END
```

where

SC is the standard composition component name from Table M8.3.1 of Sect. M8.3.

MX is the mixture number.

FD is the fuel density in grams of U or Pu per liter of solution.

AML is the acid molarity of the solution.

SPGR is the specific gravity of the solution.

VF is the density multiplier (ratio of actual to theoretical density of the solution).

TEMP is the temperature in Kelvin.

IZA is the isotope ID number from Table M8.3.1.

WTP is the weight percent of the isotope in the material.

Repeat the sequence IZA WTP until the sum of the WTPs sum to 100.

EXAMPLE 1. Solution of uranyl nitrate and plutonium nitrate.

Note that the assumptions used in processing the cross sections are likely to be inadequate for mixed-oxide solutions. This example is given purely for demonstration purposes. Create a mixture 1 consisting of a mixture of plutonium nitrate solution and uranyl nitrate solution. The specific gravity of the mixed solution is 1.4828. The solution contains 325.89 g (U + Pu)/L soln. The acid molarity of the solution is 0.53. The solution is 77.22 wt % uranium. The isotopic abundance of the uranium is 0.008% ^{234}U, 0.7% ^{235}U, 0.052% ^{236}U, and 99.24% ^{238}U. The isotopic abundance of the plutonium is 0.028% ^{238}Pu, 91.114% ^{239}Pu, 8.34% ^{240}Pu, 0.426% ^{241}Pu, and 0.092% ^{242}Pu.

The generic input specification for this solution is

SC MX FD AML SPG=SPGR VF TEMP (IZA_i WTP_i) END

where

SC is the standard composition name from Table M8.3.1 (enter SOLNPU(NO3)4 for the plutonium nitrate and SOLNUO2(NO3)2 for the uranyl nitrate).

MX is the mixture number (enter 1 for both solutions).

FD is the fuel density in grams of U or Pu per liter of solution (enter 325.89 for the plutonium nitrate and 325.89 for the uranyl nitrate).

AML is the acid molarity (enter 0.53 for both solutions).

SPGR is the specific gravity of the solution (enter SPG=1.4828 for both solutions).

VF is the density multiplier (ratio of actual to theoretical density of the solution).

TEMP is the temperature in Kelvin (enter 293).

IZA is the isotope ID number from Table M8.3.1 (enter 94238 for ^{238}Pu, 94239 for ^{239}Pu, 94240 for ^{240}Pu, 94241 for ^{241}Pu, 94242 for ^{242}Pu, 92234 for ^{234}U, 92235 for ^{235}U, 92236 for ^{236}U, and 92238 for ^{238}U).

WTP is the weight percent of the isotope in the material (enter 0.028 for ^{238}Pu, 91.114 for ^{239}Pu, 8.34 for ^{240}Pu, 0.426 for ^{241}Pu, 0.092 for ^{242}Pu, 0.008 for ^{234}U, 0.7 for ^{235}U, 0.052 for ^{236}U, and 99.24 for ^{238}U).

```
SOLNPU(NO3)4  1  325.89  0.53  SPG=1.4828  0.2278  293.  94238  .028
          94239  91.114  94240  8.34  94241  .426  94242  .092  END

SOLNUO2(NO3)2  1  325.89  0.53  SPG=1.4828  0.7722  293.  92234  .008
          92235  .700  92236  .052  92238  99.240  END
```

M7.5.5.7 Combinations of Basic and Arbitrary Standard Compositions to Define a Mixture

EXAMPLE 1. Burnable poison from B_4C and Al_2O_3.

Create a mixture 6 that is a burnable poison with a density of 3.7 g/cm^3 and composed of Al_2O_3 and B_4C. The material is 1.395 wt % B_4C. The boron is natural boron. This material can be easily specified using a combination of an arbitrary material to describe the Al_2O_3 and a simple standard composition to define the B_4C. The minimum generic input specification for this arbitrary material and the standard composition are

```
SC  ROTH  NEL  IVIS  ICP  IRS  (NCZA_i  ATPM_i)  MX  VF  END
SC  MX  VF  END
```

where

SC is the standard composition component name (enter ARBMPOIS1 for the Al_2O_3 and enter B4C for B_4C).

ROTH is the theoretical density of the compound (3.70 g/cm^3).

NEL is the number of elements in the material (there are 2 elements in Al_2O_3).

IVIS is an unused variable. A value must be entered, and 0 was chosen because it is correct for older versions of SCALE.

ICP is the compound indicator (enter a 1 for the Al_2O_3 because it is defined by a chemical formula).

IRS is an unused variable. A value must be entered, and 0 was chosen because it is correct for older versions of SCALE.

NCZA is the isotope ID number. Table M8.2.1 lists the isotope ID numbers. (Enter 13027 for aluminum and 8016 for oxygen.)

ATPM is the number of atoms of each element in the arbitrary material (enter 2 for aluminum and 3 for oxygen).

MX is the mixture number (6).

VF is the density multiplier (the density multiplier of the B_4C is the density of the material times the weight percent, divided by the theoretical density of B_4C ((3.7 × 0.01395)/2.52) or 0.02048; the density multiplier of the Al_2O_3 is 1.0 - 0.01395 or 0.98605 (the theoretical density of B_4C was obtained from Table M8.2.1).

The input data for the burnable poison are given below:

```
ARBMPOIS1  3.70  2  0  1  0  13027  2  8016  3  6  0.98605  END
B4C  6  2.048-2  END
```

The input can be specified using the DEN= parameter as shown below:

```
ARBMPOIS1  3.70  2  0  1  0  13027  2  8016  3  6  0.98605  END
B4C  6  DEN=3.7  0.01395  END
```

The density of the Al_2O_3 can be calculated. The fraction of B_4C in the mixture is $((3.7 \times 0.01395)/2.52) = 0.02048$. The fraction of Al_2O_3 in the mixture is $1.0 - 0.02048 = 0.979518$.

$$F_{Al_2O_3} * \text{Density}_{Al_2O_3} + 0.020482 * 2.52 = 3.7 = \text{Density of the mixture}$$

$$\text{Density}_{Al_2O_3} = \frac{3.7 - 0.020482 * 2.52}{0.979518} = 3.72467$$

Input data using the density of Al_2O_3 are given below:

```
ARBMPOIS1  3.72467  2  0  1  0  13027  2  8016  3  6  0.97952  END
B4C  6  2.048-2  END
```

EXAMPLE 2. Borated water from H_3BO_3 and water.

Create a mixture 2 that is borated water at 4350 parts per million by weight, resulting from the addition of boric acid, H_3BO_3 to water. The density of the borated water is 1.0078 g/cm^3 (see Ref. 9). The solution temperature is 15°C and the boron is natural boron.

An easy way to describe this mixture is to use a combination of an arbitrary material to describe the boric acid, and a basic composition to describe the water.

STEP 1. INPUT DATA TO DESCRIBE THE ARBITRARY MATERIAL

The generic input data for the boric acid arbitrary material are given below. The actual input data are derived in steps 2 through 5.

```
SC  ROTH  NEL  IVIS  ICP  IRS  (NCZA_i  ATPM_i)  MX  VF  TEMP
END
```

where

SC is the standard composition component name.

ROTH is the theoretical density of the compound (enter 0.025066 and see step 2 auxiliary calculations for the arbitrary material input data below).

NEL is the number of elements in the material (enter 3, for the H, B, and O).

IVIS is an unused variable. A value must be entered, and 1 was chosen because it is correct for older versions of SCALE.

ICP is the compound indicator (enter 1 because the boric acid is defined by a chemical formula, H3BO3).

IRS is an unused variable. A value must be entered, and 0 was chosen because it is correct for older versions of SCALE.

NCZA is the isotope ID number obtained from Table M8.2.1 (enter 5000 for boron, 1001 for hydrogen, 8016 for oxygen). Note: Boron is a multiple-isotope nuclide, so the ID number is obtained from Table M8.4.1.

ATPM is the number of atoms of this element per molecule of arbitrary material (enter 1 for boron, 3 for hydrogen, and 3 for oxygen).
Repeat the NCZA ATPM sequence until the NEL elements in the arbitrary material have been specified.

MX is the mixture number (enter 2).

VF is the density multiplier (enter 1 since the density of the H3BO3 in the borated water is used as the theoretical density).

TEMP is the temperature in Kelvin (enter 288.15).

The input data for this arbitrary material are given below.

```
ARBMH3BO3  0.025066  3  1  1  0  5000  1  1001  3  8016  3  2
1  288.15  END
```

STEP 2. AUXILIARY CALCULATIONS FOR THE ARBITRARY MATERIAL INPUT DATA

In calculating the molecular weights, use the atomic weights from SCALE, which are available in the output from COMPOZ. COMPOZ is used to create the Standard Composition Library for SCALE. The atomic weights used in SCALE may differ from some periodic tables. The SCALE atomic weights used in this problem are listed below:

H	1.0078
O	15.9954
^{10}B	10.0129
^{11}B	11.0096

The natural boron abundance obtained from Table M8.4.1 in Sect. M8.4 is given in weight percent:

^{10}B	18.30219
^{11}B	81.69782

The molecular weight of natural boron is given by:

DEN nat B/AWT nat B = DEN ^{10}B/AWT ^{10}B + DEN ^{11}B/AWT ^{11}B
DEN ^{10}B = WTF ^{10}B × DEN nat B
DEN ^{11}B = WTF ^{11}B × DEN nat B

where

DEN is density in g/cm^3,

AWT is the atomic weight in g/mol,

WTF is the weight fraction of the isotope.

Substituting,

DEN nat B/AWT nat B = DEN nat B × ((WTF ^{10}B/AWT ^{10}B) + (WTF ^{11}B/AWT ^{11}B))

Solving for AWT nat B yields:

AWT nat B = 1/((WTF ^{10}B/AWT ^{10}B) + (WTF ^{11}B/AWT ^{11}B))

The atomic weight of natural boron is thus

1.0/((0.1830219 g ^{10}B/g nat B/10.0129 g ^{10}B/mol ^{10}B) +
(0.8169782 g ^{11}B/g nat B/11.0096 g /mol ^{11}B)) = 10.81261 g nat B/mol nat B

The molecular weight of the boric acid, H_3BO_3 is given by:

(3 × 1.0078) + 10.81261 + (3 × 15.9954) = 61.8222

Calculate the grams of boric acid in a gram of solution:

Boric acid, H_3BO_3 is 61.8222 g/mol
Natural boron is 10.81261 g/mol

(4350 × 10^{-6} g B/g soln) × (1 mol/10.81261 g B) × (61.8222 g boric acid/mol) =
0.024872 g boric acid/g soln (2.4872 wt %)

Interpolating from ref. 9, the specific gravity of the boric acid solution at 2.4872 weight percent is 1.0087. This value is based on water at 15°C. The density of pure air free water at 15°C is 0.99913 g/cm^3. Therefore, the density of the boric acid solution is 1.0087 × 0.99913 g/cm^3 = 1.0078 g soln/cm^3.

Calculate ROTH, the theoretical density of the boric acid.

1.0078 g soln/cm^3 × 0.024872 g boric acid/g soln = 0.025066 g boric acid/cm^3

Calculate TEMP, the temperature in Kelvin:

273.15 + 15 = 288.15

STEP 3. DESCRIBE THE BASIC STANDARD COMPOSITION INPUT DATA

The generic input data for the basic standard composition are given below:

```
SC   MX   VF   TEMP   END
```

where

SC is the standard composition component name from Table M8.2.1 (enter H2O).

MX is the mixture number (enter 2).

VF is the density multiplier (enter the volume fraction, 0.984507, and see step 4 auxiliary calculations for the basic standard composition input data below).

TEMP is the temperature in Kelvin (enter 288.15).

The input data for this standard composition are given below.

```
H2O      2   0.984507   288.15   END
```

STEP 4. AUXILIARY CALCULATIONS FOR THE BASIC STANDARD COMPOSITION INPUT DATA

Calculate the volume fraction of the water in the solution. Each gram of solution contains 0.024872 g of boric acid, so there is 0.975128 g of water in each gram of solution. The volume fraction of water is then given by:

(1.0078 g soln/cm^3 × 0.975128 g water/g soln)/0.9982 g water/cm^3 = 0.984506

The 0.9982 is the theoretical density of water from Table M8.2.1.

Calculate TEMP, the temperature in Kelvin:

273.15 + 15 = 288.15

STEP 5. CREATE THE MIXTURE FOR BORATED WATER

```
ARBMH3BO3 0.025066 3 1 1 0 5000 1 1001 3 8016 3 2 1 288.15 END
 H2O          2 0.984506 288.15 END
```

M7.5.5.8 Combinations of Basic and Solution Standard Compositions to Define a Mixture

The solution specification is the easiest way of specifying the solutions listed in Table M8.3.1. A combination of solution and basic standard compositions can be used to describe a mixture that contains more than just a solution as demonstrated in the following example.

EXAMPLE 1. Uranyl nitrate solution containing gadolinium.
Create a 4.306% enriched uranyl nitrate solution containing 0.184 g gadolinium per liter. The uranium in the nitrate is 95.65% ^{238}U, 0.022% ^{236}U, 4.306% ^{235}U, and 0.022% ^{234}U. The uranium concentration is 195.8 g U/L and the specific gravity of the uranyl nitrate is 1.254. There is no excess acid in the solution. The presence of the gadolinium is assumed to produce no significant change in the solution density. The solution is defined to be mixture 3.

The input data for a solution are entered as follows:

```
SC   MX   FD   AML   SPG=SPGR   VF   TEMP   (IZA_i   WTP_i)   END
```

where

SC is the standard composition component name from Table M8.3.1 (enter SOLNUO2(NO3)2).

MX is the mixture number (enter 3).

FD is the fuel density in grams of U or Pu per liter of solution (enter 195.8).

AML is the acid molarity of the solution (enter 0 because there is no excess acid in the solution).

SPGR is the specific gravity of the solution (enter SPGR=1.254).

VF is the density multiplier, the volume fraction of the solution that is uranyl nitrate (enter 1.0).

TEMP is the temperature in Kelvin (enter 293).

IZA is the isotope ID number from Table M8.31 (enter 92238 for ^{238}U, 92236 for ^{236}U, 92235 for ^{235}U, and 92234 for ^{234}U).

WTP is the weight percent of the isotope in the material (enter 95.65 for ^{238}U, 0.022 for ^{236}U, 4.306 for ^{235}U, and 0.022 for ^{234}U).

Repeat the sequence IZA WTP until the sum of the WTPs sum to 100.

The input data for the uranyl nitrate solution are given as

```
SOLNUO2(NO3)2 3  195.8 0 SPG=1.254 1.0 293 92238 95.65 92236 0.022
92235 4.306 92234 0.022 END
```

The input data for a basic standard composition are entered as follows:

```
SC   MX   VF   TEMP   END
```

where

SC is the standard composition component name from Table M8.2.1 (enter GD for gadolinium).

MX is the mixture number (enter 3).

VF is the density multiplier or the ratio of actual to theoretical density. (From Table M8.2.1, the theoretical density of gadolinium is 1.0. The density of the gadolinium is 0.184 g/L or 0.000184 g/cm^3. Therefore, enter 0.000184/1.0 = 0.000184.)

TEMP is the temperature in Kelvin (293).

The input data for basic standard composition are entered as follows:

```
GD   3   0.000184   293   END
```

The input data for the mixture are given as:

```
SOLNUO2(NO3)2 3  195.8  0  SPG=1.254  1.0  293  92238  95.65
     92236  0.022  92235  4.306  92234  0.022

GD  3  0.000184  293  END
```

M7.5.5.9 Combinations of Arbitrary Material and Solution to Define a Mixture

The solution specification is the easiest way of specifying the solutions listed in Table M8.3.1. A solution specification and an arbitrary material specification can be used to describe a mixture that contains more than just a solution as demonstrated in the following example.

EXAMPLE 1. Uranyl nitrate solution with gadolinium nitrate.
Create a 4.306% enriched uranyl nitrate solution containing gadolinium in the form of $Gd(NO_3)_3$. The uranium in the nitrate is 95.65% ^{238}U, 0.022% ^{236}U, 4.306% ^{235}U, and 0.022% ^{234}U. The uranium concentration is 195.8 g U/L and the specific gravity of the uranyl nitrate is 1.254. There is no excess acid in the solution. The concentration of the gadolinium is 0.184 g/L. The solution is defined to be mixture 3.

The input data for a solution are entered as follows:

SC MX FD AML SPG=SPGR VF TEMP (IZA_i WTP_i) END

where

SC is the standard composition component name from Table M8.3.1 (SOLNUO2(NO3)2).

MX is the mixture number (3).

FD is the fuel density in grams of U or Pu per liter of solution (195.8).

AML is the acid molarity of the solution (0 because there is no excess acid in the solution).

SPGR is the specific gravity of the solution (SPG=1.254).

VF is the volume fraction of the mixture that is uranyl nitrate (0.99985 = 1.254/ (1.254 + 0.000184)).

TEMP is the temperature in Kelvin (293).

IZA is the isotope ID number from Table M8.2.1 (enter 92238 for ^{238}U, 92236 for ^{236}U, 92235 for ^{235}U, and 92234 for ^{234}U).

WTP is the weight percent of the isotope in the material (enter 95.65 for ^{238}U, 0.022 for ^{236}U, 4.306 for ^{235}U, and 0.022 for ^{234}U).
Repeat the sequence IZA WTP until the sum of the WTPs sum to 100.

The input data for the uranyl nitrate solution are given as

```
SOLNUO2(NO3)2 3 195.8 0 SPG=1.254 0.99985 293 92238 95.65
     92236 0.022 92235  4.306 92234 0.022 END
```

The generic input specification for an arbitrary material is given as:

```
SC ROTH NEL IVIS ICP IRS (NCZA_i ATPM_i) MX VF TEMP
(IZA_j WTP_j) END
```

where

SC is the standard composition component name. The first four characters **MUST** be ARBM (enter ARBMGD(NO3)3).

ROTH is the theoretical density of the compound. (In this case, the density of gadolinium nitrate in the solution will be used. The calculated density is 0.0004016. See the density calculation given below.)

NEL is the number of elements in the material. (Enter 3. This material contains gadolinium, nitrogen, and oxygen.)

IVIS is an unused variable. A value must be entered, and 0 was chosen because it is correct for older versions of SCALE.

ICP is the compound indicator [enter 1 because the gadolinium nitrate is defined by a chemical formula, $Gd(NO_3)_3$].

IRS is an unused variable. A value must be entered, and 1 was chosen because it is correct for older versions of SCALE.

NCZA is the isotope ID number from Table M8.2.1. (Enter 64000 for gadolinium, 7014 for nitrogen, and 8016 for oxygen.)

ATPM is the number of atoms of each element in the arbitrary material (enter 1 for gadolinium, 3 for nitrogen, and 9 for oxygen).
Repeat the sequence NCZA ATPM until the NEL elements in the arbitrary material have been specified.

MX is the mixture number (enter 3).

VF is the density multiplier [enter 1.0 for the volume fraction because the density of the $Gd(NO_3)_3$ in the solution was entered as ROTH; thus the contribution to the overall mixture was already accounted for in ROTH].

TEMP is the temperature in Kelvin (293).

IZA is not entered because there are no multiple-isotope nuclides in this arbitrary material.

WTP is not entered because there are no multiple-isotope nuclides in this arbitrary material.

The density of the gadolinium is given as 0.184 g/L. To describe the arbitrary material, the density of the $Gd(NO_3)_3$ is needed. The atomic weights used by COMPOZ to create the Standard Composition Library are:

Gd	157.25
N	14.0033
O	15.9945

Therefore, the density of the $Gd(NO_3)_3 = 0.000184$ g Gd/cm^3 × (157.25 + 3(14.0033 + 3(15.9945))/157.25) = 0.0004016 g/cm^3.

The input data for this arbitrary material are given below:

```
ARBMGD(NO3)3   .0004016   3   0   1   1   64000   1   7014   3   8016   9   3   1
293   END
```

The input data for the mixture of uranyl nitrate and gadolinium nitrate are given as:

```
SOLNUO2(NO3)2 3 195.8 0 SPG=1.254 0.99985 293 92238 95.65 92236 0.022
      92235 4.306 92234 0.022 END
ARBMGD(NO3)3   .0004016 3 0 1 1 64000 1 7014 3 8016 9 3 1 293 END
```

Note: Since the default temperature (293 K) is to be used, it can be omitted from the arbitrary material standard composition. The temperature must be entered if the standard composition contains a multiple-isotope nuclide whose isotopic abundance is to be specified.

M7.5.6 EXAMPLES OF UNIT CELL SPECIFICATIONS

The data that are entered as a unit cell specification are determined by the type of calculation as discussed in Sect. M7.5.4. Examples of the unit cell data follow.

M7.5.6.1 Infinite Homogeneous Medium Unit Cell Data

Unit cell data are not required for INFHOMMEDIUM. All the materials specified in the standard composition specification data are treated as infinite homogeneous media for the cross-section processing performed by BONAMI and/or NITAWL.

Cell-weighted cross sections are created by XSDRNPM when an analytical sequence that ends in X (CSAS1X, etc.) is executed. The unit cell used by XSDRNPM is assumed to consist entirely of the smallest defined mixture number. All other materials are assumed to have a number density of 1.0E-20. The most plausible reason for using XSDRNPM for an infinite homogeneous medium is to obtain the eigenvalue for an infinite mass of material. Since XSDRNPM calculates the eigenvalue for the mixture in the cell, that mixture should contain fissile material. If the smallest mixture number in the standard composition data does not contain fissile material, the mixture for the unit cell should be specified. If the unit cell does not contain fissile material, XSDRNPM will execute and calculate the eigenvalue using the 1.0E-20 number densities for the fuel.

Warning: If unit cell data are to be entered as in example 3 below, the word CELLMIX must be spelled correctly. If it is misspelled, the code will not give an error message and will attempt to use the smallest mixture number. The input data will get out of phase for CSAS and SAS sequences that expect to read data after the unit cell specification. For example, CSAS25 expects to read KENO data after the unit cell specification. If CELLMIX is misspelled, the code assumes that it is reading the KENO title card and the data reading gets out of phase.

EXAMPLE 1. A single mixture.
Consider a cylindrical configuration of 10% enriched UO_2 having a radius of 35 cm and a height of 20 cm.

Because this problem defines only one mixture, unit cell data do not need to be specified. XSDRNPM will calculate the eigenvalue of an infinite mass of 10% enriched UO_2.

EXAMPLE 2. Two mixtures.
Consider a cylindrical steel container filled with 10% enriched UO_2. The inside radius is 35 cm and inside height is 20 cm. The wall thickness of the steel is 0.32 cm. The UO_2 is defined as mixture 1, and the steel is defined as mixture 2.

Because this problem defines the fuel to be the smallest mixture number, unit cell data need not be specified. XSDRNPM will calculate the eigenvalue of an infinite mass of 10% enriched UO_2.

EXAMPLE 3. Two mixtures and specify the cell.
Consider a cylindrical steel container filled with 10% enriched UO_2. The inside radius is 35 cm, and inside height is 20 cm. The wall thickness of the steel is 0.32 cm. The steel is defined as mixture 1, and the UO_2 is defined as mixture 2.

If this problem is run using an analytical sequence that does not perform a cell-weighting calculation, unit cell data need not be specified.

If this problem is run using an analytical sequence that performs a cell-weighting calculation, unit cell data should be specified so XSDRNPM can calculate the eigenvalue, fluxes, and cell-weighted cross sections for the 10% enriched UO_2. The necessary cell data are CELLMIX 2.

M7.5.6.2 LATTICECELL Unit Cell Data

Unit cell data are always required for LATTICECELL calculations. Only one unit cell can be defined in a problem. This unit cell is always one-dimensional; infinitely long cylinders, spheres, slabs. The configuration of the unit cell is determined by the specified "type of lattice." Both "regular" and "annular" cells are allowed. The "regular" cells allow spherical, cylindrical, or symmetric slab fuel regions that are constrained to a central fuel region surrounded by an optional gap, an optional clad, and an external moderator material. The "annular" cells for spherical, cylindrical, or asymmetric slab configurations are constrained to a central (second) moderator material surrounded by a fuel region having an optional gap and optional clad on both sides of the fuel with an external (first) moderator material.

"Regular" cells are specified using SQUAREPITCH, TRIANGPITCH, SPHSQUAREP, SPHTRIANGP, or SYMMSLABCELL.

"Annular" cells are specified using ASQUAREPITCH, ASQP, ATRIANGPITCH, ATRP, ASPHSQUAREP, ASSP, ASPHTRIANGP, ASTP, or ASYMSLABCELL.

The unit cell data in a LATTICECELL problem are used (1) to provide the dimensions and shape of the lump and the moderator material for resonance cross-section processing, (2) to provide lattice

corrections for the cross-section processing, and (3) to provide information used in creating cell-weighted cross sections when XSDRNPM is executed for cross-section processing.

BONAMI and/or NITAWL perform resonance cross-section processing for the materials used in the unit cell, utilizing the shape and dimensions defined in the cell. A Dancoff correction is applied to account for lattice effects. Materials that are not used in the unit cell are treated as infinite homogeneous media. If cell-weighted cross sections are to be created by XSDRNPM, an analytical sequence ending with an X must be used. XSDRNPM calculates the eigenvalue of the cell assuming a white boundary condition. The resultant fluxes are used to weight the cross sections of the materials in the cell and to create a homogenized cell-weighted cross section having the characteristics of the heterogeneous cell configuration. This cell-weighted cross section is always labeled mixture 500. Whenever XSDRNPM is executed for cross-section processing, mixtures used in the cell description cannot be used in the heterogeneous geometry data for other codes. If they are needed in the other code, additional mixtures with identical specifications must be defined in the standard composition data.

The general input data for a LATTICECELL unit cell follow:

```
CTP   PITCH   FUELOD   MFUEL   MMOD   MMOD2   TKMOD2   CLADOD   MCLAD   CLADID
MGAP   END
```

where

CTP is the type of lattice. This defines both the shape of the fuel lump and the spacing configuration of the lattice. The LATTICECELL configurations are listed below.

(1) "Regular cells"

SQUAREPITCH	- cylindrical fuel in a square-pitched array
TRIANGPITCH	- cylindrical fuel in a triangular-pitched array
SPHSQUAREP	- spherical fuel in a square-pitched array
SPHTRIANGP	- spherical fuel in a square-triangular array
SYMMSLABCELL	- fuel slabs identically moderated on each side

(2) "Annular cells"

ASQUAREPITCH	- annular cylinders in a square-pitched array
ASQP	- annular cylinders in a square-pitched array
ATRIANGPITCH	- annular cylinders in a triangular-pitched array
ATRP	- annular cylinders in a triangular-pitched array
ASPHSQUAREP	- annular spherical fuel in a square-pitched array
ASSP	- annular spherical fuel in a square-pitched array
ASPHTRIANGP	- annular spherical fuel in a triangular-pitched array
ASTP	- annular spherical fuel in a triangular-pitched array
ASYMSLABCELL	- fuel slabs moderated differently on each side

PITCH is the center-to-center spacing of the fuel lumps (in centimeters).

FUELOD is the outside dimension (diameter or thickness) of the fuel in centimeters.

MFUEL is the mixture number of the fuel.

MMOD is the mixture number of the moderator or first moderator.

MMOD2 is the mixture number of the second moderator. ENTER ONLY FOR ANNULAR CELLS.

TKMOD2 is the dimension (diameter or thickness) of the second moderator in centimeters. ENTER ONLY FOR ANNULAR CELLS.

CLADOD is the outside dimension of the clad in centimeters. OMIT IF NO CLAD.

MCLAD is the mixture number of the clad. OMIT IF NO CLAD.

CLADID is the outside dimension of the gap or the inside dimension of the clad in centimeters. OMIT IF NO GAP.

MGAP is the mixture number. OMIT IF NO GAP.

Examples of "regular" LATTICECELL unit cells are given in Examples 1–5, and examples of "annular" LATTICECELL unit cells are given in Examples 6–10 below.

EXAMPLE 1. SQUAREPITCH (infinitely long cylindrical pins in a square-pitched array).
Consider a large array of UO_2 fuel pins having a fuel O.D. of 0.79 cm, a 0.015-cm gap, and a 0.06-cm-thick aluminum clad. The array is a square-pitched array with a center-to-center spacing of 1.60 cm and is completely flooded with water. In the standard composition data, UO_2 is defined to be mixture 1, the aluminum clad is defined to be mixture 2, and the water moderator is defined to be mixture 3.

The input data for this LATTICECELL description are entered as follows:

```
CTP  PITCH  FUELOD  MFUEL  MMOD  CLADOD  MCLAD
CLADID  MGAP  END
```

where

CTP is the type of lattice (SQUAREPITCH)

PITCH is the center-to-center spacing in cm (1.60)

FUELOD is the outside diameter of the fuel in cm (0.79)

MFUEL is the fuel mixture number (1)

MMOD is the moderator mixture number (3)

CLADOD is the outside diameter of the clad in cm (0.79 + 2*0.015 + 2*0.06 = 0.94)

MCLAD is the clad mixture number (2)

CLADID is the inside diameter of the clad or the outside diameter of the gap in cm (0.79 + 2*0.015 = 0.82)

MGAP is the gap mixture number (enter 0 for a void)

SQUAREPITCH 1.60 0.79 1 3 0.94 2 0.82 0 END

EXAMPLE 2. TRIANGPITCH (infinitely long cylinders in a triangular-pitched array). Consider an array of UO_2 pins with a diameter of 0.635 cm. The outside diameter of the clad is 0.78 cm. There is no gap between the fuel and clad. The array is a triangular-pitched array with a center-to-center spacing of 5.0 cm and is flooded with water. In the standard composition data, the UO_2 is defined to be mixture 1, the aluminum is defined to be mixture 2, and the water moderator is defined to be mixture 3.

The input data for this LATTICECELL description are entered as follows:

```
CTP   PITCH   FUELOD   MFUEL   MMOD   CLADOD   MCLAD   END
```

where

CTP is the type of lattice (TRIANGPITCH).

PITCH is the center to center spacing in cm (5.0).

FUELOD is the outside diameter of the fuel in cm (0.635).

MFUEL is the fuel mixture number (1).

MMOD is the moderator mixture number (3).

CLADOD is the outside diameter of the clad in cm (0.78).

MCLAD is the clad mixture number (2).

TRIANGPITCH 5.0 .635 1 3 .78 2 END

EXAMPLE 3. SPHSQUAREP (spheres in a square-pitched array).
Consider a large array of U_3O_8 spheres having a fuel O.D. of 18.6 cm, with an aluminum clad that is 0.18 cm thick. The array is a triangular-pitched array with a center-to-center spacing of 19.0 cm and is unmoderated. In the standard composition data, the aluminum is defined to be mixture 1 and the U_3O_8 is defined to be mixture 2. There is no moderator material, so 0 will be used to represent a void.

The input data for this LATTICECELL description are entered as follows:

```
CTP    PITCH   FUELOD   MFUEL   MMOD   CLADOD   MCLAD   END
```

where

CTP is the type of lattice (SPHSQUAREP).

PITCH is the center-to-center spacing in cm (19.0).

FUELOD is the outside diameter of the fuel in cm (18.6).

MFUEL is the fuel mixture number (2).

MMOD is the moderator mixture number (0).

CLADOD is the outside diameter of the clad in cm (18.6 + 2*0.18 = 18.96).

MCLAD is the clad mixture number (1).

```
SPHSQUAREP      19.0 18.6 2 0 18.96 1 END
```

EXAMPLE 4. SPHTRIANGP (spheres in a triangular-pitched array).
Consider a large array of U_3O_8 spheres having a fuel O.D. of 18.6 cm, with an aluminum clad that is 0.18 cm thick. The array is a triangular-pitched array with a center-to-center spacing of 19.0 cm and is flooded with water. In the standard composition data, the aluminum is defined to be mixture 1, the U_3O_8 is defined to be mixture 2, and the water moderator is defined to be mixture 3.

The input data for this LATTICECELL description are entered as follows:

```
CTP    PITCH   FUELOD   MFUEL   MMOD   CLADOD   MCLAD   END
```

where

CTP is the type of lattice (SPHTRIANGP).

PITCH is the center-to-center spacing in cm (19.0).

FUELOD is the outside diameter of the fuel in cm (18.6).

MFUEL is the fuel mixture number (2).

MMOD is the moderator mixture number (3).

CLADOD is the outside diameter of the clad in cm (18.6 + 2*0.18 = 18.96).

MCLAD is the clad mixture number (1).

SPHTRIANGP 19.0 18.6 2 3 18.96 1 END

EXAMPLE 5. SYMMSLABCELL (slabs repeated in a symmetric fashion).
Consider a system of alternating slabs of U_3O_8 and low-density water. Each U_3O_8 region is 1.27 cm thick, and each water region is 15.0 cm thick. In the standard composition data, the U_3O_8 is defined to be mixture 1, and the low-density water is defined to be mixture 2.

The input data for this LATTICECELL description are entered as follows:

```
CTP    PITCH   FUELOD   MFUEL   MMOD   END
```

where

CTP is the type of lattice (SYMMSLABCELL).

PITCH is the center-to-center spacing in cm (1.27 + 15.0 = 16.27).

FUELOD is the outside diameter of the fuel in cm (1.27).

MFUEL is the fuel mixture number (1).

MMOD is the moderator mixture number (2).

SYMMSLABCELL 16.27 1.27 1 2 END

EXAMPLE 5a. SYMMSLABCELL (slabs repeated in a symmetric fashion).
Consider a system of alternating slabs of U_3O_8 and low-density water. Each U_3O_8 region is 1.27 cm thick, and each water region is 15.0 cm thick. The U_3O_8 regions have a 0.01-cm gap and 0.24-cm-thick aluminum clad on each face. In the standard composition data, the U_3O_8 is defined to be mixture 1, the aluminum is defined to be mixture 2, and the low-density water is defined to be mixture 3.

The input data for this LATTICECELL description are entered as follows:

```
CTP  PITCH  FUELOD  MFUEL  MMOD  CLADOD  MCLAD  CLADID
MGAP  END
```

where

CTP is the type of lattice (SYMMSLABCELL).

PITCH is the center-to-center spacing in cm (15.0 + 1.27 + 2*0.01 + 2*0.24 + 15.0 = 16.77).

FUELOD is the thickness of the fuel in cm (1.27).

MFUEL is the fuel mixture number (1).

MMOD is the moderator mixture number (3).

CLADOD is the outside dimension of the clad in cm (1.27 + 2*0.01 + 2*0.24 = 1.77).

MCLAD is the clad mixture number (2).

CLADID is the inside dimension of the clad in cm (1.27 + 2*0.01 = 1.29).

MGAP is the gap mixture number (0 is used to represent a void).

```
SYMMSLABCELL  16.77  1.27  1  3  1.77  2 1.29  0  END
```

EXAMPLE 6. ASQUAREPITCH (infinitely long annular cylindrical rods in a square-pitched array). Consider an array of uranium metal pipes having an inside diameter of 5.0 cm and an outer diameter of 6.75 cm. A gap of 0.025 cm and a clad of 0.25 cm exist on both the inner and outer surfaces of the fuel. The fuel rods are arranged in a square-pitched array. The center-to-center spacing is 8.0 cm. The array is completely flooded with water. In the standard composition data, the uranium metal is defined to be mixture 1, the clad is mixture 2, the inner moderator is Plexiglas and is mixture 3, the gap is a void, and the external moderator is water, defined to be mixture 4.

The input data for this LATTICECELL description are entered as follows:

```
CTP   PITCH  FUELOD  MFUEL  MMOD  MMOD2  TKMOD2  CLADOD
MCLAD  CLADID  MGAP  END
```

where

CTP is the type of lattice (SQUAREPITCH).

PITCH is the center-to-center spacing in cm (8.0).

FUELOD is the outside diameter of the fuel in cm (6.75).

MFUEL is the fuel mixture number (1).

MMOD is the moderator mixture number (4, the external moderator).

MMOD2 is the second moderator mixture number (3, the moderator material in the innermost region).

TKMOD2 is the diameter of the moderator in the innermost region in cm (5.0 - 2*0.025 - 2*0.25 = 4.45)).

CLADOD is the outside diameter of the clad in cm (6.75 + 2*0.025 + 2*0.25 = 7.30).

MCLAD is the clad mixture number (2).

CLADID is the outside diameter of the gap (6.75 + 2*0.025 = 6.80).

MGAP is the gap mixture number (enter 0 for a void).

ASQUAREPITCH 8.0 6.75 1 4 3 4.45 7.3 2 6.8 0 END
or
ASQP 8.0 6.75 1 4 3 4.45 7.3 2 6.8 0 END

EXAMPLE 6a. ASQUAREPITCH (infinitely long annular cylindrical rods in a square-pitched array). Consider an array of uranium metal pipes having an inside diameter of 5.0 cm and an outer diameter of 6.75 cm arranged in a square-pitched array. The center-to-center spacing is 8.0 cm. The array is completely flooded with water. In the standard composition data, the uranium metal is defined to be mixture 1, and the water moderator is defined to be mixture 2.

The input data for this LATTICECELL description are entered as follows:

```
CTP    PITCH   FUELOD   MFUEL   MMOD   MMOD2   TKMOD2   END
```

where

CTP is the type of lattice (ASQUAREPITCH).

PITCH is the center-to-center spacing in cm (8.0).

FUELOD is the outside diameter of the fuel in cm (6.75).

MFUEL is the fuel mixture number (1).

MMOD is the moderator mixture number (2).

MMOD2 is the second moderator mixture number (2, the moderator material in the innermost region).

TKMOD2 is the diameter of the moderator in the innermost region in cm (5.0).

ASQUAREPITCH 8.0 6.75 1 2 2 5.0 END
or
ASQP 8.0 6.75 1 2 2 5.0 END

NOTE: This problem uses the same moderator material in the center and outside the uranium pipes. This will cause the code to print a warning message.

EXAMPLE 7. ATRIANGPITCH (infinitely long annular cylindrical rods in a triangular-pitched array). Consider an array of uranium metal pipes having an inside diameter of 8.0 cm and a wall thickness of 0.75 cm arranged in a square-pitched array. The center-to-center spacing is 9.75 cm. The array is completely flooded with water. A Plexiglas rod fills the center of the uranium pipe. In the standard compositions data, the uranium metal is defined to be mixture 1, the Plexiglas is defined to be mixture 2, and the external water moderator is mixture 3.

The input data for this LATTICECELL description are entered as follows:

```
CTP    PITCH   FUELOD   MFUEL   MMOD   MMOD2   TKMOD2   END
```

where

CTP is the type of lattice (ATRIANGPITCH).

PITCH is the center-to-center spacing in cm (9.75).

FUELOD is the outside diameter of the fuel in cm (8.0 + 2*0.75 = 9.5).

MFUEL is the fuel mixture number (1).

MMOD is the mixture number of the first (external) moderator (3).

MMOD2 is the mixture number of the second moderator (2, the moderator in the innermost region).

TKMOD2 is the diameter of the moderator in the innermost region in cm (8.0).

ATRIANGPITCH 9.75 9.5 1 3 2 8.0 END
or
ATRP 9.75 9.5 1 3 2 8.0 END

EXAMPLE 8. ASPHSQUAREP (spherical annuli in a square-pitched array).
Consider a large array of hollow U_3O_8 spheres having a fuel I.D. of 8.0 cm and O.D. of 18.6 cm. The centers of the spheres are empty. The external moderator is water. The spheres are stacked in a square-pitched array with a center-to-center spacing of 19.0 cm. In the standard composition data, the U_3O_8 is defined to be mixture 1, and the water is defined to be mixture 2. The centers of the spheres are defined to be void, mixture 0.

The input data for this LATTICECELL description are entered as follows:

```
CTP    PITCH   FUELOD   MFUEL   MMOD   MMOD2   TKMOD2   END
```

where

CTP is the type of lattice (SPHSQUAREP).

PITCH is the center-to-center spacing in cm (19.0).

FUELOD is the outside diameter of the fuel in cm (18.6).

MFUEL is the fuel mixture number (1).

MMOD is the moderator mixture number (2).

MMOD2 is the mixture number of the second moderator (0, the moderator in the innermost region).

TKMOD2 is the diameter of the moderator in the innermost region in cm (8.0).

```
ASPHSQUAREP    19.0 18.6 1 2 0 8.0 END
or
ASSP           19.0 18.6 1 2 0 8.0 END
```

EXAMPLE 9. ASPHTRIANGP (spheres in a triangular-pitched array).
Consider a large array of hollow U_3O_8 spheres having a fuel I.D. of 8.0 cm and a fuel O.D. of 18.6 cm. A 0.18-cm-thick aluminum clad exists inside and outside the fuel. The interior of each sphere is void. The array is a triangular-pitched array with a center-to-center spacing of 19.0 cm and is flooded with water. In the standard composition data, the aluminum is defined to be mixture 1, the U_3O_8 is defined to be mixture 2, and the water moderator is defined to be mixture 3. The void in the center of each sphere is entered as mixture 0.

The input data for this LATTICECELL description are entered as follows:

```
CTP    PITCH   FUELOD   MFUEL   MMOD   MMOD2   TKMOD2   CLADOD
MCLAD   END
```

where

CTP is the type of lattice (ASPHTRIANGP).

PITCH is the center-to-center spacing in cm (19.0).

FUELOD is the outside diameter of the fuel in cm (18.6).

MFUEL is the fuel mixture number (2).

MMOD is the moderator mixture number (3).

MMOD2 is the mixture number of the second moderator (0, the moderator in the innermost region).

TKMOD2 is the diameter of the moderator in the innermost region in cm (8.0 - 2*0.18 = 7.64).

CLADOD is the outside diameter of the clad in cm (18.6 + 2*0.18 = 18.96).

MCLAD is the clad mixture number (1).

```
ASPHTRIANGP     19.0  18.6  2  3  0  7.64  18.96  1  END
or
ASTP            19.0  18.6  2  3  0  7.64  18.96  1  END
```

EXAMPLE 10. ASYMSLABCELL (repeated slabs having different moderator conditions on the left and right boundaries).

Consider a system of slabs of U_3O_8 reflected by 8.0 cm of full-density water on the left face and 16.0 cm of low-density water on the right face. Each U_3O_8 region is 1.27 cm thick. In the standard composition data, the U_3O_8 is defined to be mixture 1, the full density water is defined to be mixture 2, and the low-density water is mixture 3.

The input data for this LATTICECELL description are entered as follows:

```
CTP    PITCH   FUELOD   MFUEL   MMOD   MMOD2   TKMOD2   END
```

where

CTP is the type of lattice (ASYMSLABCELL).

PITCH is the center-to-center spacing between fuel slabs, in cm (1.27 + 8.0/2 + 16.0/2 = 13.27).

FUELOD is the outside diameter of the fuel in cm (1.27).

MFUEL is the fuel mixture number (1).

MMOD is the moderator mixture number (2).

MMOD2 is the second moderator material (3).

TKMOD2 is the thickness of the second moderator in cm (8.0).

ASYMSLABCELL 13.27 1.27 1 2 3 8.0 END

EXAMPLE 10a. ASYMSLABCELL (repeated slabs having different moderator conditions on the left and right boundaries). Consider a system of slabs of U_3O_8 reflected by 8.0 cm of full-density water on the left face and 16.0 cm of low-density water on the right face. Each U_3O_8 region is 1.27 cm thick and has a 0.01-cm gap and 0.24-cm-thick aluminum clad on each face. In the standard composition data, the U_3O_8 is defined to be mixture 1, the full-density water is defined to be mixture 2, the low-density water is mixture 3, and the aluminum is mixture 4.

The input data for this LATTICECELL description are entered as follows:

```
CTP   PITCH  FUELOD  MFUEL  MMOD  MMOD2  TKMOD2  CLADOD
MCLAD  CLADID  MGAP  END
```

where

CTP is the type of lattice (ASYMSLABCELL).

PITCH is the distance from the center of the first moderator to the center of the second moderator in cm (1.27 + 2*0.01 + 2*0.24 + 8.0/2 + 16.0/2 = 13.77).

FUELOD is the fuel thickness in cm (1.27).

MFUEL is the fuel mixture number (1).

MMOD is the first moderator mixture number (2).

MMOD2 is the second moderator material (3).

TKMOD2 is the thickness of the second moderator in cm (8.0).

CLADOD is the outside dimension of the clad in cm (1.27 + 2*0.01 + 2*0.24 = 1.77).

MCLAD is the clad mixture number (4).

CLADID is the outside dimension of the gap in cm (1.27 + 2*0.01 = 1.29).

MGAP is the gap mixture number (0).

```
ASYMSLABCELL  13.77  1.27  1  2  3  8.0  1.77  4  1.29  0  END
```

M7.5.6.3 MULTIREGION Unit Cell Data

Unit cell data are always required for MULTIREGION calculations. Only one unit cell can be defined in a problem. The LATTICECELL description is rigorously constrained as to the placement of fuel, gap, clad, and moderator. MULTIREGION allows complete freedom in the placement of the materials but is constrained by shape (i.e., only concentric regions of the same shape are allowed). With the exception of the external cell boundary, MULTIREGION is capable of describing all of the configurations available in LATTICECELL. However, it does not account for lattice effects, so it is best used for problems where lattice effects are not important.

The materials specified in the unit cell are treated according to the specified shape, zone dimensions, and the moderator conditions for each zone. The resonance cross-section processing ignores lattice geometry effects.

The general input data for a MULTIREGION unit cell follow:

```
CS   BR   BL   ORGN   DY   DZ   END   (MXZ   RZ   XMOD)   END   ZONE
```

where

CS is the geometry shape. All regions in a MULTIREGION cell have the same shape and are one-dimensional. There are no restrictions on the placement of materials. The available geometric shapes are the following:

SLAB	all regions are slabs
CYLINDRICAL	all regions are infinitely long concentric cylinders
SPHERICAL	all regions are concentric spheres
BUCKLEDSLAB	all regions are slabs having the same finite height.
BUCKLEDCYL	all regions are concentric cylinders having the same finite height.

BR is the right (outside) boundary condition. This is required data for a BUCKLEDSLAB or BUCKLEDCYL and is optional for other geometries. The default value is VACUUM. The available choices are

VACUUM	Nothing returns at the boundary

	REFLECTED	Provides mirror image return at the boundary. DO NOT USE FOR CYLINDRICAL OR SPHERICAL
	PERIODIC	Provides periodic reflection at the boundary. DO NOT USE FOR CYLINDRICAL OR SPHERICAL
	WHITE	Provides isotropic return at the boundary.

BL is the left (inside) boundary condition. These data are required for a BUCKLEDSLAB or BUCKLEDCYL and are optional for other geometries. The default value is REFLECTED. The available choices are the following:

VACUUM	Nothing returns at the boundary
REFLECTED	Provides mirror image return at the boundary. RECOMMENDED FOR CYLINDRICAL OR SPHERICAL
PERIODIC	Provides periodic reflection at the boundary. DO NOT USE FOR CYLINDRICAL OR SPHERICAL
WHITE	Provides isotropic return at the boundary.

ORGN is the location of the left boundary of a slab relative to the axis that is perpendicular to the slab. The default is 0.0. DO NOT CHANGE FOR SPHERICAL OR CYLINDRICAL GEOMETRY.

DY is the buckling height in centimeters. ENTER ONLY FOR BUCKLEDSLAB OR BUCKLEDCYL.

DZ is the buckling depth in centimeters. ENTER ONLY FOR BUCKLEDSLAB.

END terminates the geometry parameters.

MXZ is the mixture number of the zone.

RZ is the outside dimension of the zone.

XMOD is an optional entry specifying the external moderator index. These data were required for older versions of SCALE but can be omitted for this version. If the user chooses to input this data, a valid option must be specified. The choices are

NOEXTERMOD	There are no moderating materials in an adjacent zone.
ONEEXTERMOD	There is moderating material in one adjacent zone.
TWOEXTERMOD	There are moderating materials in both adjacent zones.

Repeat the sequence (MXZ RZ XMOD) until all of the zones in the geometry have been described.

END ZONE terminates the MULTIREGION unit cell data.

Examples of MULTIREGION unit cells follow:

EXAMPLE 1. SLAB.
Consider a 5-cm-thick slab of fuel (mixture 1) with 0.5 cm of aluminum (mixture 3) and 15 cm of water (mixture 2) on each face. The unit cell data for this problem could be entered as follows:

CS BR BL ORGN END (MXZ RZ XMOD) END ZONE

where

CS is the geometry shape (SLAB).

BR is the right (outside) boundary condition (VACUUM).

BL is the left (inside) boundary condition (REFLECTED because it is easier to describe only half of the system and reflect at the mid-plane of the fuel.

ORGN is the location of the left boundary of a slab in cm (0).

END terminates the geometry parameters.

MXZ is the mixture number of the zone [1 for the first zone (fuel), 3 for the second zone (aluminum), and 2 for the third zone (water)].

RZ is the outside dimension of the zone. (2.5 for the half thickness of fuel in the first zone, 3.0 = 2.5 + 0.5 for the outer dimension of the aluminum in the second zone, and 18.0 = 2.5 + 0.5 + 15.0 for the outer dimension of the water in the third zone.)

XMOD is the optional external moderator index and has been omitted.

Repeat the sequence (MXZ RZ XMOD) until all of the zones in the geometry have been described.

END ZONE

The unit cell data for this problem can be entered as follow:

```
SLAB     VACUUM  REFLECTED  0  END
1  2.5      3  3.0     2  18.0     END  ZONE
```

EXAMPLE 2. CYLINDRICAL.

Consider a large array of fuel pins. Each pin is UO_2 (mixture 1) with a radius of 0.465 cm, a 0.009-cm gap (mixture 0), and a Zircaloy clad (mixture 9) 0.062 cm thick, centered in a water (mixture 8) region surrounded by a flooded support structure represented by homogenized water and Zircaloy (mixture 10). The outer radius of the water-Zircaloy region is 0.844 cm and it is 0.037 cm thick. This problem cannot be described as a LATTICECELL problem because the LATTICECELL configuration is limited to fuel-gap-clad-cell boundary and this problem is fuel-gap-clad-moderator-outer region. A white boundary condition on the outer boundary is a reasonable representation of a large array. However, lattice effects are not accounted for when MULTIREGION is used, so the user will have to enter the appropriate Dancoff factor in the optional parameter data.

The unit cell data for this problem could be entered as follows:

```
CS    BR   BL   ORGN   END   (MXZ   RZ   XMOD)   END   ZONE
```

where

CS is the geometry shape (CYLINDRICAL).

BR is the right (outside) boundary condition (WHITE).

BL is omitted because the default is REFLECTED and is appropriate for CYLINDRICAL.

ORGN is omitted because it applies only to slabs.

END terminates the geometry parameters.

MXZ is the mixture number of the zone [1 for the first zone (fuel), 0 for the second zone (gap), 9 for the third zone (clad), 8 for the fourth zone (water), and 10 for the outer water-Zircalloy region].

RZ is the outside dimension of the zone. (0.465 for the radius of the fuel in the first zone, 0.474 for the outer radius of the gap, 0.536 for the outer radius of the Zircaloy clad, 0.807 for the outer radius of the water moderator, and 0.844 for the outer radius of the outer region.)

XMOD is the optional external moderator index and has been omitted.

Repeat the sequence (MXZ RZ XMOD) until all of the zones in the geometry have been described.

END ZONE

The input data for this unit cell can be entered as follows:

```
CYLINDRICAL  WHITE  END  1  0.465  0  0.474  9  0.536
             8  0.807  10  0.844  END  ZONE
```

EXAMPLE 3. SPHERICAL.
Describe a bare sphere of uranium metal 8.72 cm in radius. The uranium metal is defined to be mixture 1. The unit cell data for this problem could be entered as follows:

```
CS  END  (MXZ  RZ  XMOD)  END  ZONE
```

where

CS is the geometry shape (SPHERICAL). Other geometry parameters need not be entered because the defaults are sufficient.

END terminates the geometry parameters.

MXZ is the mixture number of the zone (1 for the first zone (uranium)).

RZ is the outside dimension of the zone in cm (8.72 for the radius of the uranium in the first zone).

XMOD is the optional external moderator index and has been omitted.
Repeat the sequence (MXZ RZ XMOD) until all of the zones in the input have been described.

END ZONE

The input data for this unit cell can be entered as follows:

```
SPHERICAL  END  1  8.72  END  ZONE
```

EXAMPLE 4. BUCKLEDSLAB.
Consider a plate of fuel 4 cm thick, reflected by 3 cm of water on both faces. The plate is 32 cm tall and 16 cm deep. The fuel is mixture 1 and the water is mixture 2.

The unit cell data for this problem could be entered as follows:

```
CS  BR  BL  ORGN  DY  DZ  END  (MXZ  RZ  XMOD)  END  ZONE
```

where

CS is the geometry shape (BUCKLEDSLAB).

BR is the right (outside) boundary condition (VACUUM).

BL is the left boundary condition. (BL must be entered as REFLECTED even though REFLECTED is the default because the buckling height and depth must be entered.)

ORGN is the location of the left boundary on the x-axis (0.0 this value must be entered even though it is the default value because the buckling height and depth must be entered).

DY is the buckling height in cm (32.0).

DZ is the buckling depth in cm (16.0).

END terminates the geometry parameters.

MXZ is the mixture number of the zone (1 for the first zone (fuel), and 2 for the second zone (water)).

RZ is the outside dimension of the zone (2.0 cm for the half thickness of the fuel in the first zone, and 5.0 cm (4/2 + 3) for the outer dimension of the water in zone 2).

XMOD is the optional external moderator index and has been omitted.

Repeat the sequence (MXZ RZ XMOD) until all of the zones in the geometry have been described.

END ZONE

The unit cell data for this problem follow:

```
BUCKLEDSLAB  VACUUM  REFLECTED  0.0  32  16.0  END
1  2.0  2  5.0  END  ZONE
```

EXAMPLE 5. BUCKLEDCYL.

Consider a solution of uranyl nitrate contained in a cylindrical stainless-steel container reflected by 33 cm of water. The inside dimensions of the steel container are 7.62 cm in radius and 130.0 cm tall. The steel is 0.15 cm thick. The uranyl nitrate is defined to be mixture 1, the steel is defined to be mixture 2, and the water is defined to be mixture 3.

The unit cell data for this problem could be entered as follows:

```
CS   BR   BL   ORGN   DY   END   (MXZ   RZ   XMOD)   END   ZONE
```

where

CS is the geometry shape (BUCKLEDCYL).

BR is the right (outside) boundary condition (VACUUM).

BL is the left boundary condition. (The left boundary is at the center of the cylinder and must be entered as REFLECTED even though REFLECTED is the default because the buckling height must be entered.)

ORGN is the location of the left boundary on the x-axis (enter 0.0 even though it is the default value because data will be specified after it).

DY is the buckling height in cm (130.0).

END terminates the geometry parameters.

MXZ is the mixture number of the zone [enter 1 for the first zone (fuel), 2 for the second zone (stainless steel) and 3 for the third zone (water)].

RZ is the outside dimension of the zone in cm. (Enter 7.62 for the radius of the fuel in the first zone, 7.77 for the outer radius of the stainless container and 40.77 cm for the outer radius of the water reflector.)

XMOD is the optional external moderator index and has been omitted.

Repeat the sequence (MXZ RZ XMOD) until all of the zones in the geometry have been described.

END ZONE

The unit cell data for this problem follow:

```
BUCKLEDCYL   VACUUM  REFLECTED  0.0  130.0  END
1  7.62  2  7.77  3  40.77   END  ZONE
```

M7.5.7 OPTIONAL PARAMETER DATA OR MORE DATA

The optional parameter data provide a means of providing additional information or alternative data to the cross-section processing codes. The data that are provided to XSDRNPM are used only for cross-section processing. Optional parameter data will be read if the words "MORE DATA" are entered. As many parameters as are needed can be entered. Each parameter entry must be separated from the others by one or more blanks. The optional parameter data are terminated by entering the word "END." The parameter data that can be entered are listed below.

ISN= This keyword allows XSDRNPM to use an order of angular quadrature other than 8 when it is executed to perform cell-weighted cross-section processing. The value entered with this keyword is ISN, the 8th entry of the 1$ array in XSDRNPM. Section M7.2.5.7 describes the automatic quadrature generator.

SZF= This keyword allows the user to alter the number of XSDRNPM mesh intervals provided by the Material Information Processor. The default value of SZF is 1.0. The Material Information Processor automatically provides the mesh intervals used in XSDRNPM. See Sect. M7.2.5.6 for details about the automatic mesh generator. It is not uncommon for an excessive number of mesh intervals to be generated. The keyword SZF= allows a means of reducing or increasing the number of mesh intervals. A number between zero and 1.0 will provide more mesh intervals, and a number greater than 1.0 will reduce the number of mesh intervals. If SZF $\leq$ 0, the user specifies the number of intervals in each zone immediately following the MORE DATA block. If SZF > 0, the interval spacing is generated as described in M7.2.5.6; while if SZF <0, the intervals are equally spaced in each zone.

IIM= This keyword allows the user to set the maximum number of inner iterations for XSDRNPM. The value entered with this keyword is IIM, the 11th entry in the XSDRNPM 1$ array. The default value of IIM is 20.

ICM= This keyword is used to set the maximum number of outer iterations for XSDRNPM. The value entered with this keyword is ICM, the 12th entry in the XSDRNPM 1$ array. The default value of ICM is 25.

EPS= This keyword is used to set the overall convergence criteria for XSDRNPM. The default value is 0.0001. EPS is the first entry in the XSDRNPM 5* array. The convergence criteria are discussed in Sect. M7.2.5.8.

PTC= This keyword is used to set the point convergence criteria (the scalar flux convergence criteria) for XSDRNPM. The default value is 0.0001. PTC is the second entry in the XSDRNPM 5* array.

BKL= This keyword is used to set the buckling factor, BF, for XSDRNPM. The default value is 1.420892 and is two times the multiplier on the "extrapolation" distance used to determine where a linearly extrapolated line from the asymptotic flux shape will go to zero. For slabs, the extrapolation distance is approximately 0.71 λ_{tr} or approximately 1.42. The buckling factor, BF, is the 6th entry in the XSDRNPM 5* array.

IUS= This keyword is used to set the upscatter scaling factor for XSDRNPM. The default value is 0. IUS=0 does not utilize upscatter scaling. IUS=1 uses upscatter scaling to accelerate the solution and/or speed convergence. IUS= is used to set the 11th entry, IFCT, of the XSDRNPM 3$ array.

RES= This keyword is used to supply resonance data to BONAMI and NITAWL for cross-section processing. This option must be used if the problem needs more than one unit cell description or contains more than one fissile mixture. See Sect. M7.5.10 for an example illustrating the use of this feature.
The data are entered in the form: RES= **mm fgeom dimn [rinner]**
where

mm is the mixture number, **fgeom** is the lump shape (SLAB, CYLINDER, SPHERE), **dimn** is the dimension, in cm, of the lump (thickness of the slab or radius of the sphere or cylinder), and rinner is the optionally entered inner radius of an annular cylinder or sphere.

DAN(mm)= This keyword is used to supply Dancoff data to BONAMI and NITAWL for cross-section processing.
The data are entered in the form: DAN(**mm**)=**dancoff**
where
mm is the mixture number and **dancoff** is the Dancoff factor to be applied to mixture mm. The easiest way to obtain the Dancoff factor is to run a CSASN problem and specify **PARM=CHECK**. The Dancoff is printed as part of the RESONANCE DATA. See Sect. M7.5.10 for an example demonstrating the use of this feature.

BAL= This keyword controls the balance table edits in XSDRNPM. The default value is FINE. The available options are listed below.

BAL=FINE Prints the fine-group balance tables.
This corresponds to IPBT=0 in the XSDRN 2$ array.

BAL=NONE Suppresses all balance table print.
This corresponds to IPBT= -1 in the XSDRN 2$ array.

BAL=ALL Prints the fine- and broad-group balance tables.
This corresponds to IPBT=1 in the XSDRN 2$ array.

DY= This keyword allows the user to specify the first transverse dimension in centimeters used in a buckling correction to calculate leakage normal to the principal direction (i.e., the height of a slab or a cylinder). This correction is already included in the unit cell data for a MULTIREGION problem. Therefore, DY should only be specified for a LATTICECELL problem. DY= corresponds to DY, the 7th entry in the XSDRN 5* array.

DZ= This keyword allows the user to specify the second transverse dimension in centimeters used in a buckling correction (i.e., the width or depth of a slab). This correction is already included in the unit cell data for a MULTIREGION problem. Therefore, DY should only be specified for a LATTICECELL problem utilizing slab geometry. DZ= corresponds to DZ, the 8th entry in the XSDRN 5* array.

COF= This keyword is used to set the diffusion coefficient option for transverse leakage corrections in XSDRNPM. This variable corresponds to IPN, the 7th variable in the XSDRNPM 3$ array. The default value is 0. The available options are listed below.

COF=0 Set a transport cross section for each zone.
COF=1 Use a spatially averaged diffusion coefficient for all zones.
COF=2 Use a diffusion coefficient for all zones that is one-third the diffusion coefficient determined from the spatially averaged transport cross section for all zones.
COF=3 Use a flux and volume weighting across all zones.

FRD= This keyword is used to set the unit number from which the binary flux guess for XSDRNPM will be read. It corresponds to setting IFN, the 4th entry in the XSDRNPM 3$ array to a value greater than 3. In SCALE, it is prudent to choose a unit number in the 30's, 40's, or 50's so other necessary data sets are not impacted. The user is responsible for supplying job control language data that are necessary for reading the flux data set.

FWR= This keyword is used to set the unit number on which the fluxes generated by XSDRNPM will be written in binary format. It corresponds to setting ID1, the 2nd entry in the XSDRNPM 2$ array to a value greater than 3. In SCALE, it is prudent to choose a unit number in the 30's, 40's, or 50's so other necessary data sets are not impacted. The user is responsible for supplying job control language data that are necessary for creating and saving the flux data set.

ADJ= Adjoint mode flag for XSDRNPM. Set to 1 to cause XSDRNPM to solve the adjoint problem.

NBU= Unit on which balance tables will be written from XSDRNPM. If the balance tables file is to be saved, enter the unit number where they are to be written. The user is responsible for supplying job control data necessary to create and save the balance table dataset.

WGT= Cross-section weighting flag for XSDRNPM. The default is to do cross-section weighing. If a user needs to not do cross-section weighting, then a value of 0 should be entered.

ZMD(iz)= Zone width modifiers for an XSDRNPM search problem. This allows entering a zone width modifier for zone iz in the XSDRNPM search problem. The zone width data are entered in the form:
ZMD(iz)=modifier
where iz is the zone number and modifier is the width modifier.

INT(iz)= Number of mesh intervals for zone iz in XSDRNPM. The default is to calculate the number. The data are entered as:
INT(iz)=number
where iz is the zone number and number is the number of mesh intervals.

KEF= The desired value of k_{eff} for an XSDRNPM zone width search. The default is 1.0.

KFM= The first eigenvalue modifier used in an XSDRNPM search. This value is used to make the first change in the XSDRNPM search. The default value is −0.1.

DAB= This keyword is used to set the number of direct-access data blocks for the Material Information Processor direct-access device on unit 8. The default number of direct-access data blocks is 200. This feature can be used if the problem fails with the message LMP005 DA ERROR - RELATIVE BLOCK NOT IN DATA SET. RELATIVE BLOCK NUMBER IS nnn. Set DAB= to a value larger than nnn. For example, if nnn is 201, 300 or 400 would be an appropriate value to try.

AXS= This keyword is used to set the unit number on which the macroscopic ANISN library is written. If the unit number is input as 7, the ANISN library will be written in a free-form card-image format. For any other unit number, the library will be written in binary format. The user is responsible for supplying job control language data that are necessary for creating and saving the ANISN cross-section library. The only control sequences that can create an ANISN cross-section library are CSASI, CSASIX, and SAS3.

MSH= This keyword is used to set the maximum number of mesh points per resonance. This is the maximum number of mesh points allowed for the Simpson's rule integration in NITAWL, and is the MSCM variable in NITAWL's 1$ array. The default value sent from the Material Information Processor to NITAWL is 2001. See Sects. F2.3.3, F2.3.4, and F2.7 for additional information.

MLV= This keyword is used to set the highest resonance ℓ-value for which a self-shielding calculation will be performed in NITAWL. It is passed to NITAWL as variable IQM in the 1$ array. The default value on the Material Information Processor is 2. See Sects. F2.3.7 and F27 for additional information.

ID1= Scalar flux print control. The default value is -1, which suppress printing the scalar fluxes in XSDRNPM. See Section F3.5, 2$array, variable ID1 for allowed values and corresponding actions.

COLL This keyword is used to activate the collapse of the thermal groups into one group for the shielding sequences. To activate this feature, simply enter COLL in MORE DATA. For example, MORE DATA COLL END would activate this feature. MORE DATA EPS=.00005 COLL END DATA would tighten the convergence criteria for XSDRNPM and collapse all of the thermal groups into one group.

M7.5.7.1 Sample Optional Parameter Data

Consider a problem in which it is desirable to increase the number of inner iterations in XSDRN to 30 and to tighten the overall convergence criteria to a value of 0.000075. This could be accomplished by entering the data as follows:

```
MORE DATA    IIM=30   EPS=0.000075   END
```

The order of the data entry is not important. The data must start with MORE or MORE DATA and end with an END. It need not be entered as a single "card," but can be strung out across several "cards." However, a keyword cannot be separated across "card" boundaries. The terminator for the optional parameter data, END, must not begin in column 1 unless you assign a name to it. An alternative method of entering the above data is given below.

```
MORE   DATA
IIM=30   EPS=0.000075
END   MORE
```

or

```
MORE   DATA   IIM=30   EPS=0.000075   END   MORE   DATA
```

M7.5.8 EXAMPLES OF COMPLETE MATERIAL INFORMATION PROCESSOR INPUT DATA

The Material Information Processor data consist of:

(1) TITLE
(2) CROSS-SECTION LIBRARY NAME
(3) TYPE OF CALCULATION
(4) STANDARD COMPOSITIONS SPECIFICATION DATA
(5) UNIT CELL SPECIFICATION
(6) OPTIONAL PARAMETER DATA (MORE DATA)

Items 1 through 6 have been discussed in Sects. M7.5.1 through M7.5.7.

M7.5.8.1 Infinite Homogeneous Medium Input Data

Examples of Material Information Processor input data for infinite homogeneous media problems are given below.

EXAMPLE 1. Default Cell Definition.
Consider a cylindrical billet of 20 wt % enriched UO_2, having a density of 10.85 g/cc that is 26 cm in diameter and 26 cm tall.

The average mean-free path in the uranium dioxide is on the order of 2.5 cm. Because only a small fraction of the billet is within a mean-free path of the surface, the material can be treated as an infinite homogeneous medium. The Material Information Processor data utilizing the 27-group ENDF/B-IV SCALE cross-section library follows:

```
20%  ENRICHED  UO2  BILLET
27GR  INF
UO2  1  0.99  293  92235  20  92238  80  END
END  COMP
```

The volume fraction used for the UO_2, 0.99, is calculated by dividing the actual density yy the theoretical density obtained from Table M8.2.1 (10.85/10.96). Since the enrichment was specified as 20%, it is reasonable to assume that the remainder is ^{238}U.

An alternative input data description follows:

```
20% ENRICHED UO2 BILLET
27G INF
UO2 1 DEN=10.85  1  293  92235  20  92238  80  END
END COMP
```

EXAMPLE 2. Specify the Cell Definition.

Consider a 5-l Plexiglas bottle with an inner radius of 9.525 cm and inner height of 17.78 cm that is filled with highly enriched uranyl nitrate solution at 415 g/L, a specific gravity of 1.555, and 0.39 mg of excess nitrate per gram of solution. The uranium isotopic content of the nitrate solution is 92.6 wt % ^{235}U, 5.9 wt % ^{238}U, 1.0 wt % ^{234}U, and 0.5 wt % ^{236}U.

The size of the nitrate solution is on the order of 16 to 20 cm in diameter and height. The average mean-free path in the nitrate solution is on the order of 0.5 cm. Therefore, infinite homogeneous medium is an appropriate choice for this problem.

If the Plexiglas is defined to be mixture 1 and the uranyl nitrate solution is defined to be mixture 2, unit cell data must be entered. This is done by entering the word "CELLMIX" followed by the mixture that is to be used to define the cell. The Material Information Processor data for this problem utilizing the 16-group Hansen-Roach cross-section library is given below.

```
SET UP 5 LITER URANYL NITRATE SOLUTION IN A PLEXIGLAS CONTAINER
HANSEN-ROACH     INFHOMMEDIUM
PLEXIGLAS    1  END
SOLNUO2(NO3)2    2  415  9.783-3  SPG=1.555  1.0  293  92235  92.6
       92238  5.9   92234  1.0   92236  0.5  END
END  COMP
CELLMIX  2
```

M7.5.8.2 LATTICECELL Input Data

Examples of Material Information Processor input data for LATTICECELL problems are given below.

EXAMPLE 1. SQUAREPITCH.

Consider an infinite planar array (infinite in x and y and 1 layer in z) of 20 wt % enriched U metal rods with a 1-cm pitch. Each fuel rod is bare uranium metal, 0.75 cm OD x 30.0 cm long. The rods are submerged in water.

Because the diameter of the fuel rod, 0.75 cm, is only slightly larger than the average mean-free path in the uranium metal, approximately 0.5, and because the configuration is a regular array, LATTICECELL is the appropriate choice for proper cross-section processing. The Material Information Processor data using the 27-group ENDF/B-IV cross-section library follows:

```
INFINITE  PLANAR  ARRAY  OF  20%  U  METAL  RODS
27GROUP  LATTICECELL
URANIUM  1  1  293  92235  20  92238  80  END
H2O      2  END
END  COMP
SQUAREPITCH   1.0  0.75  1  2  END
```

EXAMPLE 2. SQUAREPITCH.

Consider an infinite planar array (infinite in x and y and 1 layer in z) of PWR-like fuel pins of 2.35% enriched UO_2 clad with zirconium. The density of the UO_2 is 9.21 g/cc. The fuel in each pin is 0.823 cm in diameter, the clad is 0.9627 cm in diameter, and the length of each pin is 366 cm. The fuel pins are separated by 0.3124 cm of water in the horizontal plane.

Because the diameter of the fuel rod, 0.823 cm, is only slightly larger than the average mean-free path in the uranium metal, approximately 0.5, and because the configuration is a regular array, LATTICECELL is the appropriate choice for proper cross-section processing. The Material Information Processor data using the 16-group Hansen-Roach cross-section library follows:

```
PWR-LIKE  FUEL  BUNDLE
HANSEN-ROACH  LATTICECELL
UO2   1  .84  293.  92235  2.35  92238  97.65  END
ZR   2  1  END
H2O   3  1  END
END  COMP
SQUAREPITCH   1.2751  .823  1  3  .9627  2  END
```

EXAMPLE 3. SPHTRIANGP.

Consider an infinite array of spherical pellets of 2.67% enriched UO_2 with a density of 10.3 g/cc and a diameter of 1.0724 cm arranged in a "triangular" pitch, flooded with borated water at 4350 WPPM. The boron is natural boron, the borated water is created by adding boric acid, H_3BO_3, and has a density of 1.0078 g/cc. The temperature is 15°C, and the pitch is 1.1440 cm. The standard composition data for the borated water are given in Example 2 of Sect. M7.5.5.7.

Because the diameter of the fuel pellet, 1.0724 cm, is smaller than the average mean-free path in the UO_2, approximately 1.5 cm, and because the configuration is a regular array, LATTICECELL is the appropriate choice for proper cross-section processing.

The density fraction for the UO_2 is the ratio of actual to theoretical density (10.3/10.96 = 0.9398). Assume that the U is all ^{235}U and ^{238}U.

To describe the boric acid, first calculate the grams of boric acid in a gram of solution:
Boric acid, H_3BO_3, is 61.8222 g/mol
Natural boron is 10.81261 g/mol
$(4350 \times 10^{-6}$ g B/g soln) × (1 mol/10.81261 g B) × (61.8222 g boric acid/mol) = 0.0248715 g boric acid/g soln.

Then calculate the theoretical density of the boric acid.
1.0078 g soln/cc × 0.024871 g boric acid/g soln = 0.025066 g boric acid/cc

Then calculate the volume fraction of the water in the solution. Each gram of solution contains 0.024871 g of boric acid, so there is 0.975129 g of water in each gram of solution.

The volume fraction of water is then given by:
(1.0078 g soln/cc × 0.975129 g water/g soln)/0.9982 g water/cc = 0.984507
The 0.9982 is the theoretical density of water from Table M8.2.1.

The temperature in degrees Kelvin is 273 + 15 = 288.

The Material Information Processor data using the 27-group ENDF/B-IV cross-section library follows:

```
SPHERICAL  PELLETS  IN  BORATED  WATER
27GR  LATT
UO2   1  .9398  288  92235  2.67  92238  97.33  END
ARBMH3BO3  0.025066  3  1  1  0  5000  1  1001  3  8016  3
      2  1  288  END
H2O   2  0.984507  288  END
END  COMP
SPHTRIANGP   1.1440  1.0724  1  2  END
```

M7.5.8.3 MULTIREGION Input Data

Examples of Material Information Processor input data for MULTIREGION problems are given below.

EXAMPLE 1. SPHERICAL.

Consider a small highly enriched uranium sphere supported by a Plexiglas collar in a tank of water. The uranium metal sphere has a diameter of 13.1075 cm, is 97.67% enriched, and has a density of 18.794 g/cc. The cylindrical Plexiglas collar has a 4.1275-cm-radius central hole, extends to a radius of 12.7 cm and is 2.54 cm thick. The water filled tank is 60 cm in diameter.

The density fraction of the uranium metal is the ratio of actual to theoretical density, where the theoretical density is obtained from Table M8.2.1. Thus the density multiplier is 18.794/19.05 = 0.9866. The abundance of uranium is not stated beyond 97.67% enriched, so it is reasonable to assume the remainder is ^{238}U. The Plexiglas collar is not significantly different from water and does not surround the fuel, so it can be ignored. If it is ignored, the problem becomes a one-dimensional geometry that can be defined using the MULTIREGION type of calculation, and the eigenvalue of the system can be obtained without additional data by executing CSAS1X. However, the Plexiglas has been included in this data so it can be passed to a code such as KENO V.a which can describe the geometry rigorously. Using the 27-group ENDF/B-IV cross-section library, the Material Information Processor data follow:

```
SMALL  WATER  REFLECTED  SPHERE  ON  PLEXIGLAS  COLLAR
27GR  MULT
URANIUM     1  .9866  293.  92235  97.67  92238  2.33  END
PLEXIGLAS   2  END
H2O         3  END
END  COMP
SPHERICAL END 1 6.55375 3 30.0 END ZONE
```

EXAMPLE 2. BUCKLEDSLAB.

This example features a dense 93.2% enriched uranyl-fluoride solution inside a Plexiglas container immersed in water. The fissile solution contains 570.8 g of heavy metal per liter and has no excess acid. The critical thickness of the fuel is 5.384 cm. The finite height of the fuel slab is 147.32 cm, and the depth is 71.58 cm. The Plexiglas container is 1.905 cm thick and is reflected by 20.32 cm of water.

The half thickness of the fuel (2.692) will be used with a reflected left boundary and a vacuum right boundary. The Material Information Processor data using the 27-group ENDF/B-IV cross-section library are given below:

```
CRITICAL  SLAB  EXPERIMENT  USING  URANYL-FLUORIDE  SOLUTION
27GR  MULTIREGION
SOLNUO2F2  1  570.8  0  1  293  92235  93.2  92238  6.8  END
PLEXIGLAS  2  END
H2O        3  END
END  COMP
BUCKLEDSLAB  VACUUM  REFLECTED  0  71.58  147.32  END
1  2.692  2  4.597  3  24.917  END  ZONE
```

M7.5.9 THREE METHODS OF SPECIFYING A SOLUTION

The standard composition specification data offer flexibility in the choice of input data. This section illustrates three methods of specifying the same solution. Section M7.5.9.1 lists the number densities calculated by the Material Information Processor for each method.

Create a mixture 3 that is aqueous uranyl nitrate solution:

$UO_2(NO_3)_2$, sp. gr. = 1.555
0.2669 g U/g-soln., 0.415 g U/cc; excess nitrate = 0.39 mg/g-soln
Uranium isotopic content: 92.6 wt % U-235 5.9 wt % U-238
1.0 wt % U-234 and 0.5 wt % U-236

In calculating the molecular weights, use the atomic weights from SCALE, which are available in the output from COMPOZ. COMPOZ was run to create the Standard Composition Library for SCALE on your computer. The atomic weights used in SCALE may differ from some periodic tables. The SCALE atomic weights used in this problem are listed as follows:

H	1.0078
O	15.9954
N	14.0033
U-234	234.0406
U-235	235.0442
U-236	236.0458

U-238 238.0510

Three methods of describing the uranyl nitrate solution will be demonstrated. Method 1 is more rigorous, method 2 is easier and is as accurate, and method 3 is approximate.

METHOD 1:

This method involves breaking the solution into its component parts [(HNO_3, $UO_2(NO_3)_2$, and H_2O)] and entering the basic standard composition specifications for each.

1. Calculate the density of the HNO_3 0.39×10^{-3} g NO_3/g soln × ((62.997 g HNO_3/mol HNO_3)/(61.990 g NO_3/mol NO_3)) × 1.555 g soln/cc soln = 6.16×10^{-4} g HNO_3/cc soln.

2. Calculate the density fraction of HNO3 (actual density/theoretical density). In the Standard Composition Library the theoretical density of HNO_3 is $1.0 \times 6.16 \times 10^{-4}/1.0 = 6.16 \times 10^{-4}$.

3. Calculate the molecular weight of the uranium

   The number of atoms in a mol of uranium is the sum of the number of atoms of each isotope in the mol of uranium.

   Let AU = the average molecular weight of uranium, g U/mol U
   GU = the density of uranium in g/cc

   Then the number of atoms in a mol of uranium =
   (6.023 × 10+23 * 10-24 * GU)/AU
   or 0.6023 * GU/AU

   The weight fraction of each isotope is the weight % * 100
   Therefore, F235 = 0.926, the weight fraction of U-235 in the U
   F238 = 0.059, the weight fraction of U-238 in the U
   F236 = 0.005, the weight fraction of U-236 in the U
   F234 = 0.010, the weight fraction of U-234 in the U
   A235 = 235.0442, the molecular weight of U-235
   A238 = 238.0510, the molecular weight of U-238
   A236 = 236.0458, the molecular weight of U-236
   A234 = 234.0406, the molecular weight of U-234

   Then the number of atoms of isotopes in a mol of uranium =
   6.023 × 10+23 * 10-24 * ((GU*F235/A235) + (GU*F238/A238) +
   GU*F236/A236) + (GU*F234/A234))
   or

   0.6023*GU * (0.926/235.0442 + 0.059/238.0510 +
   0.005/236.0458 + 0.010/234.0406)

Because the number of atoms of uranium equals the sum of the atoms of isotopes,

$$0.6023 * GU/AU = 0.6023 * GU *(0.926/235.0442 + 0.059/238.0510 + 0.005/236.0458 + 0.010/234.0406)$$

$$1/AU = 0.926/235.0442 + 0.059/238.0510 + 0.005/236.0458 + 0.010/234.0406$$

$$AU = 235.2144$$

4. Calculate the molecular weight of the $UO_2(NO_3)_2$.
   $235.2144 + (8 \times 15.9954) + (2 \times 14.0033) = 391.184$ g $UO_2(NO_3)_2$/mol

5. Calculate the density of $UO_2(NO_3)_2$
   0.415 g U/cc × ((391.184 g $UO_2(NO_3)_2$/mol)/(235.2144 g U/mol)) =
   0.69018 g $UO_2(NO_3)_2$/cc soln.

6. Calculate the density fraction (actual density/theoretical density) of $UO_2(NO_3)_2$.
   (In the Standard Composition Library the theoretical density of $UO_2(NO_3)_2$ is given as 2.2030 g/cc.)
   The density fraction is 0.69018/2.2030 = 0.31329

7. Calculate the amount of water in the solution
   1.555 g soln/cc soln - 6.16×10^{-4} g HNO_3/cc soln - 0.69018 g $UO_2(NO_3)_2$LL/cc soln =
   0.8642 g H_2O/cc soln.

8. Calculate the density fraction (actual density/theoretical density) of water.
   (In the Standard Composition Library the theoretical density of water is given as 0.9982 g/cc.)
   The density fraction is 0.8642/0.9982 = 0.86575

The solution specification data follow:

```
HNO3     3    6.16-4    293   END
UO2(NO3)2    3    .31329   293   92235   92.6   92238   5.9   92234   1.0
      92236   0.5   END
H2O      3    .86575   293   END
```

METHOD 2:

This method utilizes the solution option available in the standard composition specification data. Because the specific gravity is specified in the input data, this method should yield correct number densities that should agree with method 1 except for calculational round-off. The option allowing the specific gravity to be input in the solution data was not available prior to SCALE 4.0.

1. Calculate the fuel density
   0.415 g U/cc is 415 g U/L.

2. The molecular weight of nitrate NO_3 is 61.9895.

3. Calculate the molarity of the solution.
   0.39 mg nitrate/g soln × 1000 cc soln/L soln × 1 g/1000 mg × 1.555 g soln/cc soln = 0.60645 g excess nitrate/L soln
   A 1-molar solution is 1 mol of acid/L of solution:
   (For nitric acid 1 molar is 1 normal because there is only one atom of hydrogen per molecule of acid in HNO_3.)
   (0.60645 g nitrate/L soln)/(61.9895 g NO_3/mol NO_3) = 9.783×10^{-3} mol nitrate/L is identical to mol of acid/L is identical to molarity.

4. The density fraction of the solution is 1.0. Do not try to use the density (specific gravity) of the solution divided by the theoretical density of $UO_2(NO_3)_2$ from the Standard Composition Library for your density multiplier. The $UO_2(NO_3)_2$ listed there is the solid, not the solution.

   The solution specification data follow:

```
SOLNUO2(NO3)2   1  415  9.783-3  SPG=1.555  1.0  293  92235  92.6
     92238  5.9   92234   1.0  92236  0.5  END
```

METHOD 3:

This method utilizes the solution option available in the standard composition specification data without specifying the specific gravity. Because the specific gravity is not specified in the input data, the specific gravity is approximated by the Material Information Processor. The option allowing the specific gravity to be input in the solution data was not available prior to SCALE 4.0.

1. Calculate the fuel density
   0.415 g U/cc is 415 g U/L.

2. The molecular weight of nitrate NO_3 is 61.9895.

3. Calculate the molarity of the solution
   0.39 mg nitrate/g soln × 1000 cc soln/L soln × 1 g/1000 mg × 1.555 g soln/cc soln = 0.60645 g excess nitrate/L soln.
   A 1-molar solution is 1 mol of acid/L of solution:
   (For nitric acid 1 molar is 1 normal because there is only one atom of hydrogen per molecule of acid in HNO_3.)
   (0.60645 g nitrate/L soln)/(61.9895 g NO_3/mol NO_3) = 9.783×10^{-3} mols nitrate/L is identical to mols of acid/L is identical to molarity.

4. The density multiplier of the solution is 1.0. Do not try to use the density (specific gravity) of the solution divided by the theoretical density of $UO_2(NO_3)_2$ from the Standard Composition Library for your density fraction. The $UO_2(NO_3)_2$ listed there is the solid, not the solution.

The solution specification data follow:

```
SOLNUO2(NO3)2    1  415  9.783-3  1.0  293  92235  92.6  92238  5.9
                          92234   1.0  92236  0.5  END
```

M7.5.9.1 Comparison of Number Densities from the Three Methods

The number densities of methods 1 and 2 should agree within the limits of the input data. The density multipliers in method 1 are 5 digits and the density multipliers in method 2 are 4 digits. Therefore, the number densities calculated by the two methods should agree to 4 or 5 digits. Methods 2 and 3 are identical except for the specification of the specific gravity. It is specified as input data in method 2 and is calculated by the Material Information Processor for method 3. The differences in the two specific gravities are responsible for the difference in the hydrogen and oxygen number densities. It is recommended that method 2 be used when the specific gravity of the solution is given.

METHOD 1		METHOD 2		METHOD 3	
NUCLIDE NO.	ATOM DENSITY	NUCLIDE NO.	ATOM DENSITY	NUCLIDE NO.	ATOM DENSITY
92235	9.84590E-04	92235	9.84599E-04	92235	9.84599E-04
92238	6.19407E-05	92238	6.19413E-05	92238	6.19413E-05
92234	1.06783E-05	92234	1.06784E-05	92234	1.06784E-05
92236	5.29380E-06	92236	5.29385E-06	92236	5.29385E-06
7014	2.13089E-03	7014	2.13092E-03	7014	2.13092E-03
8016	3.74127E-02	8016	3.74130E-02	8016	3.74826E-02
1001	5.77959E-02	1001	5.77964E-02	1001	5.79356E-02

M7.5.10 MULTIPLE FISSILE CELLS IN A SINGLE PROBLEM

Consider a problem that involves three different UO_2 fuel assemblies: a 1.98%-enriched assembly, a 2.64%-enriched assembly, and a 2.96%-enriched assembly. All fuel rods are UO_2 at 10.138 g/cc and are 0.94 cm in diameter. The Zircaloy-4 clad has an inside radius of 0.4875 cm and an outside radius of 0.545 cm. The rod pitch is 1.44 cm. Each fuel assembly is a 15 x 15 array of fuel pins with water holes, instrumentation holes, and burnable poison rods. For cross-section processing, the presence of the water holes, instrumentation holes, and burnable poison rods in the assemblies are ignored.

The Material Information Processor allows only one unit cell specification per problem. Therefore, a special effort must be made to provide the correct cross-section processing for the three different fuels. This can be achieved by specifying one of the fuel mixtures in the unit cell and entering the resonance and Dancoff data for the other two mixtures in the optional parameter data (MORE DATA).

To obtain the Dancoff data necessary for correct cross-section treatment of the three different fuels, run CSASN with PARM=CHECK specified. Note that **PARM=CHECK** must begin beyond column 10. Because all three fuels have the same physical dimensions (gap, clad, moderator and pitch), their Dancoff

factors will be identical. Therefore, only one CSASN run is required. Find the Dancoff factors in the output. The final Material Information Processor data will specify one of the fuel mixtures in the unit cell and the Dancoff factors for the other two fuels will be entered in MORE DATA. This is done using the keyword DAN(_)=. The correct resonance information for the two fuel mixtures that are not specified in the unit cell must also be entered in MORE DATA by specifying the mixture number, physical shape, and fuel lump dimension via the keyword RES=.

The input data used to determine the Dancoff factors are given below. It is not necessary to specify all three fuel mixtures in the data. Only mixtures that are used in the unit cell data are required for the purpose of determining the Dancoff factors. This problem will determine the Dancoff factors for mixture 3 because it is used in the unit cell data (SQUAREPITCH).

```
=CSASN          PARM=CHK
DEMONSTRATION PROBLEM WITH MULTIPLE RESONANCE CORRECTIONS REQUIRED
27GROUPNDF4   LATTICECELL
UO2           1   .925      300   92235   1.98   92238   98.02   END
UO2           2   .925      300   92235   2.64   92238   97.36   END
UO2           3   .925      300   92235   2.96   92238   97.04   END
ZIRCALLOY     4   1.0       300   END
H2O           5   1.0       300   END
END   COMP
SQUAREPITCH     1.44   .94   3   5   1.09   4   .975   0   END
END
```

A portion of the computer printout from the above problem is given below. Locate the Dancoff factor for mixture 3 (2.31161E-01). The value 1092235 is the ^{235}U of mixture 1, 2092235 is the ^{235}U of mixture 2, 3092235 is the ^{235}U of mixture 3. Notice that Dancoff factors are calculated ONLY for the mixtures that are used in the unit cell data.

RESONANCE DATA (3* ARRAY)

ID	TEMP	GEOM	ABAR	DANCOFF	INNER RAD.	NSUB0	ITA	M1	SIGMA1	IT1	M2	SIGMA2	IT2	LUMP VOL
1092235	300.00	0	0.00000E+00	0.00000E+00	0.00000E+00	4.53377E-04	1	15.991	3.87761E+02	1	238.051	6.02510E+02	1	1.0000
2092235	300.00	0	0.00000E+00	0.00000E+00	0.00000E+00	6.04497E-04	1	15.991	2.90846E+02	1	238.051	4.48840E+02	1	1.0000
3092235	300.00	2	4.70000E-01	2.31161E-01	0.00000E+00	6.77765E-04	1	15.991	2.59414E+02	1	238.051	3.99001E+02	1	1.0000
1092238	300.00	0	0.00000E+00	0.00000E+00	0.00000E+00	2.21610E-02	1	15.991	7.93296E+00	1	235.044	2.43505E-01	1	1.0000
2092238	300.00	0	0.00000E+00	0.00000E+00	0.00000E+00	2.20115E-02	1	15.991	7.98741E+00	1	235.044	3.26875E-01	1	1.0000
3092238	300.00	2	4.70000E-01	2.31161E-01	0.00000E+00	2.19391E-02	1	15.991	8.01408E+00	1	235.044	3.67704E-01	1	1.0000
4040302	300.00	2	5.45000E-01	4.39454E-01	4.87500E-01	4.33078E-02	1	0.000	0.00000E+00	0	0.000	0.00000E+00	0	1.0000

The following Material Information Processor data will calculate the Dancoff factors and resonance data for fuel mixture 1 because they are used in the unit cell data. The Dancoff factor and resonance data provided in MORE DATA will be used for fuel mixtures 2 and 3. Thus, appropriate cross-section processing will be achieved for all three fuel mixtures. The Dancoff factor for mixtures 2 and 3 was determined above. The resonance data are determined from the problem description (cylindrical pins with a radius of 0.47 cm).

```
DEMONSTRATION PROBLEM WITH MULTIPLE RESONANCE CORRECTIONS REQUIRED
27GROUPNDF4   LATTICECELL
UO2           1   .925      300   92235   1.98   92238   98.02   END
UO2           2   .925      300   92235   2.64   92238   97.36   END
```

```
UO2          3   .925      300   92235   2.96   92238   97.04   END
ZIRCALLOY    4   1.0       300   END
SS304        6   1.0       300   END
H2O          5   1.0       300   END
END   COMP
SQUAREPITCH    1.44   .94   1   5   1.09   4   .975   0   END
MORE   DATA
RES=2   CYLINDER     .47       DAN(2)=0.231161
RES=3   CYLINDER     .47       DAN(3)=0.231161
END   MORE
```

If the geometric configuration or density of the fuel or moderator for each of the three fuel cells is different, a CSASN run should be made for the two configurations that will not be specified in the final unit cell description. These two CSASN runs will provide Dancoff data to be entered in the MORE DATA portion of the final Material Information Processor data. The third configuration is specified in the unit cell data. Thus, two CSASN runs should be made with PARM=CHK specified. The first run specifies the first configuration in the unit cell. The second run specifies the second configuration in the unit cell. The Dancoff factors are located in the CSASN computer printouts and specified in MORE DATA in the final Material Information Processor data using the third fuel cell configuration in the unit cell. In addition, the shape and dimensions of those two fuel lumps must be entered in MORE DATA. In this way, the cross sections are correctly processed for the three different fuel cell configurations.

M7.5.11 MULTIPLE FISSILE MIXTURES IN A SINGLE PROBLEM

Extreme caution should be exercised when an attempt is made to treat multiple fissile mixtures in a single problem. The Material Information Processor and the SCALE cross-section processing codes do not adequately treat multiple fissile mixtures having significant interaction with each other in the resonance range.

The following problem involves large units having the bulk of their fissile material more than one mean-free path away from the surface of the unit. The interaction between the units that occurs in the resonance range is a very small fraction of the total interaction because an overwhelming percentage of the interaction occurs deep within each unit. Therefore, the resonance range interaction between the units can be ignored, and the cross-section processing in the resonance range can be considered adequate for this particular application.

Consider a problem that consists of four 20.96-kg 93.2%-enriched uranium metal cylinders, density 18.76 g/cc, and four 5-l Plexiglas bottles filled with highly enriched uranyl nitrate solution at 415 g/L, a specific gravity of 1.555, and 0.39 mg of excess nitrate per gram of solution. The isotopic content of the uranium metal is 93.2 wt % ^{235}U, 5.6 wt % ^{238}U, 1.0 wt % ^{234}U, and 0.2 wt % ^{236}U. The uranium isotopic content of the nitrate solution is 92.6 wt % ^{235}U, 5.9 wt % ^{238}U, 1.0 wt % ^{234}U and 0.5 wt % ^{236}U. The size of the metal cylinders is between 10 and 12 cm in diameter and height, and the size of the nitrate solution is on the order of 16 and 20 cm in diameter and height. The average mean-free path in the uranium metal is on the order of 1.5 cm, and the average mean free path in the nitrate solution is on the order of 0.5 cm. Therefore, infinite homogeneous medium is an appropriate choice for this problem.

See Examples 1 and 3 of Sect. M7.5.5.1 for data input details for the Plexiglas and uranium metal. See Example 1 of Sect. M7.5.5.3 for data input details for the uranyl nitrate solution. The Material Information Processor data for this problem using the 16-group cross-section library follow:

```
SET  UP  4 AQUEOUS  4  METAL  IN  CSAS25
HANSEN-ROACH     INFHOMMEDIUM
URANIUM      1  0.985  293   92235  93.2  92238  5.6  92234  1.0  92236  0.2  END
SOLNUO2(NO3)2    2  415  9.783-3  SPG=1.555  1.0  293  92235  92.6  92238  5.9
                                92234  1.0   92236  0.5  END
PLEXIGLAS    3  END
END  COMP
```

M7.5.12 CELL WEIGHTING

Cell-weighted cross sections are created by XSDRNPM when an analytical sequence that ends in X (CSAS1X, CSAS2X, etc.) is executed. The unit cell description is then used by XSDRNPM to calculate the eigenvalue of the cell. For LATTICECELL problems, a white boundary condition is assumed. For MULTIREGION problems, the boundary conditions specified in the unit cell are used. The resultant fluxes are used to weight the cross sections of the materials in the cell and create a homogenized cell-weighted cross section having the characteristics of the heterogeneous cell configuration. This cell-weighted cross section is always labeled mixture 500. Whenever XSDRNPM is executed for cross-section processing, mixtures used in the cell description cannot be used in the heterogeneous geometry data for other codes. If they are needed in other codes, additional mixtures with identical specifications must be defined in the standard composition data.

M7.5.12.1 Cell weighting an infinite homogeneous problem

Cell weighting an infinite homogeneous medium has no effect on the cross sections because there is only one zone and one set of cross sections. However, mixture 500 is created, and if a subsequent code uses the mixture number utilized in the unit cell, a warning message will be printed. However, mixture 500 can be used in a subsequent code, and it is identical to the cell cross section. CSAS1X is usually run to obtain the k-infinity for the mixture and not to obtain a cell-weighted cross section.

EXAMPLE 1

This problem would probably be run to provide the k-infinity of 20%-enriched UO_2.

```
20%  ENRICHED  UO2  BILLET
27GR  INF
UO2  1  0.99  293  92235  20  92238  80  END
END  COMP
```

M7.5.12.2 Cell weighting a LATTICECELL problem

Cell weighting used with a LATTICECELL problem creates cell-weighted homogeneous cross sections that represent the characteristics of the heterogeneous system. This cell-weighted cross section can then be used in a subsequent code for the overall volume where the cells are located without having to mock up the actual three-dimensional heterogeneous array of cells. This cell-weighted homogeneous mixture is always designated as mixture 500. Note that the mixtures used in the unit cell description cannot be used in a

subsequent code because they have been flux weighted to create mixture 500. Therefore, if a mixture used in the unit cell description is also to be used in a subsequent code, another mixture must be created that is identical except for the mixture number. Every mixture that is to be used in a subsequent code must be defined in the standard composition data.

A byproduct of the cell-weighting calculation is the eigenvalue (k-effective) of an infinite array of the cell described as the unit cell.

EXAMPLE 1

Consider a cylindrical stainless steel tank filled with spherical pellets of 2.67%-enriched UO_2 arranged in a close-packed "triangular" pitch, flooded with borated water at 4350 WPPM. The cylindrical stainless tank is sitting in a larger tank filled with borated water at 4350 WPPM.

The data for the UO_2 and borated water were developed in detail in Example 3 of Sect. M7.5.8.2. The stainless steel must be defined, and mixture 3 was chosen because mixture 1 was the UO_2 and mixture 2 was the borated water. Because the borated water will be used as a reflector for the stainless steel tank, and has been used in the unit cell data, it must be repeated with a different mixture number (in this case, as mixture 4).

In the subsequent code, mixture 500 will be used to represent the UO_2 pellets in the borated water, mixture 3 will represent the stainless steel tank, and mixture 4 will represent the borated water reflector around the stainless-steel tank.

The Material Information Processor data for creating the cell-weighted cross sections using the 27-group ENDF/B-IV cross-section library follow:

```
SPHERICAL  PELLETS  IN  BORATED  WATER
27GR  LATT
UO2   1  .9398  293.  92235  2.67  92238  97.33  END
ARBMH3BO3  0.025066  3  1  1  0  5000  1  1001  3  8016  3  2  1  293  END
H2O      2  0.984507  293  END
SS304    3  1  293  END
ARBMH3BO3  0.025066  3  1  1  0  5000  1  1001  3  8016  3  4  1  293  END
H2O      4  0.984507  293  END
END  COMP
SPHTRIANGP   1.1440  1.0724  1  2  END
```

M7.5.12.3 Cell weighting a MULTIREGION problem

A MULTIREGION problem is cell weighted primarily to obtain a cell-weighted homogeneous cross section that represents the characteristics of the heterogeneous system. The eigenvalue obtained for a MULTIREGION problem with cylindrical or spherical geometry having a white boundary condition specified on the right boundary approximates an infinite array of the cells. A vacuum boundary condition would represent a single cell. A slab with reflected boundary conditions for both boundaries represents an infinite array of slab cells. The cell-weighted cross sections for spherical or cylindrical geometries with a white right boundary condition do not have a Dancoff correction and thus may not be accurate for representing a large array of the specified units. However, the Dancoff can be specified in the optional parameter data, Sect. M7.5.7, to make the cross sections more accurately represent an array of units.

EXAMPLE 1

Consider a small, highly enriched uranium sphere supported by a Plexiglas collar in a tank of water. The uranium metal sphere has a diameter of 13.1075 cm, is 97.67% enriched, and has a density of 18.794 g/cc. The cylindrical Plexiglas collar has a 4.1275-cm radius central hole, extends to a radius of 12.7 cm and is 2.54 cm thick. The water-filled tank is 60 cm in diameter.

The Plexiglas collar is not significantly different from water and does not surround the fuel, so it will be ignored. Because this makes the problem a one-dimensional geometry, it can be defined using the MULTIREGION type of calculation and the eigenvalue of the system can be obtained without additional data by executing CSAS1X. The abundance of uranium is not stated beyond 97.67% enriched, so assume the remainder is ^{238}U. Using these assumptions and the 27-group ENDF/B-IV cross-section library, the Material Information Processor data follow:

```
SMALL  WATER  REFLECTED  SPHERE  ON  PLEXIGLAS  COLLAR
27GR  MULT
URANIUM     1  DEN=18.794  1  293.  92235  97.67  92238  2.33  END
H2O         2  END
END  COMP
SPHERICAL  END   1  6.5537  2  30.0  END  ZONE
```

M7.6 DESCRIPTION OF OUTPUT

This section describes the computer printout from the Material Information Processor. The order of the printout is the following:

1. Title – The title of the problem is printed.

2. Problem Parameters – The parameters used in the problem are listed.

3. Problem Composition Description – All of the standard compositions used in describing the mixtures for the problem are listed.

4. Problem Geometry – The data defining the unit cell for the problem is listed.

5. Optional Parameter Data – If optional parameter data are entered, the optional parameter data table is printed.

6. Library Information Table – A table defining data libraries is printed for quality assurance purposes.

7. Additional Data – These data are printed only if the Material Information Processor is to check the data without executing (PARM=CHECK on the analytical sequence card). Data that will be used in cross-section processing are printed.

M7.6.1 PROBLEM TITLE

The Problem Title is the first entry printed by the Material Information Processor. It is located immediately above the problem parameters, as shown in Figure M7.6.1. See Sect. M7.4.3 for the data input requirements.

```
        problem to generate material information processor printout

**** problem parameters ****

lib 44groupndf5 library
mxx     9 mixtures
msc    10 composition specifications
izm     4 material zones
ge  latticecell geometry
more    1 0/1 do not read/read optional parameter data
msln    1 fuel solutions
```

Figure M7.6.1 Example of problem title and problem parameters

M7.6.2 PROBLEM PARAMETERS

The Problem Parameters is a list of the parameters entered by the user and those counted by the code as the problem input data are processed. Sample input data specifying the title, cross-section library, and type of calculation are given below.

```
PROBLEM TO GENERATE MATERIAL INFORMATION PROCESSOR PRINTOUT
HANSEN-ROACH  LATTICECELL
```

The resulting Problem Parameters printout is shown in Figure M7.6.1. The problem title is printed exactly as it was entered. The cross-section library, LIB, and the geometry, GE, were set by the above data. The other parameters were determined from other data entered for the problem. The left column contains the variable name associated with the data. LIB, the cross-section library, is the first parameter item and is input as data. The data input requirements for LIB are defined in Sect. M7.4.3, item 2, CROSS SECTION LIBRARY NAME. The number of mixtures, MXX, the number of composition specifications, MSC, and the number of material zones, IZM, are determined by the code. The number of mixtures are counted when the standard composition specification data are read and is the total number of mixtures defined in the standard composition specification data. The number of composition specifications is the number of standard composition definitions used in the standard composition specifications data. The geometry type, GE, is input as data and governs the type of geometry data required to define the unit cell. It also influences the type of resonance treatment applied to the cross sections. The data input requirements for GE are given in Sect. M7.4.3, item 3, TYPE OF CALCULATION. The optional parameter flag, MORE, is set by the code. It is set to 1 if optional parameter data are entered. Otherwise, it is zero. The number of fuel solutions, MSLN, is determined by the code from the standard composition specification data and is the number of standard compositions whose name begins with SOLN.

M7.6.3 PROBLEM COMPOSITION DESCRIPTION

This portion of the Material Information Processor printout lists all of the standard compositions used in the problem and their associated data, as shown in Figure M7.6.2. The standard composition data are printed in the order in which the standard compositions are entered. For example, if data for mixture 5 are entered first, and data for mixture 1 are entered last, the standard composition defining mixture 5 will be printed first, and that for mixture 1 will be printed last. Furthermore, if several standard composition specifications are required to define a single mixture, they need not be entered contiguously. They will then be printed in the order in which they were entered, interspersed exactly as they were in the input data.

In each set of data shown in Figure M7.6.2, the far left column lists the variable name or data name of the input data for each standard composition. These variable names correspond to those used in the Standard Composition input data described in Sect. M7.4.4. The middle column lists the data, and the right column contains either an explanation, or additional data.

The first set of data illustrates the data for a basic standard composition (see Sect. M7.5.5.1 for detailed input data examples) in which the user did not enter the density. The standard composition name is UO2, the mixture number is 1, the volume fraction is 0.96, and the theoretical density (obtained by the code from Table M8.2.1), is 10.96 g/cc. When the code supplies the density, the explanation to the right of the density, ROTH, is stated as THEORETICAL DENSITY. The temperature is 293 degrees Kelvin. After the temperature, the ZA number of the nuclides comprising the standard composition are listed in the center

```
**** problem composition description ****

 sc  uo2          standard composition
 mx             1 mixture no.
 vf         .9600 volume fraction
 roth     10.9600 theoretical density
 nel            2 no. elements
 icp            1 0/1 mixture/compound
 temp       293.0 deg kelvin
            92000      1.00 atom/molecule
                         92235     3.250 wt%
                         92238    96.750 wt%
             8016      2.00 atoms/molecule
 end

 sc  uo2          standard composition
 mx             7 mixture no.
 vf        1.0000 volume fraction
 roth     10.5216 specified density
 nel            2 no. elements
 icp            1 0/1 mixture/compound
 temp       293.0 deg kelvin
            92000      1.00 atom/molecule
                         92235     3.250 wt%
                         92238    96.750 wt%
             8016      2.00 atoms/molecule
 end

 sc  zr           standard composition
 mx             2 mixture no.
 vf        1.0000 volume fraction
 roth      6.4900 theoretical density
 nel            1 no. elements
 icp            1 0/1 mixture/compound
            40000      1.00 atom/molecule
 end

 sc  h2o          standard composition
 mx             3 mixture no.
 vf        1.0000 volume fraction

 roth       .9982 theoretical density
 nel            2 no. elements
 icp            1 0/1 mixture/compound
             1001      2.00 atoms/molecule
             8016      1.00 atom/molecule
 end

 sc  boron        standard composition
 mx             4 mixture no.
 vf         .0086 volume fraction
 roth      7.7600 specified density
 nel            1 no. elements
 icp            1 0/1 mixture/compound
             5000      1.00 atom/molecule
 end

 sc  ss304        standard composition
 mx             4 mixture no.
 vf         .9914 volume fraction
 roth      7.7600 specified density
```

Figure M7.6.2 Example of standard composition printout

```
nel             4 no. elements
icp             0 0/1 mixture/compound
           24304    19.000 wt%
           25055     2.000 wt%
           26304    69.500 wt%
           28304     9.500 wt%
end

sc  ss304         standard composition
mx              5 mixture no.
vf         1.0000 volume fraction
roth       7.9200 theoretical density
nel             4 no. elements
icp             0 0/1 mixture/compound
           24304    19.000 wt%
           25055     2.000 wt%
           26304    69.500 wt%
           28304     9.500 wt%
end

sc  arbmatl1      standard composition
mx              6 mixture no.
vf         1.0000 volume fraction
roth       7.1500 specified density
nel             3 no. elements
icp             0 0/1 mixture/compound
            6012     3.250 wt%
           14000     1.350 wt%
           26000    95.400 wt%
end

sc  solnuo2(no3) standard composition
mx              8 mixture no.
fd       325.8900 solution fuel density
aml         .5300 acid molarity
vf         1.0000 volume fraction
temp        293.0 deg kelvin
spg        1.4828 specified specific gravity
sc  uo2(no3)2     standard composition
           92000      1.00 atom/molecule
                         92234      .008 wt%
                         92235      .700 wt%
                         92236      .052 wt%
                         92238    99.240 wt%
            7014      2.00 atoms/molecule
            8016      8.00 atoms/molecule
sc  hno3          standard composition
            1001      1.00 atom/molecule
            7014      1.00 atom/molecule
            8016      3.00 atoms/molecule
sc  h2o           standard composition
            1001      2.00 atoms/molecule
            8016      1.00 atom/molecule
end

sc  arbmuo2puo2   standard composition
mx              9 mixture no.
vf         1.0000 volume fraction
roth      11.2000 specified density
nel             3 no. elements
icp             0 0/1 mixture/compound
```

Figure M7.6.2 (continued)

```
temp        293.0 deg kelvin
              8016     11.889 wt%
             92000     44.982 wt%
                                 92235     93.200 wt%
                                 92238      5.600 wt%
                                 92234      1.000 wt%
                                 92236       .200 wt%
             94000     43.130 wt%
                                 94239     95.000 wt%
                                 94240      2.500 wt%
                                 94241      2.000 wt%
                                 94238       .500 wt%
 end
```

Figure M7.6.2 (continued)

column and the corresponding number of atoms per molecule are listed in the right column (URANIUM, 92000 at 1 atom/molecule and OXYGEN, 8016 at 2 atoms/molecule). If the nuclide is a multiple isotope nuclide, both the ZA number of the isotopes and their corresponding isotopic weight percents are listed in the right column immediately after the multiple isotope nuclide. The input data for this entry are shown below.

```
UO2 1  0.96 293 92235 3.25 92238 96.75 END
```

The second set of data illustrates the same standard composition used as mixture 7, with a user-supplied density. When the user supplies the density, the explanation to the right of the density, ROTH, is stated as SPECIFIED DENSITY. The input data for this entry are shown below.

```
UO2 7 DEN=10.5216 1.0 293 92235 3.25 92238 96.75 END
```

The third and fourth sets of data also illustrate data for basic standard compositions. The third standard composition name is ZR, the mixture number is 2, the volume fraction is 1.0, and the theoretical density, obtained from Table M8.2.1 by the code, is 6.44 g/cc. The fourth standard composition name is H2O, the mixture number is 3, the volume fraction is 1.0, and the theoretical density, obtained by the code from Table M8.2.1, is 0.9982 g/cc. The input data are shown below.

```
ZR 2 1.0 END
H2O 3 1.0 END
```

The fifth and sixth sets of data illustrate the creation of a single mixture using two basic standard compositions (see Sect. M7.5.5.4 for examples). Mixture 4 is borated stainless steel with a density of 7.76 g/cc, and is 0.86 wt % natural boron. The input data for this mixture are shown below.

```
BORON  4  DEN=7.76 0.0086  END
SS304  4  DEN=7.76 0.9914  END
```

The seventh set of data is another basic standard composition, stainless steel 304. The standard composition name is SS304, the mixture number is 5, the volume fraction is 1.0, and the theoretical density, determined by the code, is 7.92 g/cc. The input data for this mixture are shown below:

```
SS304  5  1.0  END
```

The eighth set of data illustrates data for an arbitrary material standard composition. Examples of arbitrary material input data are given in Sect. M7.5.5.2. The standard composition name defined by the user is ARBMATL1; the mixture number, MX, is 6; the volume fraction, VF, is 1.0; the density, ROTH, is always entered by the user for an arbitrary material and for this problem is 7.15 gm/cc. NEL is the number of elements required to define the arbitrary material and is entered as 3. The mixture/compound indicator, ICP, is 0, indicating that the material is defined by weight percents as in an alloy, rather than by a chemical formula. The data printed after the mixture/compound indicator, ICP, lists the isotope ID numbers, NCZA, in the center column and the corresponding weight percents, ATPM, in the right column. The input data for this arbitrary material follow.

```
ARBMATL1  7.150  3 0 0 0 6012  3.25  14028  1.35  26000  95.4  6  END
```

The ninth set of data describe a solution standard composition. Examples of solution standard composition input data are given in Sect. M7.5.5.3. The standard composition name, SC, for a solution must be chosen from Table M8.3.1. The mixture number, MX, is 8; the fuel density, FD, is 325.89 g U/L soln. The acid molarity, AML, is 0.53 moles of acid/liter of solution; the volume fraction, VF, is 1.0; the temperature, TEMP, is 293 °K; and the specific gravity, SPG, is 1.4828. When the user specifies the specific gravity, it is labeled SPECIFIED SPECIFIC GRAVITY. If the code determines the specific gravity, it is labeled DEFAULT SPECIFIC GRAVITY. Following the specific gravity, the three components that make up the solution are listed. The first component listed is the salt followed by the list of elements and their atoms/salt molecule that make up the salt. If more than one isotope is in an element the isotopic breakdown and weight percents of each element follow the element. The second component listed is the acid followed by the list of elements in the acid and their atoms/acid molecule. The final component listed is the H2O in the solution followed by the list of elements in the H2O and their atoms/H2O molecule. The input data for this solution are given below.

```
SOLNUO2(NO3)2  8 325.89 0.53 SPG=1.4828 1.0 293.
92234 .008 92235 .700 92236 .052 92238 99.240 END
```

The last set of data describes an arbitrary material standard composition that contains two multiple isotope elements. The standard composition name defined by the user is ARBMUO2PUO2; the mixture number, MX, is 9; the volume fraction, VF, is 1.0; the specified density, ROTH, which is always entered by the user for an arbitrary material is 11.2 gm/cc; the number of elements used to define the arbitrary material, NEL, is 3; the mixture/compound indicator, ICP, is 0 indicating it is a mixture defined by weight percents of the elements; and the temperature, TEMP, is 293°K. Directly following the above information is the list of elements and their respective weight percents that make up the arbitrary material. Any element that has more than one isotope is immediately followed by a list of isotopes and their respective weight percents in that element. First in the list of elements is oxygen with a ZA number of 8016 comprising 11.889 wt % of the material. Next in the list of elements is uranium comprising 44.982 wt % of the arbitrary material. The ZA number 92000 specifies natural uranium. However when isotopic data is entered this data overrides the default isotopic data. The isotopic composition and weight percents for uranium immediate follows the

uranium elements ZA number and weight percent. The final element in the list is plutonium comprising 43.130 wt % of the arbitrary material. The ZA number 94000 specifies a material composed entirely of Pu-239. However when isotopic data is entered this data overrides the default isotopic data. The isotopic composition and weight percents for plutonium immediate follows the plutonium elements ZA number and weight percent. The input data for this solution are given below.

```
ARBMUO2PUO2   11.2   3   0   0   1   8016   11.8885   92000   44.9819
   94000  43.1296 1.0 293
92235  93.2  92238  5.6  92234  1.0  92236  0.2
94239  95.0  94240  2.5  94241  2.0  94238  0.5 END
```

M7.6.4 PROBLEM GEOMETRY SPECIFICATION

This portion of the Material Information Processor printout lists the geometry description for the problem based on the unit cell description that was entered as data. The unit cell description provides data that are used in processing the cross sections. It follows the standard composition data in the printout. The three types of unit cells are (1) infinite homogeneous medium, (2) LATTICECELL, and (3) MULTIREGION. The printout for each is shown below.

M7.6.4.1 Problem Geometry Description for an Infinite Homogeneous Medium

The mixture that is to be used to calculate the eigenvalue if XSDRNPM is to be executed is printed for an infinite homogeneous medium. An example of the printout is given in Figure M7.6.3. See Sect. M7.4.5 for input data instructions. The input data corresponding to this example are:

CELLMIX 6

```
**** problem geometry ****

**** infinite homogeneous medium ****
mfuel          6 mixture no. of the infinite homogeneous medium
```

Figure M7.6.3 Example of geometry description printout for Infinite Homogeneous Medium

M7.6.4.2 Problem Geometry Description for a LATTICECELL

Figure M7.6.4 illustrates the geometry output for a square-pitch lattice. The left column lists the data name corresponding to the input specifications as listed in Sect. M7.4.6 and examples presented in Sect. M7.5.6.2. The input data for this example are given below.

```
SQUAREPITCH 1.43 .9322 1 3 1.0718 2  .9498 0 END
```

```
**** problem geometry ****

ctp squarepitch  cell type
pitch     1.4300 cm center to center spacing
fuelod     .9322 cm fuel diameter or slab thickness
mfuel         1 mixture no. of fuel
mmod          3 mixture no. of moderator
cladod    1.0718 cm clad outer diameter
mclad         2 mixture no. of clad
gapod      .9498 cm gap outer diameter
mgap          0 mixture no. of gap
```

Figure M7.6.4 Example of geometry description printout for LATTICECELL

M7.6.4.3 Problem Geometry Description for a MULTIREGION Cell

Figure M7.6.5 illustrates the geometry output for a MULTIREGION cell. The left column lists the data name corresponding to the input specifications as listed in Sect. M7.4.7. Examples of MULTIREGION input data are given in Sect. M7.5.6.3. The input data for this example are given below.

```
BUCKLEDCYL  VACUUM  REFLECTED  0.0 130.0  END
1 7.62  2 7.77  3 40.77
END ZONE
```

The printed results for the above MULTIREGION description are given in Figure M7.6.5.

```
**** problem geometry ****

cs   buckledcyl   coordinate system
br   vacuum       right boundary
bl   reflected    left boundary
orgn          .00 cm left boundary location
dy         130.00 cm buckling height
dz            .00 cm buckling depth
end

zone number     1
mzx             1 mixture no.
rz           7.62 cm right boundary location
xmod                external moderator index

zone number     2
mzx             2 mixture no.
rz           7.77 cm right boundary location
xmod                external moderator index

zone number     3
mzx             3 mixture no.
rz          40.77 cm right boundary location
xmod                external moderator index
```

Figure M7.6.5 Example of geometry description printout for MULTIREGION cell

M7.6.5 OPTIONAL PARAMETER DATA OR MORE DATA

The optional parameter data are printed only if the keyword MORE and optional parameters are entered after the unit cell data. The title "**** SPECIAL PARAMETERS ****" and the first 17 parameters listed in Figure M7.6.6 are always in the printout when optional parameter data are entered. See Sect. M7.4.8 for input data instructions and Sect. M7.5.7 for additional details. The following additional special data may be printed if specified: The number of direct access blocks, a message saying all thermal groups were collapsed into one group, three lines for each mixture with resonance data, and Dancoff factor data consisting of the title line "dancoff factor specification" followed by a line containing the words "mixture factor" followed by the mixture number and Dancoff factor for each Dancoff factor entered. The 3 lines of resonance data and the Dancoff factor data are included in Figure M7.6.6. The input data for an example that supplies resonance and Dancoff data for material 7 are given below:

```
MORE DATA  RES=7  SLAB  0.5  DAN(7)=0.23  END MORE
```

```
 **** special parameters ****

 isn            8 order of angular quadrature
 iim           20 inner iteration maximum
 icm           25 outer iteration maximum
 szf  1.00000e+00 size factor for spatial mesh
 eps  1.00000e-04 overall problem convergence
 pto  1.00000e-04 scalar flux convergence
 bkl  1.42089e+00 buckling factor
 ius            0 thermal upscatter scaling
 bal         fine balance table print flag
 dy   0.00000e+00 buckling height
 dz   0.00000e+00 buckling depth
 ipn            0 diffusion coefficient option
 frd            0 logical unit number to read flux guess
 fwr           -1 logical unit number to write flux guess
 msh         2001 number of intervals for res. intgrtns
 mlv            2 max lvalue for res. intgrtns
 axs            0 logical unit number to write anisn lib
 res            7 mixture with special resonance correction
  *          Slab geometry for special resonance correction
  *   5.00000e-01 dimension (lbar) for special resonance correction

 dancoff factor specification
 mixture     factor
       7     .23000
```

Figure M7.6.6 Example of optional parameter printout

M7.6.6 ZONE SPECIFICATIONS FOR A LATTICECELL

The zone specifications for a LATTICECELL problem are printed after the special parameters (optional parameter data or MORE DATA), described in Sect. M7.6.5. If optional parameter data are not entered in the problem, the zone specifications for a LATTICECELL are printed immediately after the problem geometry. See Figure M7.6.7 for an example of the zone specifications for LATTICECELL geometry. The input data that generated this printout are:

```
    squarepitch 1.43 .9322 1 3 1.0718 2 .9498 0 end
zone specifications for latticecell geometry

                zone  1 is fuel
                zone  2 is gap
                zone  3 is clad
                zone  4 is mod
```

Figure M7.6.7 Example of LATTICECELL zone specifications

M7.6.7 LIBRARY INFORMATION TABLE

The Material Information Processor provides a Library Information Table for quality assurance purposes. An example of this table is given in Figure M7.6.8. The table contains information about the Standard Composition Library, the master format cross-section library, the short problem-dependent master format cross-section library, and the direct-access dataset for saving input data. The Material Information Processor creates the short cross-section library by copying only the nuclides utilized in the problem from the master format cross-section library. It also saves input data as a direct-access dataset. For these four data libraries, the table lists (1) the unit number used to reference the library, (2) the data set name of the library, (3) the volume where the dataset resides, and (4) unit function, which is a brief description of the type of library or the library function.

Additional data provided for the Standard Composition Library include the unit number, the dataset name, the title read from the Standard Composition Library, and the date the Standard Composition Library was created. The additional cross-section library data printed in the table include the unit number, the dataset name, and the title read from the master format cross-section library.

M7.6.8 ADDITIONAL DATA

The Material Information Processor data can be checked by executing CSASN and specifying PARM=CHECK on the analytical sequence indicator. When this is done, the printout will contain additional data as discussed in this section. If PARM=CHECK is not specified, the problem printout includes only the printout preceding this section. The data included in the additional data are (1) the mixing table and a table of parameters, (2) resonance data, and (3) NITAWL, XSDRNPM, and BONAMI data.

M7.6.8.1 Mixing Table Data

The first information printed under the heading additional data is the mixing table generated by the Material Information Processor. Multiple occurrences of the same nuclide are distinguished from each other by adding 1000000 × MIXNO to the nuclide ID number, where MIXNO is the mixture number. For example, in Figure M7.6.9, 1008016 is oxygen used in mixture 1 and 3008016 is oxygen used in mixture 3. The atom density is given in atoms/barn-cm. The far right column, labeled N.I.T. POINTER, is the internal code pointer to the beginning of the data needed to generate resonance processing data for NITAWL.

```
*** problem to generate material information processor printout ***

********** data library information **********

 unit                                                volume
number              data set name                    name        unit function
------              -------------                    ----        -------------

  89     /scale4.3p/data/scale.rev10.sclib                       standard composition library

  83     /scale4.3p/data/scale.rev03.xn44                        cross section library

  11     ft11f001                                                short cross section library

  90     ft90f001                                                input data direct access

                          standard composition library data
                          ---------------------------------

   unit number  :  89

   dataset name :  /scale4.3p/data/scale.rev10.sclib

   library title:  scale-4 standard composition library
                   637 standard compositions, 490 nuclides
                   90 elements with variable isotopic distrbutions.

   creation date:   9/19/95

                             cross section library data
                             --------------------------

   unit number  :  83

   dataset name :  /scale4.3p/data/scale.rev03.xn44

   library title:  scale 4.3 - 44 neutron group library        based on endf-b version 5 data
                     collapsed with a light water reactor cell flux spectrum from 238 groups
                       compiled for nrc       9/01/94
                         last updated         8/07/95
                           m.d.dehart & l.m.petrie   nuclear eng. appl. - cped - ornl
```

Figure M7.6.8 Example of data library information table

```
    **** additional data ****

 mixing table from standard compositions data

  mixture    nuclide      atom          n.i.t.
    no.        no.       density       pointer
     1      1092235   7.72325e-04       455
     7      7092235   7.72325e-04       455
     8      8092235   5.84484e-06       455
     9      9092235   1.20302e-02       455
     1      1092238   2.27011e-02       458
     7      7092238   2.27011e-02       458
     8      8092238   8.18160e-04       458
     9      9092238   7.13714e-04       458
     1      1008016   4.69468e-02        33
     7      7008016   4.69468e-02        33
     3      3008016   3.33846e-02        33
     8      8008016   3.79897e-02        33
     9      9008016   5.01454e-02        33
     2      2040000   4.28457e-02       171
     3      3001001   6.67692e-02         6
     8      8001001   6.11914e-02         6
     4      4005010   7.39771e-04        23
     4      4005011   2.97767e-03        24
     4      4024304   1.69296e-02        96
     5      5024304   1.74286e-02        96
     4      4025055   1.68662e-03        98
     5      5025055   1.73633e-03        98
     4      4026304   5.76586e-02       106
     5      5026304   5.93579e-02       106
     4      4028304   7.49967e-03       117
     5      5028304   7.72070e-03       117
     6      6006012   1.16616e-02        26
     6      6014000   2.06972e-03        50
     6      6026000   7.35568e-02       100
     8      8092234   6.70843e-08       454
     9      9092234   1.29633e-04       454
     8      8092236   4.32343e-07       456
     9      9092236   2.57063e-05       456
     8      8007014   1.96818e-03        30
     9      9094239   1.15604e-02       466
     9      9094240   3.02953e-04       467
     9      9094241   2.41362e-04       468
     9      9094238   6.11007e-05       465


    mmt          38 nuclides from cross section library
    ires         25 resonance nuclides
    ibl           1 left  bdy condition 0/1/2/3
vacuum/reflected/periodic/white
    ibr           3 right bdy condition 0/1/2/3
vacuum/reflected/periodic/white
    ms           38 entries in the mixing table
    isct          3 order of scattering
    dy       0.0000 first  transverse buckling dimension
    dz       0.0000 second transverse buckling dimension
    vsc      0.0000 void streaming
```

Figure M7.6.9 Mixing table and parameters from the Material Information Processor data check

The second set of data lists parameters for BONAMI, ICE, NITAWL, and XSDRN. The left column contains the parameter name or variable name. The center column contains the value assigned to the parameter. The right column contains an explanation of the parameter.

M7.6.8.2 Resonance Data for NITAWL

The data shown in Figure M7.6.10 are used by NITAWL to provide the cross-section resonance processing to create problem-dependent cross sections. Only nuclides having resonance data are listed in this table. ID is the nuclide ID number. TEMP is the temperature in degrees Kelvin. GEOM specifies the geometry shape, 0/1/2/3 corresponding to homogeneous/slab/cylinder/sphere. ABAR is the absorber lump dimension in centimeters (thickness of a slab, radius of a sphere or cylinder, zero for homogeneous). DANCOFF is the calculated Dancoff factor. INNER RAD is the inner radius of the characteristic absorber lump. NSUB0 is the absorber number density in the lump. ITA, IT1, and IT2 are the type of treatment used to determine the contribution in the interior of the absorber lump to the collision density for the absorber, the first moderator, and the second moderator. The available treatment options are: no moderator (0) and Nordheim's integral method (1). M1 and M2 are the mass of the first and second moderator, respectively, for the given nuclide. SIGMA1 and SIGMA2 are the first and second moderator scattering cross section per absorber atom. LUMP VOL is the volume fraction of the absorber lump in the cell. This is used in NITAWL to provide a crude cell weighting in the resonance range. SCALE always sets this to 1.0, which eliminates this weighting in NITAWL.

resonance data (3* array)

id	temp	geom	abar	dancoff	inner rad.	nsub0	ita	m1	sigma1	it1	m2	sigma2	it2	lump vol
1092235	293.00	2	4.66100e-01	2.27234e-01	0.00000e+00	7.72325e-04	1	15.991	2.36274e+02	1	238.051	3.62311e+02	1	1.0000
7092235	293.00	1	5.00000e-01	2.30000e-01	0.00000e+00	7.72325e-04	1	15.991	2.36274e+02	1	238.051	3.62311e+02	1	1.0000
8092235	293.00	0	0.00000e+00	0.00000e+00	0.00000e+00	5.84484e-06	1	1.008	2.13374e+05	1	16.669	3.01473e+04	1	1.0000
9092235	293.00	0	0.00000e+00	0.00000e+00	0.00000e+00	1.20302e-02	1	15.991	1.62020e+01	1	238.989	1.25668e+01	1	1.0000
1092238	293.00	2	4.66100e-01	2.27234e-01	0.00000e+00	2.27011e-02	1	15.991	8.03840e+00	1	235.044	4.04941e-01	1	1.0000
7092238	293.00	1	5.00000e-01	2.30000e-01	0.00000e+00	2.27011e-02	1	15.991	8.03840e+00	1	235.044	4.04941e-01	1	1.0000
8092238	293.00	0	0.00000e+00	0.00000e+00	0.00000e+00	8.18160e-04	1	1.008	1.52432e+03	1	15.751	2.03127e+02	1	1.0000
9092238	293.00	0	0.00000e+00	0.00000e+00	0.00000e+00	7.13714e-04	1	15.991	2.73097e+02	1	237.023	4.00123e+02	1	1.0000
2040000	293.00	2	5.35900e-01	4.29362e-01	4.74900e-01	4.28457e-02	1	0.000	0.00000e+00	0	0.000	0.00000e+00	0	1.0000
4024304	293.00	0	0.00000e+00	0.00000e+00	0.00000e+00	1.69296e-02	1	55.845	3.45332e+01	1	40.417	9.08934e+00	1	1.0000
5024304	293.00	0	0.00000e+00	0.00000e+00	0.00000e+00	1.74286e-02	1	55.845	3.45332e+01	1	58.486	8.11545e+00	1	1.0000
4025055	293.00	0	0.00000e+00	0.00000e+00	0.00000e+00	1.68662e-03	1	55.845	3.46630e+02	1	43.529	1.35351e+02	1	1.0000
5025055	293.00	0	0.00000e+00	0.00000e+00	0.00000e+00	1.73633e-03	1	55.845	3.46630e+02	1	55.925	1.25576e+02	1	1.0000
4026304	293.00	0	0.00000e+00	0.00000e+00	0.00000e+00	5.76586e-02	1	58.687	2.26242e+00	1	33.215	1.81728e+00	1	1.0000
5026304	293.00	0	0.00000e+00	0.00000e+00	0.00000e+00	5.93579e-02	1	58.687	2.26242e+00	1	52.216	1.53133e+00	1	1.0000
4028304	293.00	0	0.00000e+00	0.00000e+00	0.00000e+00	7.49967e-03	1	55.845	7.79546e+01	1	33.215	1.39715e+01	1	1.0000
5028304	293.00	0	0.00000e+00	0.00000e+00	0.00000e+00	7.72070e-03	1	55.845	7.79546e+01	1	52.216	1.17731e+01	1	1.0000
6026000	293.00	0	0.00000e+00	0.00000e+00	0.00000e+00	7.35568e-02	1	12.000	7.50921e-01	1	28.085	5.84943e-02	1	1.0000
8092234	293.00	0	0.00000e+00	0.00000e+00	0.00000e+00	6.70843e-08	1	1.008	1.85906e+07	1	16.675	2.62766e+06	1	1.0000
9092234	293.00	0	0.00000e+00	0.00000e+00	0.00000e+00	1.29633e-04	1	15.991	1.50358e+03	1	237.070	2.25862e+03	1	1.0000
8092236	293.00	0	0.00000e+00	0.00000e+00	0.00000e+00	4.32343e-07	1	1.008	2.88459e+06	1	16.675	4.07710e+05	1	1.0000
9092236	293.00	0	0.00000e+00	0.00000e+00	0.00000e+00	2.57063e-05	1	15.991	7.58230e+03	1	237.055	1.14390e+04	1	1.0000
9094239	293.00	0	0.00000e+00	0.00000e+00	0.00000e+00	1.15604e-02	1	15.991	1.68604e+01	1	235.428	1.39455e+01	1	1.0000
9094240	293.00	0	0.00000e+00	0.00000e+00	0.00000e+00	3.02953e-04	1	15.991	6.43378e+02	1	237.020	9.60560e+02	1	1.0000
9094238	293.00	0	0.00000e+00	0.00000e+00	0.00000e+00	6.11007e-05	1	15.991	3.19003e+03	1	237.051	4.80210e+03	1	1.0000

Figure M7.6.10 Resonance data for NITAWL

M7.6.8.3 Additional Data for NITAWL, XSDRNPM, and BONAMI

The data shown in Figure M7.6.11 list additional data that are provided by the Material Information Processor for cross-section processing. The NITAWL data are the 2$ and 4* arrays. The CSAS(XSDRN) data include the zone boundaries, mixture by zone, and scatter by zone. The BONAMI data are the extra cross-section data.

	nitawl data		csas(xsdrn) data			bonami data	
	nuclide identifier	thermal scatter temp.	zone boundaries	mixture numbers	scatter by zone	sigma h by mixture	temperature by mixture
1	1092235	2.93000e+02	0	1	3	1.12690e+00	0
2	7092235	2.93000e+02	4.66100e-01	0	0	5.81696e+00	0
3	8092235	2.93000e+02	4.74900e-01	2	3	0	0
4	9092235	2.93000e+02	5.35900e-01	3	3	0	0
5	1092238	2.93000e+02	8.06791e-01			0	0
6	7092238	2.93000e+02				0	0
7	8092238	2.93000e+02				8.76209e-01	0
8	9092238	2.93000e+02				0	0
9	1008016	2.93000e+02				0	0
10	7008016	2.93000e+02					
11	3008016	2.93000e+02					
12	8008016	2.93000e+02					
13	9008016	2.93000e+02					
14	2040000	2.93000e+02					
15	3001001	2.93000e+02					
16	8001001	2.93000e+02					
17	4005010	2.93000e+02					
18	4005011	2.93000e+02					
19	4024304	2.93000e+02					
20	5024304	2.93000e+02					
21	4025055	2.93000e+02					
22	5025055	2.93000e+02					
23	4026304	2.93000e+02					
24	5026304	2.93000e+02					
25	4028304	2.93000e+02					
26	5028304	2.93000e+02					
27	6006012	2.93000e+02					
28	6014000	2.93000e+02					
29	6026000	2.93000e+02					
30	8092234	2.93000e+02					
31	9092234	2.93000e+02					
32	8092236	2.93000e+02					
33	9092236	2.93000e+02					
34	8007014	2.93000e+02					
35	9094239	2.93000e+02					
36	9094240	2.93000e+02					
37	9094241	2.93000e+02					
38	9094238	2.93000e+02					

Figure M7.6.11 Additional data for NITAWL, XSDRNPM, and BONAMI

M7.7 WARNING AND ERROR MESSAGES

The Material Information Processor is responsible for reading and checking the SCALE data used to create a problem-dependent AMPX working format cross-section library. Error messages are printed if the code determines that an error has occurred. Warning messages are printed if the code recognizes a possible error.

It is the responsibility of the user to verify whether the data are correct when a warning message is encountered. The functional modules activated by the control module and related sequences will be executed even though a warning message has been generated.

When an error is recognized, an error message is written and an error flag is set so the functional modules will not be activated. The code stops immediately if the error is too severe to allow continuation of input. However, it will continue to read and check the data if it is able. When the data reading has been completed, execution will be terminated if an error flag was set when the data were being processed. The STOP codes associated with the severe error messages are listed in Sect. M7.7.2.

M7.7.1 MATERIAL INFORMATION PROCESSOR MESSAGES

The following messages originate in the Material Information Processor, that portion of the analytical sequence that reads the parameter data, standard composition specification data, and geometry data necessary for preparing the required information for the cross-section processing codes.

MP-1 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine KNIGHT indicates that the allocated computer storage will not hold the directories and isotope information tables. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the space allocation using the "SIZE" parameter on the analytical sequence indicator (Sect. M7.4.2) and resubmit the problem. A STOP 300 is executed when this message is printed.

MP-2 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine KNIGHT indicates that the allocated computer storage will not hold the directories and isotope information tables. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the space allocation using the "SIZE" parameter on the analytical sequence indicator (Sect. M7.4.2) and resubmit the problem. A STOP 310 is executed when this message is printed.

MP-3 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine KNIGHT indicates that the allocated computer storage will not hold the directories and isotope information tables. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the space allocation using the "SIZE" parameter on the analytical sequence indicator (Sect. M7.4.2) and resubmit the problem. A STOP 320 is executed when this message is printed.

MP-4 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine SETUPA indicates that the allocated computer storage will not hold the directories and isotope information tables. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the space allocation using the "SIZE" parameter on the analytical sequence indicator (Sect. M7.4.2) and resubmit the problem. A STOP 330 is executed when this message is printed.

MP-5 ***ERROR*** SYSTEM GEOMETRY NAME INCORRECT. INSTEAD OF (_____), THE USER SHOULD HAVE ENTERED LATTICECELL, MULTIREGION, OR INFHOMMEDIUM AS THE SECOND ITEM ON THE PARAMETER CARD. CHECK SPELLING.

This self-explanatory message is from subroutine SETUPB. The user has misspelled the word defining the type of calculation to be performed or the parameter data preceding it were entered incorrectly. See Sect. M7.7.3 for assistance in correctly specifying the parameter data.

MP-6 ***ERROR*** _____ NOT FOUND IN STANDARD COMPOSITION LIBRARY. MAKE SURE THE COMPOSITION NAME USED IS IN THE STANDARD COMPOSITION LIBRARY.

This self-explanatory message from subroutine STDCMP indicates that a standard composition name is misspelled, the standard composition specification data are out of order, or the "END" has been omitted from the preceding standard composition specification. Check the standard composition specification data carefully. See Sect. M7.7.4 for assistance with standard composition specification cards. See Sect. M8 for the materials available in the Standard Composition Library.

MP-7 ***ERROR*** THE USER ENTERED A VOLUME FRACTION (VF) OF 0.0 FOR ONE OF THE STANDARD COMPOSITIONS (_____). THIS INDICATES THAT HE INTENDS

TO ENTER A NUMBER DENSITY FOR THE STANDARD COMPOSITION. THAT, HOWEVER, CAN ONLY BE DONE WHEN THE STANDARD COMPOSITION NAME REPRESENTS A SINGLE NUCLIDE (LIKE H, O, PB, B-10, U-238, ETC.). CHECK THE STANDARD COMPOSITION LIBRARY.

This self-explanatory message is from subroutine STDCMP. Check the Standard Composition Library, Sect. M8, for the available standard composition names. See Sect. M7.7.4 for the correct method of specifying standard composition specification data.

MP-8 ***ERROR*** CELL TYPE NAME (_____) IS INCORRECT. CHECK THE SPELLING. THE ALLOWED NAMES ARE: SQUAREPITCH, TRIANGPITCH, SPHSQUAREP, SPHTRIANGP, SYMMSLABCELL, ASYMSLABCELL, ASQUAREPITCH, ATRIANGPITCH, ASPHSQUAREP, ASPHTRIANGP, ASQP, ATRP, ASSP, ASTP.

This self-explanatory message is from subroutine LATCEL. The data are misspelled or out of order. Some data items may be missing or extra ones may have been entered. Errors in the standard composition specification data can cause this message to be printed. See Sect. M7.7.6 for additional assistance.

MP-9 ***ERROR*** THE NUMBER OF ZONES (IZM=_____) IS INCORRECT FOR ASYMSLABCELL GEOMETRY. FOR AN ASYMMETRIC LATTICECELL CALCULATION, ONE SHOULD HAVE IZM=3, 5, OR 7, DEPENDING ON THE MATERIALS PRESENT.

This self-explanatory message is from subroutine LATCEL. See Sect. M7.7.6 for an explanation of the ASYMSLABCELL geometry data. A code error is responsible for this message.

MP-10 ***ERROR*** INSUFFICIENT DATA SUPPLIED ON THE GEOMETRY DESCRIPTION CARD.

This message from subroutine LATCEL can be caused by having an error in the standard composition specification data, thereby causing the reading routines to get out of phase. If no error messages precede this message, it may indicate that a code error exists. The number of material zones (IZM) has been destroyed or altered in some manner.

MP-11 ***ERROR*** MIXTURE _____ IN THE CSAS GEOMETRY DESCRIPTION WAS NOT SPECIFIED IN THE STANDARD COMPOSITION DATA.

This message from subroutine LATCEL indicates that a mixture number used in the geometry description was not defined in the standard composition specification data. Check the input data for consistency. If the specified mixture number is zero, and the problem is a LATTICECELL problem using mixture zero for the clad or moderator, it will be necessary to specify a low-density mixture in the standard composition data and use it in the cell specification.

MP-12 ***ERROR*** THE GAP WAS SPECIFIED AS MIXTURE _____ ON THE LATTICECELL. IT SHOULD BE ZERO OR A VALID MIXTURE NUMBER.

This message from subroutine LATCEL indicates that the mixture number used for the GAP was not defined in the standard composition specification data. Check the input data for consistency.

MP-13 **WARNING** NUMBER OF ENTRIES ON THE GEOMETRY DESCRIPTION CARD EXCEEDS THE NUMBER EXPECTED. THIS MESSAGE MAY BE GENERATED IF THE USER FORGOT TO ENTER THE END ON THE GEOMETRY DESCRIPTION CARD.

This message from subroutine LATCEL may result from a code error or from omitting the word "END" from the geometry description card.

MP-14 ***ERROR*** THE COORDINATE SYSTEM NAME (_____) IS INCORRECT. FOR THIS MULTIREGION CALCULATION, THE USER SHOULD HAVE ENTERED SLAB, CYLINDRICAL, SPHERICAL, BUCKLEDSLAB OR BUCKLEDCYL ON THE GEOMETRY DESCRIPTION CARD. CHECK SPELLING.

This self-explanatory message is from subroutine MULTRG.

MP-15 ***ERROR*** ALPHANUMERIC DESCRIPTION OF THE RIGHT-HAND BOUNDARY CONDITION (_____) IS INCORRECT. ONLY VACUUM, REFLECTED, PERIODIC, AND WHITE BOUNDARY CONDITIONS ARE ALLOWED. CHECK SPELLING. CHECK GEOMETRY DESCRIPTION CARD INPUT INSTRUCTIONS FOR ADDITIONAL ASSISTANCE.

This self-explanatory message is from subroutine MULTRG. See Sect. M7.7.6 for additional assistance.

MP-16 ***ERROR*** ALPHANUMERIC DESCRIPTION OF THE LEFT-HAND BOUNDARY CONDITION (_____) IS INCORRECT. ONLY VACUUM, REFLECTED, PERIODIC, AND WHITE BOUNDARY CONDITIONS ARE ALLOWED IN SLAB GEOMETRY. IN THE CASE OF CYLINDRICAL OR SPHERICAL GEOMETRY, ONLY THE REFLECTED BOUNDARY CONDITION IS ALLOWED ON THE LEFT. CHECK SPELLING. CHECK GEOMETRY DESCRIPTION CARD INPUT INSTRUCTIONS FOR ADDITIONAL INSTRUCTIONS.

This self-explanatory message is from subroutine MULTRG. See Sect. M7.7.6 for additional assistance.

MP-17 ***ERROR*** MIXTURE _____ FROM THE MULTIREGION DATA WAS NOT SPECIFIED IN THE STANDARD COMPOSITION DATA.

This message is from subroutine MULTRG. It indicates that a mixture number specified in the MULTIREGION data was not defined in the standard composition specification data. Check the input data for consistency.

MP-18 ***ERROR*** USER MADE AT LEAST _____ DATA ERRORS. PROBLEM WILL NOT BE RUN. HOPEFULLY, EACH OF THESE ERRORS WILL HAVE GENERATED ITS OWN SELF-EXPLANATORY ERROR MESSAGE. IF NOT, CHECK DATA CAREFULLY BEFORE RESUBMITTING.

This self-explanatory message is from subroutine SETUPB. Check through the problem printout and correct all errors that have occurred.

MP-19 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message is from subroutine SETUPB. It indicates that the allocated computer storage will not hold the data that must be loaded to calculate the information that must be passed to BONAMI. The first number is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that is required to hold these data. The third number is the minimum additional words of storage required to hold these data. Subsequent portions of the program may require even more storage. Increase the space allocation using the "SIZE" parameter on the analytical sequence indicator (Sect. M7.4.2) and resubmit the problem. A STOP 390 is executed when this message is printed.

MP-20 ***ERROR*** MIXTURE NUMBER _____ ON A STANDARD COMPOSITION CARD IS LESS THAN 1.

This message is from subroutine SETUPB. A mixture number specified on a standard composition specification card must always be greater than zero. This message is triggered if a MP-6 message is printed. Fixing the MP-6 error should eliminate this message. If the printed mixture number is a positive number, a code error is responsible for the message.

MP-21 ***WARNING*** STANDARD COMPOSITION CARD NUMBER _____ IMPLIES THAT MIXTURE NUMBER _____ HAS A TEMPERATURE OF _____ DEGREES KELVIN, WHEREAS STANDARD COMPOSITION SPECIFICATION CARD _____ IMPLIES THAT MIXTURE NUMBER _____ HAS A TEMPERATURE OF _____ DEGREES KELVIN. (ONE OF THESE MAY HAVE BEEN THE VALUE SPECIFIED BY DEFAULT.) THE CODE WILL ASSUME THE HIGHER OF THE TWO AND PROCEED. IF THIS IS NOT SATISFACTORY, THE USER

SHOULD ENTER THE CORRECT TEMPERATURE ON EACH OF THE STANDARD COMPOSITION SPECIFICATION CARDS INDICATED.

This self-explanatory message is from subroutine SETUPB.

MP-22 **WARNING** STANDARD COMPOSITION SPECIFICATION CARD(S) MISSING FOR MIXTURE NUMBER _____.

This message from SETUPB is printed to remind the user that the mixture numbers specified in the standard composition specification data are not contiguous. This may result in wasted storage space, but is not necessarily indicative of an error.

MP-23 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine MTABLE indicates that the allocated computer storage will not hold the nuclide ID numbers that will be processed by subroutine IDENTS. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage needed to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the space allocation using the "SIZE" parameter on the analytical sequence indicator (Sect. M7.4.2) and resubmit the problem. A STOP 340 is executed when this message is printed.

MP-24 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine MIXTAB indicates that the allocated computer storage will not hold the three mixing table arrays that will be processed by subroutine ARRAY3. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage needed to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the space allocation using the "SIZE" parameter on the analytical sequence indicator (Sect. M7.4.2) and resubmit the problem. A STOP 350 is executed when this message is printed.

MP-25 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine MIXTAB indicates that the allocated computer storage will not hold the three mixing table arrays that will be processed by subroutine ARRAY3. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage needed to hold

the data to this point. Subsequent portions of the program may require even more storage. Increase the space allocation using the "SIZE" parameter on the analytical sequence indicator (Sect. M7.4.2) and resubmit the problem. A STOP 360 is executed when this message is printed.

MP-26 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine MIXTAB indicates that the allocated computer storage will not hold the three mixing table arrays that will be processed by subroutine ARRAY3. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage needed to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the space allocation using the "SIZE" parameter on the analytical sequence indicator (Sect. M7.4.2) and resubmit the problem. A STOP 370 is executed when this message is printed.

MP-27 ***ERROR*** THE NUMBER OF MIXTURES FOUND IN THE MIXING TABLE IS INCONSISTENT WITH THE INPUT DATA. THE NUMBER FOUND IS _____, BUT THE INPUT DATA INDICATED _____.

This message from subroutine REORDR indicates that an error was found in the mixing table during operations to reorder and load it in permanent storage. The number of mixtures found in the mixing table should be the same as the number indicated by the input data. A code error is the likely cause of this message. A STOP 380 is executed when this message is printed.

MP-28 ***ERROR*** NUCLIDE ID ____ SPECIFIED IN THE INPUT DATA WAS NOT FOUND IN THE STANDARD COMPOSITION LIBRARY.

This message is from subroutine IDENTS or subroutine SLNS. A STOP 395 is printed with this message. Check the standard composition specification data, Sect. M7.7.4, and assure that the "ZA" ID numbers were entered correctly. This message is also printed if an arbitrary material specifies a value other than 0 or 1 for the MULTIPLE-ISOTOPE INDICATOR (IVIS in Sect. M7.7.4).

MP-29 ***ERROR*** AN ARGUMENT OF ____ IS INVALID FOR AN ARCSIN OR ARCCOS.

This message from subroutine ARCHK is indicative of a code error. ARCHK is called from subroutine DAN to assure that proper arguments are supplied to the ARCSIN and ARCCOS functions in determining cylinder Dancoff factors. This error can be caused by specifying a center-to-center spacing that is smaller than is physically possible.

MP-30 ***ERROR*** THE MATRIX WAS SINGULAR WHEN THE NUMBER FRACTION OF AN ISOTOPE IN AN ELEMENT WAS BEING DETERMINED. MAKE SURE THE SPECIFIED ISOTOPE DISTRIBUTION (WEIGHT PERCENT) SUMS TO 100.0.

This message from subroutine NOFRAC is caused by an isotope distribution that does not sum to 100.0 percent for an element. Entry A7 of Sect. M7.4.4 illustrates the correct procedure for specifying the weight percent of the various isotopes in an element.

MP-31 ***ERROR*** THE CALCULATED NUMBER FRACTIONS DO NOT REPRODUCE THE WEIGHT PERCENTS ENTERED AS INPUT DATA OR OBTAINED FROM THE STANDARD COMPOSITION LIBRARY.

WTFRAC=nnnnnnnnnn NOFRAC=mmmmmmmmmm MASS=ℓℓℓℓℓℓℓℓℓℓ

This message is printed from subroutine NOFRAC. WTFRAC, NOFRAC, and MASS are printed for each isotope in the standard composition. WTFRAC is the specified input weight percent for the isotope converted to weight fraction instead of weight percent. NOFRAC is the adjusted atom percent converted to atom fraction for the isotope corresponding to a total weight percent of 100% for the isotopes in the standard composition. MASS is the atomic weight of the isotope. The adjusted isotopic weight percents are not printed in MP-31 but can be calculated according to:

$$ADJ_i = \frac{NOFRAC_i \times MASS_i}{\sum_i NOFRAC_i \times MASS_i} \times 100$$

where

ADJ_i is the adjusted weight percent of isotope i,

$NOFRAC_i$ is the number fraction of isotope i printed in MP-31, and

$MASS_i$ is the atomic weight of isotope i printed in MP-31.

Message MP-31 is printed if the adjusted weight percent of any individual isotope differs by 0.4% or more from the isotopic weight percent specified for that particular isotope in the standard composition data. An error flag is set, and the problem will not execute. If the isotopic weight percents specified in the input data do not sum to 100%, the weight percent of the first isotope whose specified weight percent is greater than 0.1% is adjusted to force the total weight percent to sum to 100%. If this adjustment results in a calculated weight percent for that isotope that is less than 0.4% different from that specified in the input data, the problem is run using the adjusted data. If message MP-31 is printed, correct the isotopic weight percents specified in the standard composition input data to sum to 100 or specify the isotope with the largest weight percent first, and resubmit the problem.

MP-32 ***ERROR*** END COMP WAS EXPECTED, BUT ____ WAS READ INSTEAD.

This message from subroutine SETUPA is printed if the data are out of order or the keywords END COMP or END COMPOSITIONS are omitted after the last standard composition specification. An END followed by blanks is also allowed. Check the data and the spelling of the END COMP. See Sect. M7.4.4.

MP-33 ***ERROR*** END OF FILE WAS ENCOUNTERED WHILE READING MULTIREGION ZONE DESCRIPTION. VERIFY THAT THE END ZONE CARD WAS ENTERED.

This self-explanatory message from subroutine SETUPA is printed if the END ZONE is omitted following the MULTIREGION zone description data. See Sect. M7.4.7.

MP-34 ***ERROR*** END ZONE WAS EXPECTED, BUT ____ WAS READ INSTEAD.

This message from subroutine SETUPA is printed if data are out of order or the keywords END ZONE are omitted at the end of the MULTIREGION zone description data. Check the data and the spelling of the END ZONE. See Sect. M7.4.7.

MP-35 ***ERROR*** END OF FILE WAS ENCOUNTERED WHEN THE GEOMETRY DESCRIPTION CARD WAS EXPECTED.

This self-explanatory message from subroutine SETUPA is printed if data are omitted or out of order. See Sect. M7.4.

MP-36 ***ERROR*** ILLEGAL SOLUTION NAME _____. ALLOWED NAMES INCLUDE SOLNUO2F2, SOLNUO2(NO3)2 AND SOLNPU(NO3)4.

This self-explanatory message from subroutines SLNS and SLNAME is printed if a solution name is misspelled or data are out of order. See Sect. M7.4.4 for assistance in specifying solution names correctly.

MP-37 ***ERROR*** ____ IS AN INVALID NAME WHEN READING MORE DATA.

This message is printed from subroutine MOREDT when extra parameter data are to be entered as explained in Sect. M7.4.8. The data are out of order or a parameter name is misspelled.

MP-38 ***ERROR*** INVALID GEOMETRY WORD _____. ONLY INFHOMMEDIUM, MULTIREGION, OR LATTICECELL ARE ALLOWED.

This self-explanatory message is from subroutine SETUPA. Correct the input data and resubmit the problem. Check the spelling of the geometry word, assure that the data are in order, and resubmit the problem.

MP-39 ***WARNING*** AN END DATA WAS READ BEFORE IT WAS EXPECTED. AN END WAS PROBABLY OMITTED FROM A STANDARD COMPOSITION.

This message from subroutine SETUPA indicates that an "END" was omitted from a standard composition specification or the END for a standard composition specification was followed by COMP. The first four characters following the END on a standard composition specification card cannot be COMP. The words END COMP terminate the standard composition specification data. Check the standard composition specification data carefully.

MP-40 ***ERROR*** NUCLIDE ID _____ IN MIXTURE _____ DOES NOT OCCUR IN THE STANDARD COMPOSITION LIBRARY.

This self-explanatory message is from subroutine REORDR. A STOP 385 is executed in conjunction with this message.

MP-41 ***ERROR*** A NUCLIDE ID OF _____ IS INVALID FOR _____ IN THE FOLLOWING STANDARD COMPOSITION SPECIFICATION.

This message from subroutine STDCMP indicates that a nuclide ID is not compatible with a standard composition name. For example: UO2 3 1 300 94240 50 94238 50 END would cause this error because plutonium is invalid for a uranium standard composition specification. If this message is printed for a solution, the specific gravity of the solution may have been entered without the required keyword SPG=.

MP-42 ***ERROR*** AN END WAS ENCOUNTERED BEFORE MORE DATA WAS COMPLETED.

This message from MOREDT indicates incomplete input for MORE DATA. See Sect. M7.4.8 for assistance.

MP-43 ***WARNING*** BAL= _____ IS AN INVALID BALANCE TABLE SPECIFICATION. ALL BALANCE TABLES WILL BE PRINTED.

This message from subroutine MOREDT indicates that the value entered following BAL= is incorrect. Available options are NONE, FINE, and ALL. If any other value is entered, this message will be printed.

MP-44 ***ERROR*** NUCLIDE _____ WAS NOT FOUND ON THE CROSS SECTION LIBRARY AND IS NOT A MULTIPLE ISOTOPE NUCLIDE IN THE STANDARD COMPOSITION LIBRARY.

ERROR

This message from subroutine SCDATA indicates that the nuclide ID specified was not found on the cross section library or in the multiple isotope table in the Standard Composition Library. An error flag is set to prevent execution, and checking is continued.

MP-45 ***** ERROR ***** _____ IS NOT A VALID CALCULATION TYPE. USE INFHOMMEDIUM, LATTICECELL, OR MULTIREGION. EXECUTION IS TERMINATED.

This message from subroutine CSPARM indicates that the TYPE OF CALCULATION (see entry 3 of Sect. M7.4.3) was spelled incorrectly, entered out of order, or was improperly specified.

MP-46 *** ERROR *** THE FUELOD CANNOT BE GREATER THAN THE PITCH.

This self-explanatory message from subroutine LATCEL results from an error in the UNIT CELL SPECIFICATION for a LATTICECELL problem (see Sect. M7.4.6). The value of PITCH must be at least as large as the value of FUELOD.

MP-47 *** ERROR *** THE CLADOD CANNOT BE LESS THAN THE FUELOD, NOR GREATER THAN THE PITCH.

This message from subroutine LATCEL indicates an error in the UNIT CELL SPECIFICATION for a LATTICECELL problem. See Sect. M7.4.6 and verify the values of PITCH, FUELOD, and CLADOD.

MP-48 *** ERROR *** THE GAPOD CANNOT BE LESS THAN THE FUELOD, NOR GREATER THAN THE CLADOD.

This message from subroutine LATCEL indicates an error in the UNIT CELL SPECIFICATION for a LATTICECELL problem. See Sect. M7.4.6 and verify the values of FUELOD, CLADOD, and CLADID (note that CLADID is the GAPOD and is equal to FUELOD + twice the gap thickness).

MP-49 *** ERROR *** THE ABOVE RADIUS MUST BE GREATER THAN THE PREVIOUS RADIUS.

This message from subroutine MULTRG indicates an error in the GEOMETRY SPECIFICATION for a MULTIREGION problem. See Sect. M7.4.7 and check to assure that each value of RZ is greater than the previous value of RZ.

MP-50 *** WARNING *** IN MORE DATA, RESONANCE INFORMATION (RES=) WAS SUPPLIED FOR MIXTURE _____. IT WILL NOT BE USED BECAUSE THAT MIXTURE OCCURS IN THE CELL DESCRIPTION.

This message from subroutine MOREDT is printed if resonance data (RES=) are entered for a mixture in MORE DATA (Sect. M7.4.8) and is also used in the cell description (Sects. M7.4.6 and M7.4.7).

MP-51 *** ERROR *** IN MORE DATA _____ IS AN INVALID GEOMETRY TYPE FOR USE IN SPECIFYING RESONANCE DATA. CYLINDER, SPHERE, OR SLAB MUST BE ENTERED.

This message from subroutine MOREDT is printed if resonance data (RES=) are entered in MORE DATA (Sect. M7.4.8) and an incorrect shape is specified. The correct specification for a sphere of mixture 3 having a radius of 1.5 cm is: RES=3 SPHERE 1.5

MP-52 *** WARNING *** IN MORE DATA, DANCOFF INFORMATION (DAN( )=) WAS SUPPLIED FOR MIXTURE _____. THIS VALUE WILL BE USED INSTEAD OF CALCULATING THE DANCOFF FROM THE CELL DESCRIPTION.

This message from subroutine MOREDT is printed to alert the user that the Dancoff information calculated from the unit cell (Sects. M7.4.6 and M7.4.7) specification is being overridden by the value that was entered in MORE DATA (Sect. M7.4.8).

MP-54 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine C4DATA indicates that the allocated computer storage will not hold the volume fraction data from subroutine VERIFY. The first number printed is the amount of storage, in words, needed to hold this data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the space allocation using the "SIZE" parameter on the analytical sequence indicator (Sect. M7.4.2) and resubmit the problem.

MP-55 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine C4DATA indicates that the allocated computer storage will not hold the mixing table data required for subroutine BONAMI. The first number printed is the amount of storage, in words, needed to hold this data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the space allocation using the "SIZE" parameter on the analytical sequence indicator (Sect. M7.4.2) and resubmit the problem.

MP-56 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine C4DATA indicates that the allocated computer storage will not hold the mixture number, outer radii, temperature, sigma-H, and zone identifiers for each BONAMI zone. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the space allocation using the "SIZE" parameter on the analytical sequence indicator (Sect. M7.4.2) and resubmit the problem.

MP-57 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine C4DATA indicates that the allocated computer storage will not hold the BONAMI control parameters. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the space allocation using the "SIZE" parameter on the analytical sequence indicator (Sect. M7.4.2) and resubmit the problem.

MP-58 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine C4DATA indicates that the allocated computer storage will not hold the cross-section data required by subroutines EPSIG and XSMESH. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the space allocation using the "SIZE" parameter on the analytical sequence indicator (Sect. M7.4.2) and resubmit the problem.

MP-59 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine C4DATA indicates that the allocated computer storage will not hold the data required by subroutine XSDRN. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent

portions of the program may require even more storage. Increase the space allocation using the "SIZE" parameter on the analytical sequence indicator (Sect. M7.4.2) and resubmit the problem.

MP-60 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine C4DATA indicates that the allocated computer storage will not hold the data required by subroutine ICE. The first number printed is the amount of storage, in words, needed to hold this data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the space allocation using the "SIZE" parameter on the analytical sequence indicator (Sect. M7.4.2) and resubmit the problem.

MP-61 *** ERROR *** THE CROSS-SECTION LIBRARY NAME ENTERED IN THE MATERIAL INFORMATION PROCESSOR DATA FOR THIS CSAS PROBLEM IS INCORRECT. SEE TABLE M8.2.2 OF THE SCALE MANUAL.

This message from subroutine C4DATA indicates that an invalid CROSS-SECTION LIBRARY NAME (see item 2 of Sect. M7.4.3) was entered. The name was misspelled, out of order, or improperly specified.

MP-62 ***ERROR*** A MIXTURE NUMBER IS OUT OF RANGE. ENTRY _____ IN THE MIXING TABLE IS _____. IT SHOULD FALL BETWEEN 1 AND ____, THE LARGEST NUMBER USED IN THE STANDARD COMPOSITION DATA.

This message is from subroutine EPSIG. Because the largest mixture number is determined by the code as the input data are read, this message may be the result of a code error introduced when changes were made to the code.

MP-63 ***ERROR*** A POINTER INTO THE NUCLIDE DATA IS OUT OF RANGE. ENTRY _____ IN THE MIXING TABLE IS _____. IT SHOULD FALL BETWEEN 1 AND _____, THE NUMBER OF NUCLIDES IN THE STANDARD COMPOSITION LIBRARY.

This message is from subroutine EPSIG. It may result from a code error introduced when changes were made to the code.

MP-64 TAPE COPY NEEDS _____ WORDS, BUT ONLY HAS _____ WORDS.

This message from subroutine SHORTX indicates that the allocated computer storage is insufficient to create the short cross-section library utilized by the Material Information Processor. Increase the space allocation using the "SIZE" parameter on the analytical sequence indicator (Sect. M7.4.2) and resubmit the problem. A STOP 200 is executed when this message is printed.

MP-65 ***** ERROR ***** THE FOLLOWING NUCLIDES WERE NOT FOUND ON THE MASTER LIBRARY:

This message from subroutine SHORTX indicates that the user specified a standard composition which contains a nuclide that is not available on the specified master library. For example, nuclide ID 25304, which is stainless-steel-weighted manganese, is not available on any of the libraries but is listed in the Standard Composition Library. 25055 could be used instead.

MP-66 ***ERROR*** THE MIX. NO. (MIXZ=_____) ASSIGNED TO ZONE IZ=_____WAS OUTSIDE THE RANGE 0 TO MXX=_____.

This message from subroutine VERIFY indicates that the mixture number is out of range. A code error is the likely cause of this error.

MP-67 **WARNING** MIXTURE _____ WAS ASSIGNED TO ZONES _____ AND __ ____. THIS MAY BE CORRECT IF THE MIXTURE HAS NO RESONANCE NUCLIDES AND HAS THERMAL SCATTERING DATA AT ONLY ONE TEMPERATURE. USUALLY, UNIQUE MIXTURE NUMBERS SHOULD BE USED IN EACH ZONE, EVEN THOUGH THE MIXTURE SPECIFICATIONS MAY BE IDENTICAL. THIS ALLOWS BONAMI AND NITAWL TO PRODUCE SEPARATE CROSS SECTIONS BASED ON THE APPROPRIATE NUMBER OF EXTERNAL MODERATORS AND THE ACTUAL MEAN CHORD LENGTH FOR EACH SPECIFIED ZONE AS WELL AS THE ACTUAL TEMPERATURE FOR THAT ZONE.

This self-explanatory message is from subroutine VERIFY. The user should verify that the multiple use of the stated mixture number was intentional and correct.

MP-68 ERRONEOUS MIXING TABLE LENGTH FOR XSDRN.

This message from subroutine XSDRN is indicative of a code error. The computed mixing table length, MS, passed to subroutine XSDRN, does not match the counted length in subroutine XSDRN.

MP-69 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine XSMESH indicates that the allocated computer storage will not hold the interval boundaries and zone number for each interval. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the space allocation using the "SIZE" parameter on the analytical sequence indicator (Sect. M7.4.2) and resubmit the problem. Specification (by the control module) of too many mesh intervals in a given zone is the most frequent cause of failure. In MULTIREGION calculations where one has a large zone containing a strong absorber (such as a tank of uranyl-fluoride solution), it may be necessary to reduce the number of mesh intervals by

increasing the size factor (SZF) in the Optional Parameter Data (Sect. M7.7.7). Making this factor large enough (SZF=10, 15, 20, 30, etc.) will generally allow any problem to run in the space allocated. Once the problem runs, one should check the number density of all strong absorbers to see if they are realistic. Occasionally a user will accidentally specify an unrealistic concentration of a strong absorber in one or more zones. Such a mistake dramatically increases the number of mesh intervals the code thinks it needs.

MP-70 ***ERROR*** MORE THAN ONE ZONE WAS ENCOUNTERED FOR THIS INFINITE HOMOGENEOUS MEDIA PROBLEM.

This self-explanatory message is from subroutine XSMESH. Correct the input data and resubmit the problem.

MP-71 ***WARNING*** THE TEMPERATURE FOR STANDARD COMPOSITION _____WAS SPECIFIED AS _____ DEGREES CELSIUS.
DENSITY DATA AT 25 DEGREES CELSIUS WILL BE USED FOR THIS SOLUTION.

This message from subroutine SLNS is printed if SOLNUO2F2 or SOLNPU(NO3)4 were specified in the standard composition data with a temperature outside the range of 15 to 30 degrees CELSIUS. The Standard Composition Library does not contain data for these solutions outside that temperature range.

MP-72 *** ERROR *** KEYWORD SPG= OR DEN= TO SPECIFY THE SPECIFIC GRAVITY OF THE SOLUTION WAS EXPECTED. KEYWORD _____ WAS READ INSTEAD.

This message from subroutine STDCMP indicates an error in the specification of solution data in the standard composition specification. If the specific gravity of a solution is to be entered, it is the fourth entry after the solution name. Check the solution input data carefully.

MP-73 ***ERROR*** EXTERNAL MODERATOR INDEX IS INCORRECT IN ZONE ____OF THE MULTIREGION DATA. ENTER NOEXTERMOD, ONEEXTERMOD, OR TWOEXTERMOD INSTEAD OF _____. CHECK SPELLING.

This self-explanatory message is printed from subroutine MULTRG and subroutine RESDA or subroutine MULTRG. The user has misspelled the word defining the external moderator index of the specified zone or the MULTIREGION data are out of order. See Sect. M7.4.7.

MP-74 *** ERROR *** FIRST MODERATOR HAS NEGATIVE THICKNESS

This message from subroutine DANCOF indicates that the dimensions specified for an ASYMSLABCELL are inconsistent. The array pitch (PITCH) is smaller than the sum of the second moderator thickness (TKMOD2) and *MAX* where *MAX* is the outside diameter of the clad (CLADOD) if entered; otherwise, *MAX* is the outside diameter of the fuel (FUELOD). Correct the data and resubmit the problem. See Sect. M7.4.6 and Figure M7.4.3 for assistance.

MP-75 *** ERROR *** KEYWORD DEN= OR SPG= TO SPECIFY THE DENSITY OF THE BASIC STANDARD COMPOSITION WAS EXPECTED. KEYWORD _____ __WAS READ INSTEAD.

This message from subroutine STDCMP indicates an error in the specification of the density in the basic standard composition data. If the density of the material is to be entered, it is the second entry after the standard composition name. The density is optional data. If the density is entered, it is multiplied by the volume fraction to obtain the density actually used for this composition.

MP-76 *** ERROR *** THE LOWER BOUND OF XSDRN INTERVAL _____ IS _____ WHICH MUST BE LESS THAN THE UPPER BOUND OF _____.

This message from subroutine XSMESH indicates that the specified XSDRN mesh interval is incorrect. Each mesh interval must have a finite positive thickness. This message can be caused by an error in the unit cell data. Either a zero-thick region was specified or the unit cell dimensions were incorrectly specified. Carefully check the unit cell dimensions. If a LATTICECELL annular cell is specified, verify that the FUELOD is at least as large as TKMOD2+2(CLADOD-FUELOD).

MP-77 A NEGATIVE DIMENSION WAS ENCOUNTERED IN THE UNIT CELL DATA. CHECK AND CORRECT THE GEOMETRY DIMENSION.

This message from subroutine LATCEL is printed if a negative number is read for a cell dimension. Check the printed problem geometry and correct the input data (Sect. M7.4.6).

MP-78 THE FUEL THICKNESS IS NEGATIVE. THE ANNULAR CELL DIMENSIONS FOR TKMOD2, CLADOD, AND FUELOD ARE INCONSISTENT.

This message from subroutine LATCEL indicates an error in the description of a cylindrical or spherical annular cell. The cell description must provide a finite fuel thickness. The inside diameter of the fuel is calculated using the diameter of the second moderator, TKMOD2, and the outer diameter of the clad, CLADOD. If the calculated inside diameter of the fuel is greater than or equal to the specified outer diameter of the fuel, there is no fuel in the cell and this message is printed. The thickness of the gap and clad is ½(CLADOD–FUELOD), so the inside diameter of the fuel is TKMOD2+CLADOD–FUELOD. See Sect. M7.4.6 for data input instructions.

MP-79 *** ERROR *** THE ORIGIN MUST BE 0.0 FOR SPHERICAL OR CYLINDRICAL GEOMETRY.

This message from subroutine MULTRG is printed if the origin, ORGN of Table M7.4.8, Sect. M7.4.7, is nonzero for a cylinder or sphere. Either the MULTIREGION unit cell data are out of order or a nonzero number has been entered for ORGN. Correct the data and resubmit the problem.

MP-80 *** ERROR *** NOT ENOUGH STORAGE IN CLAPSE—FIRST NUMBER IS THE AMOUNT NEEDED, SECOND IS THE AMOUNT AVAILABLE.

PERTINENT CONSTANTS

This message from subroutine CLAPSE indicates that the allocated computer storage is insufficient to allow collapsing the thermal cross sections to one group for shielding calculations. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated. A STOP 201 is executed when this message is printed.

MP-81 *** ERROR *** DANCOFF FACTOR MUST BE BETWEEN 0.0 AND 1.0

This message from subroutine MOREDT is printed if DAN(n)= is specified in MORE DATA with a value greater than 1.0 or less than 0.0. Dancoff factors must lie between 0 and 1. The problem will not be run if message MP-81 is printed. Correct the data and resubmit the problem. See Sect. M7.4.7 for assistance.

MP-82 THE FIRST MODERATOR THICKNESS IS NEGATIVE. THE ASYMMETRIC SLAB CELL DIMENSIONS FOR TKMOD2, CLADOD, AND PITCH ARE INCONSISTENT

This message from subroutine LATCEL indicates an error in the description of an asymmetric slab cell. The thickness of the first moderator is not specified in the input data and is calculated as PITCH–TKMOD2/2–CLADOD. If the thickness of the first moderator is negative, this message is printed.

MP-83 *** ERROR *** AN INPUT DATA ERROR HAS BEEN ENCOUNTERED IN THE MATERIAL INFORMATION PROCESSOR DATA ENTERED FOR THIS PROBLEM.

This message from subroutine C4DATA is printed if the subroutine library routine LRDERR returns a value of "TRUE," indicating that a reading error was encountered in the Material Information Processor input data. Locate the unnumbered message stating "***** ERROR IN INPUT. CARD IMAGE PRINTED ON NEXT LINE *****." Correct the data and resubmit the problem.

MP-84 *** WARNING *** FOR MIXTURE ____ THE DANCOFF FACTOR OF ____ IS OUTSIDE THE RANGE OF 0 TO 1. IT WILL BE RESET TO THE CLOSER BOUND.

This message from subroutine RESDA is printed when the DANCOFF factor is less than 10^{-4} outside the allowed range of 0 to 1. This is usually due to roundoff in calculating the Dancoff factor.

MP-85 *** ERROR *** FOR MIXTURE ____ THE DANCOFF FACTOR OF ____ IS OUTSIDE THE RANGE OF 0 TO 1. IT WILL BE RESET TO THE CLOSER BOUND. THE PROBLEM WILL NOT BE EXECUTED.

This message from subroutine RESDA is printed when the Dancoff factor is more than 10^{-4} outside the allowed range of 0 to 1. Check the input data to be sure that the specified Dancoff factor is between 0 and 1. See Sect. M7.4.8 or C4.4.8 for input specifications for the Dancoff factor. If the Dancoff factor was not specified in the optional parameter data, the message is due to a code error.

MP-86 ***ERROR*** THE FUEL DENSITY FOR SOLUTION ____ IN MIXTURE ____ SPECIFIES A FUEL DENSITY OF _____ G/L, WHICH EXCEEDS THE FUEL DENSITY OF A HYDRATED CRYSTAL, AND WILL LEAD TO ERRONEOUS DENSITIES WHEN USED AS A SOLUTION

This message from subroutine SLNS is printed only for solution standard compositions (those that begin with SOLN) that are incorrectly specified. Each solution standard composition is composed of (1) a fuel-salt, **fs**, (2) water, $\mathbf{H_2O}$, and (3) an acid. A fully hydrated fuel-salt is defined as $\mathbf{fs \cdot nH_2O}$ where **n** defines the number of water molecules associated with the fuel-salt crystal (water of hydration). The values of **n** are:

n	Solution	Hydrated Salt
2	UO_2F_2	$UO_2F_2 \cdot 2H_2O$
6	$UO_2(NO_3)_2$	$UO_2(NO_3)_2 \cdot 6H_2O$
5	$Pu(NO_3)_4$	$Pu(NO_3)_4 \cdot 5H_2O$

If the fuel density is so large that there is not enough water in the solution to form fully hydrated crystals of fuel-salt, this message will be printed. The solution name, mixture number, and specified fuel density are printed in the error message. The problem will not run if this message is printed. Correct the input data for this solution standard composition in the specified mixture and resubmit the problem.

MP-87 ***WARNING*** THE FUEL DENSITY FOR SOLUTION ____ IN MIXTURE ___ SPECIFIES A FUEL DENSITY OF _____ G/L. THIS MAY BE GREATER THAN THE SATURATED SOLUTION FUEL DENSITY, AND MAY GIVE INCORRECT DENSITIES AS A SOLUTION. CHECK THE DENSITIES CAREFULLY.

This message from subroutine SLNS is printed because the fuel density for the specified solution standard composition may be high enough to allow precipitation of the fuel-salt. Each solution standard composition is composed of (1) a fuel-salt (**fs**), (2) water ($\mathbf{H_2O}$), and (3) an acid. The water/fuel-salt ratio, **n**, is the ratio of the moles of water to moles of fuel-salt. The minimum threshold values of **n** used to trigger this message are:

n	Solution
8	UO_2F_2
17	$UO_2(NO_3)_2$
17	$Pu(NO_3)_4$

The solution name, mixture number, and specified fuel density are printed in the error message. The problem will run and it is the responsibility of the user to verify that the resulting solution is correct.

MP-88 ***ERROR*** THE LIBRARY SPECIFIED IS A PRE-NITAWL-II LIBRARY

This error message from subroutine SETUPA indicates the specified library was created to be used with a version of NITAWL prior to NITAWL-II. See Table M8.2.2 of Table M4.1.1 for a list of acceptable cross-section libraries. If the library is correctly specified, its format is not consistent with the NITAWL-II format.

MP-89 THE MATERIAL SPECIFIED IN THE ___TH STANDARD COMPOSITION SPECIFICATION DOES NOT ALLOW MULTIPLE ISOTOPES.
THE FOLLOWING ISOTOPE SPECIFICATIONS WERE ENTERED:
NCZA(i) ATPM(i) NCZA(i+1) ATPM(i+1) . . . .

This error message from subroutine SCDATA indicates that the nth standard composition specification does not contain multiple isotopic nuclides but isotopic data (NCZA and ATPM) were included. It could possibly indicate a missing END statement. When determining the nth specification, arbm and basic standard composition specifications count as one each and solution specifications count as three each (fuel salt, water, and an acid).

MP-90 TOO MANY ISOTOPES WERE SPECIFIED FOR ELEMENT _____OF THE _____TH STANDARD COMPOSITION SPECIFICATION.

This error message from subroutine SCDATA indicates that element ____ of the ___th standard composition specification contains more isotopes than are allowed. Reduce the number of isotopes used to describe the material. When determining the ___th standard composition specification, arbitrary materials and basic standard composition specifications count as one each and solution specifications count as three each (fuel salt, water, and an acid).

MP-91 ***ERROR*** THE USER SPECIFIED A NEGATIVE VOLUME FRACTION FOR _____.

This self-explanatory error message from subroutine STDCMP indicates a negative density multiplier or volume fraction (VF). It was entered for the standard composition named in the message.

MP-92 ***ERROR*** THE USER SPECIFIED A NEGATIVE OR 0 MIXTURE NUMBER FOR ____
-.

This self-explanatory error message from subroutine STDCMP indicates that a negative or zero mixture number (MX) was entered for the standard composition named in the message.

MP-93 ***ERROR*** THE USER SPECIFIED A NEGATIVE OR 0 DENSITY FOR _____.

This self-explanatory error message from subroutine STDCMP indicates that a negative or zero density or specific gravity (SPGR or ROTH) was specified for the standard composition named in the message.

MP-94 ***ERROR*** THE USER SPECIFIED A NEGATIVE OR 0.0 FUEL DENSITY FOR SOLUTION _____.

This self-explanatory error message from subroutine STDCMP indicates that a negative of zero fuel density (FD) was specified for the solution standard composition named in the message.

MP-95 ***ERROR*** THE USER SPECIFIED A NEGATIVE ACID MOLARITY FOR SOLUTION
_____.

This self-explanatory error message from subroutine STDCMP indicates that a negative or zero acid molarity (AML) was specified for the solution standard composition named in the message.

MP-96 ***ERROR*** ILLEGAL ENDING KEYWORD FOR DANCOFF.)= SHOULD HAVE BEEN ENTERED, BUT _____WAS READ INSTEAD.

This error from MOREDT indicates a DAN(keyword was read, but after the mixture number, the required)= keyword was not found. Correct the Dancoff specification.

MP-97 ***ERROR*** A ZONE WIDTH MODIFIER WAS SPECIFIED FOR ZONE ___. IT MUST BE BETWEEN 1 AND _____.

This error from MOREDT indicates that a zone width search modifier was specified for a zone greater than the number of zones, or less than 1. Correct the zone number.

MP-98 ***ERROR*** THE NUMBER OF INTERVALS WAS SPECIFIED FOR ZONE____. IT MUST BE BETWEEN 1 AND ____.

This error for MOREDT indictes that the number of intervals was specified for a zone greater than the number of zones, or less than 1. Correct the zone number.

M7.7.2 STOP CODES

The STOP codes that are utilized in the Material Information Processor are listed in Table M7.7.1 indicating the subroutine where they occur and the associated error message. A STOP is executed when a fatal error is recognized. Locate the associated message number to determine the appropriate corrective measures. A traceback may be generated whenever subroutine STOP is called to print a message. If no traceback is indicated in the STOP CODE table, a STOP is printed at the completion of the associated message.

Table M7.7.1 STOP Codes Utilized in Material Information Processor

STOP NUMBER	SUBROUTINE	TRACEBACK	ASSOCIATED MESSAGE
20			see Sect. M7.7.3
200	SHORTX	No	MP-64
201	CLAPSE	No	MP-80
300	KNIGHT	Yes	MP-1
310	KNIGHT	Yes	MP-2
320	KNIGHT	Yes	MP-3
330	SETUPA	Yes	MP-4
340	MTABLE	Yes	MP-23
350	MIXTAB	Yes	MP-24
360	MIXTAB	Yes	MP-25
370	MIXTAB	Yes	MP-26
380	REORDR	No	MP-27
385	REORDR	No	MP-40
390	SETUPB	Yes	MP-19
395	IDENTS	No	MP-28
395	SLNS	No	MP-28
396	CSPARM	No	MP-45

M7.7.3 MESSAGES ASSOCIATED WITH STOP 20 IN CSAS

The following messages from subroutine library routines will result in a STOP 20 in the material information processor and CSAS.

LMP001 DA ERROR - INVALID UNIT NUMBER.
THE LOGICAL UNIT NUMBER IS _____.

This message from a subroutine library direct-access routine indicates that an invalid unit number was specified as a direct-access device. In CSAS, this message is indicative of a code error.

LMP002 DA ERROR - FORTRAN USING THIS UNIT.
THE LOGICAL UNIT NUMBER IS _____.

This message from a subroutine library direct-access routine indicates that the specified unit number is open as a sequential dataset rather than a direct-access dataset. In CSAS, this error may be caused by entering a direct-access unit number for FRD= or FWR= in MORE DATA. See Sect. M7.4.8.

LMP003 DA ERROR - DCB NOT OPEN.
THE LOGICAL UNIT NUMBER IS _____.

This message from a subroutine library direct-access routine indicates that the program attempted to read or write on a direct-access device but the data control block was not open. In CSAS this message is indicative of a code error.

LMP004 DA ERROR - UNABLE TO OPEN DCB.
THE LOGICAL UNIT NUMBER IS _____.

This message from a subroutine library direct-access routine indicates that the program is unable to open the data control block for the direct-access device. This message indicates that the job control language did not include proper specification of the above named unit.

LMP005 DA ERROR - RELATIVE BLOCK NOT IN DATA SET. RELATIVE BLOCK NUMBER IS _____.

This message from a subroutine library direct-access routine indicates that the number of direct-access blocks is too small for the problem. Increase the number of direct-access blocks in MORE DATA by entering the parameter DAB=nnn where nnn is larger. For example, if the relative block number is 201, try increasing the number of direct-access blocks to 300 or more. For CSAS25, CSAS2X, CSAS4, and CSAS4X, it may also be necessary to set NB8=nnn in the KENO parameter data. See Sect. M7.4.8 or C4.4.8, entry number 18, and Sect. F11.4.3, parameter NB8.

LMP006 DA ERROR - INVALID BLOCK LENGTH.
THE BLOCK LENGTH IS _____.

This message from a subroutine library direct-access routine indicates that the length of the direct-access blocks is invalid. A valid block length must be positive. In CSAS, this message is indicative of a code error.

LMP007 DA ERROR - DCB ALREADY OPEN.
THE LOGICAL UNIT NUMBER IS _____.

This message from a subroutine library direct-access routine indicates that the data control block for the above named unit was previously opened and not closed.

LMP008 DA ERROR - PERMANENT I/O ERROR.

This message from a subroutine library direct-access routine indicates that a permanent I/O error has occurred.

M7.7.4 UNNUMBERED MESSAGES

Occasionally the code may terminate without printing a message that can be located via the message number. Some of these messages are contained in this section.

***** END OF FILE READ ON UNIT n *****

This message is from subroutine ENFILE in the Subroutine Library. Unit n is the device from which data are being read. This message can be caused by lack of a double blank between the END for the last standard composition and the END COMP. It can also be caused by omitting the END COMP or misspelling COMP in the END COMP entry. Other causes include incomplete or missing data. A traceback accompanies this message. Correct the data and resubmit the problem. See Sect. M7.4.4 or C4.4.4 for assistance.

***** ERROR IN INPUT. CARD IMAGE PRINTED ON NEXT LINE *****
card image is printed here
ON THE ABOVE CARD, CHARACTER NUMBER m (IMAGE=c) IS NOT VALID.

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M7.A NOTES ON SOME ELEMENTARY RESONANCE SELF-SHIELDING TECHNIQUES USED IN SCALE

M7.A.1 THE NORDHEIM INTEGRAL METHOD FOR THE TWO-REGION PROBLEM

Multigroup cross-section data must be determined from the basic nuclear data in a fashion that is consistent with the way in which the data are to be used. For most processes (absorption, fission, etc.) that means averaging the actual data over the various energy groups, with the scalar flux (of a similar system) being used as a weighting function:

$$\sigma^g = \frac{\int_{E^g}^{E^{g-1}} \phi(E)\,\sigma(E)\,dE}{\int_{E^g}^{E^{g-1}} \phi(E)\,dE}. \qquad \text{(M7.A.1)}$$

Even though slightly different expressions might be used for the transport cross section and/or the group-to-group scattering terms,[11] it is still necessary to determine the flux spectrum. In the resonance range $\phi(E)$ and $\sigma(E)$ may both vary dramatically, and this weighting, referred to as "resonance self-shielding," is most important.

To determine $\phi(E)$, it is convenient to write an expression for the collision density at energy E in terms of the scattering density at all higher energies. For energies in the resonance region, virtually all of the slowing-down source is due to elastic scattering. Thus, neutrons of energy E′ may scatter down to α', and the probability of a neutron at energy E′ scattering down to some energy within dE about E is given by

$$P(E' \to E)dE = \left(\frac{1}{1-\alpha}\right)\left(\frac{1}{E'}\right) dE, \qquad \text{(M7.A.2)}$$

where

$$\alpha = \left(\frac{A-1}{A+1}\right)^2. \qquad \text{(M7.A.3)}$$

For simplicity, let us now consider a two-zone problem with a single nuclide in each zone. In the Nordheim method,[3] the flux in the fuel $\phi_F(E)$ and the flux in the moderator $\phi_M(E)$ are assumed to be spatially flat over their respective regions. Gross spatial effects are accounted for by allowing $P^{\circ}_{F\to M}(E)$ to represent the probability that a neutron of energy E escapes from the fuel without a collision, while $1 - P^{\circ}_{F\to M}(E)$ represents the probability that the neutron has its next interaction within the fuel. If V_F and V_M represent the volume of the fuel and moderator regions, then the total collision rate in each region is given by[12]

$$V_F\Sigma_{tF}(E)\phi_F(E) = V_F[1 - P^{\circ}_{F\to M}(E)]\int_E^{E/\alpha_F} \phi_F(E')\Sigma_{sF}(E')\left(\frac{1}{1-\alpha_F}\right)\left(\frac{1}{E'}\right)dE'$$

$$+ V_M P^{\circ}_{M\to F}(E)\int_E^{E/\alpha_M} \phi_M(E')\Sigma_{sM}(E')\left(\frac{1}{1-\alpha_M}\right)\left(\frac{1}{E'}\right)dE' \qquad \text{(M7.A.4)}$$

and

$$V_M\Sigma_{tM}(E)\phi_M(E) = V_F P^{\circ}_{F\to M}(E)\int_E^{E/\alpha_F} \phi_F(E')\Sigma_{sF}(E')\left(\frac{1}{1-\alpha_F}\right)\left(\frac{1}{E'}\right)dE'$$

$$+ V_M[1 - P^{\circ}_{M\to F}(E)]\int_E^{E/\alpha_M} \phi_M(E')\Sigma_{sM}(E')\left(\frac{1}{1-\alpha_M}\right)\left(\frac{1}{E'}\right)dE' . \qquad \text{(M7.A.5)}$$

Note that this is a coupled set of integral equations where $\phi_F(E)$ depends on $\phi_M(E)$ and vice versa. To produce self-shielded cross-section data for the fuel, one must first determine $\phi_F(E)$. Obviously, if one had additional nuclides in the fuel or moderator, one would have additional integrals whose range of integration would be defined by α_F^{25}, α_F^{28}, α_F^{oxy}, α_M^{H}, α_M^{oxy} and whose scattering density would depend on Σ_{sF}^{25}, Σ_{sF}^{28}, Σ_{sF}^{oxy}, Σ_{sM}^{H}, Σ_{sM}^{oxy}. Non-resonance nuclides inside the fuel are frequently referred to as "internal moderators," and all nuclides in the moderator region are frequently referred to as "external moderators." In the Nordheim method, the external moderators are accounted for only implicitly, as described below.

Before considering the detailed solution of Eqs. (M7.A.4) and (M7.A.5), it is convenient to note that the asymptotic solutions [i.e., the fluxes $\phi_F(E)$ and $\phi_M(E)$ in the absence of absorption] are identical. By direct substitution, it can be shown that

$$\phi_F^{\infty} = \phi_M^{\infty} = \frac{1}{\xi\Sigma_s E}, \qquad \text{(M7.A.6)}$$

where

$$\xi\Sigma_s \equiv \frac{1}{V}(\xi_F\Sigma_{sF}V_F + \xi_M\Sigma_{sM}V_M) \approx \text{constant} \qquad \text{(M7.A.7)}$$

and δ is defined as the average increase in lethargy per collision.[12] In the asymptotic range far from resonances, Σ_{sF} is simply the potential scattering cross section, Σ_{pF}.

Armed with knowledge of the asymptotic solution, it is then possible to invoke the Narrow Resonance (NR) approximation *for the external moderator*, and eliminate the integral(s) over $\phi_M(E)$ in Eq. (M7.A.4).

If the average energy loss in an elastic collision with the moderator [$1/2\ (1-\alpha)E_{res}$] is much larger than the practical width of the resonance (Γ_p), then it is very unlikely that a neutron will have a second collision within the resonance. Under these conditions, the contribution to $\Sigma_{tF}(E)\phi_F(E)$ due to the integration of $\phi_M(E')\Sigma_{sM}(E')$ over the narrow energy range associated with the resonance will be negligible compared to the contribution due to the integration of $\phi_M(E')\Sigma_{sM}(E')$ over the rest of the range (from just above the resonance [$E' = E_2 \approx E$] to $E' = E/\alpha$). Figure M7.A.1 is an attempt to illustrate this situation. For energies E′ just above the resonance there is very little absorption, and the flux there assumes the asymptotic form:

$$\phi_M(E') = \phi_M^{\infty} = \frac{1}{\bar{\xi}\bar{\Sigma}_s E'} \qquad \text{(M7.A.8)}$$

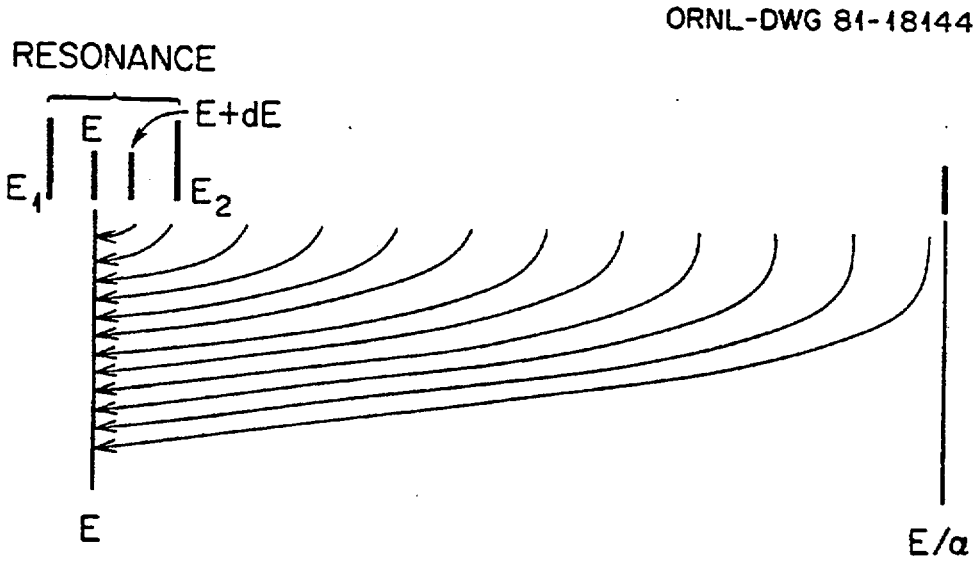

Figure M7.A.1 Elastic scattering into dE about E when E lies inside a narrow resonance

Substituting this expression in Eq. (M7.A.4) effectively decouples it from Eq. (M7.A.5). More precisely, the expression

$$\int_{E}^{E/\alpha_M} \phi_M(E')\Sigma_{sM}(E')\left(\frac{1}{1-\alpha_M}\right)\left(\frac{1}{E'}\right)dE'$$

$$= \int_{E}^{E_2=E+\epsilon} [\quad]dE' + \int_{E_2=E+\epsilon}^{E/\alpha_M} \frac{1}{\xi\Sigma_s E'}\Sigma_{sM}(E')\left(\frac{1}{1-\alpha_M}\right)\left(\frac{1}{E'}\right)dE'$$

0 (first integral) ; constant (second integral)

$$= \left(\frac{\Sigma_{sM}}{\xi\Sigma_s}\right)\left(\frac{1}{1-\alpha_M}\right)\int_{E}^{E/\alpha_M}\frac{1}{x^2}dx = \left(\frac{\Sigma_{sM}}{\xi\Sigma_s}\right)\left(\frac{1}{E}\right) \qquad \text{(M7.A.9)}$$

is substituted in Eq. (M7.A.4) to yield

$$V_F\Sigma_{tF}(E)\phi_F(E) = V_F[1-P^{o}_{F\to M}(E)]\int_{E}^{E/\alpha_F}\phi_F(E')\Sigma_{sF}(E')\left(\frac{1}{1-\alpha_F}\right)\left(\frac{1}{E'}\right)dE'$$

$$+ V_M P^{o}_{M\to F}(E)\left(\frac{\Sigma_{sM}}{\xi\Sigma_s}\right)\left(\frac{1}{E}\right) . \qquad \text{(M7.A.10)}$$

When the fuel and moderator fluxes are assumed to be flat, it can be shown using the reciprocity theorem that $P^{o}_{F\to M}(E)$ and $P^{o}_{M\to F}(E)$ are related by the equation

$$V_M P^{o}_{M\to F}(E)\Sigma_{sM}(E) = V_F P^{o}_{F\to M}(E)\Sigma_{tF}(E) . \qquad \text{(M7.A.11)}$$

Substituting this expression into Eq. (M7.A.10) yields

$$\Sigma_{tF}(E)\phi_F(E) = [1 - P^{o}_{F\to M}(E)]\int_{E}^{E/\alpha_F}\phi_F(E')\Sigma_{sF}(E')\left(\frac{1}{1-\alpha_F}\right)\left(\frac{1}{E'}\right)dE'$$

This integral equation for the flux, $\phi_F(E)$, is the basis of the Nordheim method. Note that the (1/E) slowing down source coming from the external moderator is represented by a single term on the right-hand side of

$$+ \frac{P^{\circ}_{F\text{-}M}(E)\Sigma_{tF}(E)}{\bar{\xi}\bar{\Sigma}_s E} \quad . \qquad \text{(M7.A.12)}$$

Eq. (M7.A.12). Internal moderators (such as the oxygen in UO_2) may be accounted for by including additional integrals whose range of integration would be defined by α_F^{25}, α_F^{28}, α_F^{oxy}, etc. The Nordheim method as implemented in the NITAWL code allows up to three such integrals – one for the absorber and two for "internal moderators." To solve the Nordheim integral equation, NITAWL expands the integral in a three-point formula corresponding to Simpson's Rule and then marches from the highest to the lowest energy, developing numerical values for the energy-dependent flux and collision density as it goes. For computational efficiency, NITAWL does not carry out this process over all energy but instead it (1) assumes the resonances are well isolated, (2) uses the asymptotic solution for the flux between resonances, and (3) assumes the asymptotic value for the flux [$\phi^{\infty} = 1/(\bar{\xi}\bar{\Sigma}_s E)$] at the upper end of each resonance.

In the interest of clarity, it must be pointed out that the flux spectrum in an isolated fuel lump [$\phi_F(E)$] is independent of the material properties of the surrounding moderator and that the NITAWL code does, in fact, solve Eq. (M7.A.12) without knowledge of the properties of the surrounding moderator. At first glance, this may appear to be contradictory since the term

$$\bar{\xi}\bar{\Sigma}_s \equiv \frac{1}{V}(\xi_F\Sigma_{sF}V_F + \xi_M\Sigma_{sM}V_M) \approx \text{constant} \qquad \text{(M7.A.13)}$$

appears explicitly in the Nordheim integral equation for the flux [cf. Eq. (M7.A.12)]. That equation, you will recall, gives the collision density at energy E[$\Sigma_{tF}(E)\phi_F(E)$] in terms of the flux at all higher energies [$\phi_F(E')$]. For energies (E) near the upper end of the highest energy resonance, the flux term appearing in the integrand will correspond to the asymptotic flux given by

$$\phi_F(E') = \phi_F^{\infty}(E') = \left(\frac{1}{\bar{\xi}\bar{\Sigma}_s E'}\right) . \qquad \text{(M7.A.14)}$$

Since the constant $\xi\Sigma_s$ appears in *both* terms on the right-hand side of Eq. (M7.A.12), the flux at all lower energies [$\phi_F(E)$] will be directly proportional to ($1/\xi\Sigma_s$). That constant will, of course, cancel out when the flux [$\phi_F(E)$] is used in Eq. (M7.A.1) to obtain the group-averaged cross sections. The Nordheim integral equation solved by NITAWL is, therefore, frequently written as

$$\Sigma_{tF}(E)\phi_F(E) = [1 - P^{o}_{F\to M}(E)]\int_{E}^{E/\alpha_F} \phi_F(E')\Sigma_{sF}(E')\left(\frac{1}{1-\alpha_F}\right)\left(\frac{1}{E'}\right) dE'$$

$$+ \left(\frac{1}{E}\right) P^{o}_{F\to M}(E)\Sigma_{tF}(E) \qquad \text{(M7.A.15)}$$

with the initial condition written as simply

$$\phi_F(E') \equiv \left(\frac{1}{E'}\right) \text{ at } E' > E^{max}_{res} . \qquad \text{(M7.A.16)}$$

In systems having multiple fuel lumps, the material properties of the external moderator will become important only to the extent that they affect the transmission probability through the moderator (i.e., the Dancoff factor, C) and the "effective" escape probability for a typical fuel lump, $P_{F\to M}(E)$. See Sect. M7.A.2 for additional details.

M7.A.2 EXACT EXPRESSIONS FOR THE FIRST-FLIGHT ESCAPE PROBABILITY USED IN THE NORDHEIM INTEGRAL METHOD, AND THE ROLE OF THE DANCOFF FACTOR (C) IN LATTICECELL CALCULATIONS

Before leaving our discussion of the Nordheim method as implemented in the NITAWL code, a few words must be said about $P^{o}_{F\to M}(E)$ and how it is calculated. Obviously, if one had a single fuel lump embedded in an infinite sea of moderator, $P^{o}_{F\to M}(E)$ would simply be the first-flight escape probability for the fuel lump, $P_{FO}(E)$. Assuming a uniform source of isotropically emitted neutrons, Case, deHoffman and Placzek[13] have derived exact analytic expressions for $P_{FO}(E)$ as a function of $\Sigma_{tF}(E)$ and the characteristic lump dimension of the fuel, where

$$\bar{a} = \begin{cases} t, & t = \text{thickness of an infinite slab,} \\ r, & r = \text{radius of an infinite cylinder,} \\ r, & r = \text{radius of a sphere.} \end{cases} \qquad \text{(M7.A.17a)}$$

Letting

$$x = \bar{a}\,\Sigma_{tF}(E) \qquad \text{(M7.A.17b)}$$

these exact analytic expressions for the first-flight escape probability may be written as

$$\text{slab:}\quad P_{FO}(E) = \frac{1}{x}\left[\frac{1}{2} - E_3(x)\right] \tag{M7.A.18}$$

$$\text{cylinder:}\quad P_{FO}(E) = \frac{4}{3}(x)\{2[xK_1(x)I_1(x) + K_0(x)I_0(x) - 1] + \left(\frac{1}{x}\right)K_1(x)I_1(x) - K_0(x)I_1(x) + K_1(x)I_0(x)\} \tag{M7.A.19}$$

$$\text{sphere:}\quad P_{FO}(E) = \left(\frac{3}{8x^3}\right)[2x^2 - 1 + (1 + 2x)e^{-2x}]\ . \tag{M7.A.20}$$

Tables of these functions are given in ref. 13. These tables, along with appropriate interpolation schemes, have also been incorporated in the NITAWL code.

In the derivation of Eq. (M7.A.12), $P^{\circ}_{F\to M}(E)$ was taken to represent the probability that a neutron born in the fuel will have its next collision in the moderator. In the usual situation where one has a lattice of fuel pins, this probability is not the same as the escape probability from a single fuel rod since some of the escaping neutrons may pass through the moderator without a collision and be absorbed in the next fuel lump or succeeding fuel lumps. Figure M7.A.2 shows the probability that a neutron escaping from a single fuel lump will enter and leave each succeeding fuel lump. It also shows the probability that a neutron escaping from a single fuel lump will experience a collision in each of the succeeding moderator regions. Using C to represent the free-flight transmission probability through the moderator and P_t to represent the free-flight transmission probability through the fuel:

$$P^{\circ}_{F\to M}(E) = P_{FO}(1-C)\left[1 + CP_t + C^2P_t^2 + ...\right] \tag{M7.A.21}$$

and

$$P^{\circ}_{F\to M}(E) = P_{FO}(1-C)\left(\frac{1}{1-CP_t}\right)\ . \tag{M7.A.22}$$

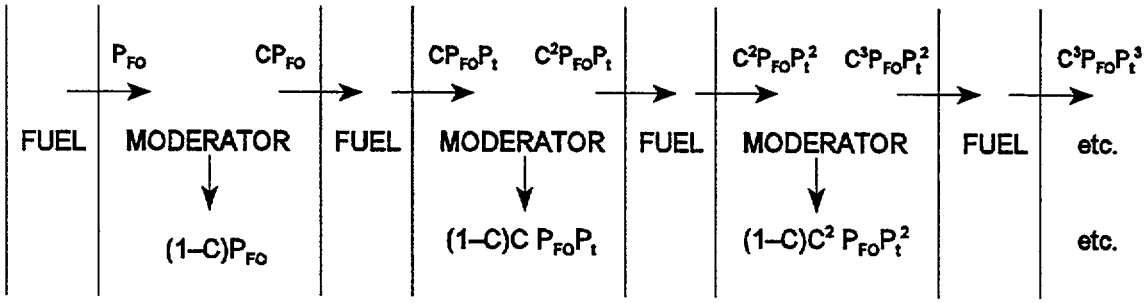

Figure M7.A.2 Transmission of an uncollided neutron through a lattice

The traditional form of Eq. (M7.A.22) is obtained by writing the transmission probability for the fuel lump, P_t, in terms of the escape probability, P_{FO}. To obtain the approximate relationship typically used, consider a monodirectional beam of neutrons impingent on a slab of thickness ℓ. The free-flight transmission probability is simply $P_t = e^{-\ell\Sigma_t}$. Now consider a monodirectional source of neutrons (S) uniformly distributed throughout the slab. The average free-flight escape probability, P_{FO} is then given by

$$P_{FO} = \frac{\int_o^\ell S\, e^{-x\Sigma_t} dx}{\int_o^\ell S\, dx} = \frac{1 - e^{-\ell\Sigma_t}}{\ell\Sigma_t} . \qquad \text{(M7.A.23)}$$

Rearranging terms, we have

$$\Rightarrow e^{-\ell\Sigma_t} = 1 - \ell\Sigma_t P_{FO} . \qquad \text{(M7.A.24)}$$

$$\Rightarrow P_t = 1 - \ell\Sigma_t P_{FO} . \qquad \text{(M7.A.25)}$$

Even though this relationship is strictly valid only for a monodirectional source, a reasonable first-order approximation for other cases may be obtained by setting ℓ equal to $\bar{\ell}$, the mean chord length through the fuel lump. The mean chord length is estimated as $4*V_F/S_F$ as well. Plugging Eq. (M7.A.25) into Eq. (M7.A.22) yields the standard approximation for $P^o_{F\to M}(E)$:

$$P^o_{F\to M}(E) = P_{FO}\left[\frac{1 - C}{1 - (1 - \bar{\ell}\Sigma_{tF}P_{FO})C}\right] \qquad \text{(M7.A.26)}$$

where P_{FO} and Σ_{tF} are energy-dependent [$P_{FO}(E)$ and $\Sigma_{tF}(E)$] and where C, the free-flight transmission probability through the moderator (also known as the Dancoff factor), depends only on the dimensions and the (relatively constant) cross section for the moderator. Approximations for the Dancoff factor in various types of lattice-cell arrangements are described in Sect. M7.2.4. Equations (M7.A.18–20) are thus used in conjunction with Eq. (M7.A.26) when solving the Nordheim integral equation for the flux.

M7.A.3 APPROXIMATE EXPRESSIONS FOR THE FIRST-FLIGHT ESCAPE PROBABILITY, THE DEFINITION OF THE ESCAPE CROSS SECTIONS, AND THE RELATIONSHIP BETWEEN THE TWO QUANTITIES

Before developing an expression for the flux based on the NR approximation and showing how that might be used to determine self-shielding factors for use in the Bondarenko method, it is convenient to make a few additional remarks concerning the first-flight escape probability.

From Eq. (M7.A.23), it is apparent that

$$P_{FO}(E) \rightarrow \frac{1}{\bar{\ell}\Sigma_{tF}(E)}, \quad \bar{\ell}\Sigma_{tF}(E) >> 1 \tag{M7.A.27}$$

whenever the fuel lump is very large or very black. While less obvious, it can be shown that Eqs. (M7.A.18–20) obey the same limit. On the other hand, $P_{FO}(E) \rightarrow 1$ whenever the fuel lump is very small. One convenient expression which fits both end-points is Wigner's rational approximation:

$$P_{FO}(E) \doteq \frac{1}{1 + \bar{\ell}\Sigma_{tF}(E)} . \tag{M7.A.28}$$

Substituting this expression into Eq. (M7.A.26) and performing a small amount of algebra yields:

$$P^{o}_{F\rightarrow M}(E) \doteq \frac{1}{1 + \left(\frac{\bar{\ell}}{1-C}\right)\Sigma_{tF}(E)} . \tag{M7.A.29}$$

Physically this says that the effect of the additional fuel in the lattice is the same as increasing the size of a single equivalent fuel rod.

As shown in Fig. M7.A.3, Wigner's rational approximation for $P_{FO}(E)$ fits the exact results given by Eqs. (M7.A.18–20) fairly well.

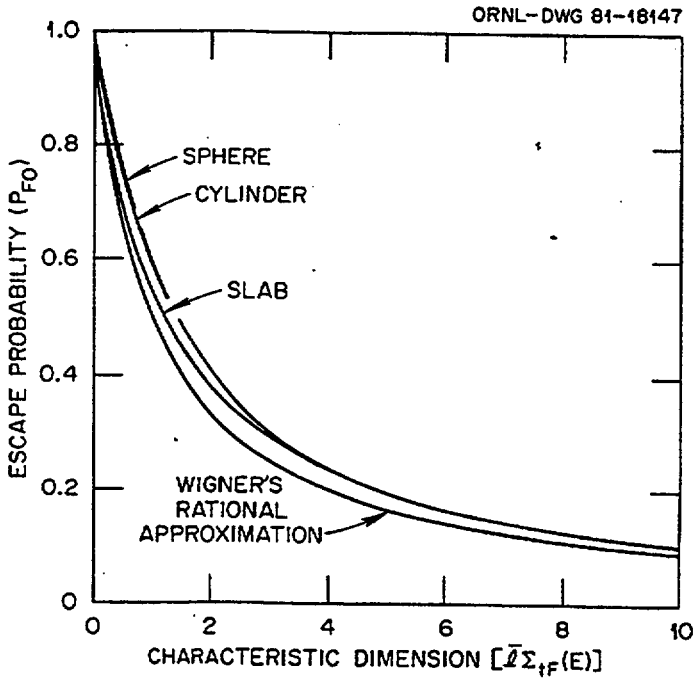

Figure M7.A.3 The escape probability (P_{FO}) and Wigner's rational approximation, as functions of the characteristic dimension [$\ell\Sigma_{tF}(E)$]

Others, in an attempt to improve the Wigner rational approximation, have suggested alternate forms such as

$$P_{FO}(E) \doteq \frac{1}{1 + a\bar{\ell}\Sigma_{tF}(E)} \qquad \text{(M7.A.30)}$$

where "a" is a fitted parameter between 0 and 1 which may be a constant, or a weak function of $\bar{\ell}\,\Sigma_{tF}(E)$. Substituting this expression in Eq. (M7.A.26) yields

$$P^{o}_{F\to M}(E) = \frac{1}{1+a\left(\frac{\bar{\ell}}{1-C}\right)\Sigma_{tF}(E)}$$

$$= \frac{N_F\left(\frac{1-C}{N_F a\bar{\ell}}\right)}{N_F\left(\frac{1-C}{N_F a\bar{\ell}}\right) + N_F\sigma_{tF}(E)} = \frac{\sigma_{esc}}{\sigma_{esc} + \sigma_{tF}(E)} \qquad \text{(M7.A.31)}$$

where σ_{esc} is a constant, or a very weak, function of $\bar{\ell}\,\Sigma_{tF}(E)$. Otter[14] has carefully fitted the modified Wigner approximation [cf. Eq. (M7.A.30)] to the exact results given by Eqs. (M7.A.18–20). He claims that using

$$a = C + \frac{1-C}{A} \qquad \text{(M7.A.32)}$$

[where A is a slowly varying function of $\bar{\ell}\,\Sigma_{tF}(E)$ as given in Table M7.A.1] will reproduce the exact escape probabilities to within ~0.5%. Substituting Eq. (M7.A.32) into the expression for the escape cross-section yields

$$\sigma_{esc} = \left(\frac{1}{N_F}\right)\left(\frac{1-C}{\bar{\ell}}\right)\left(\frac{A}{1+(A-1)C}\right) \qquad \text{(M7.A.33)}$$

To account for the fact that A is a very slowly varying function of $\bar{\ell}\,\Sigma_{tF}(E)$, one typically uses the infinitely dilute group-averaged value, $\Sigma^{g,\infty}_{tF}$, to define a group-dependent escape cross section σ^{g}_{esc}. Hence,

$$P^{o}_{F\to M}(E) = \frac{\sigma^{g}_{esc}}{\sigma^{g}_{esc} + \sigma_{tF}(E)} \qquad \text{(M7.A.34)}$$

where σ^{g}_{esc} is taken to be constant within any given energy group.

Table M7.A.1 Recommended "A" factors used in the modified Wigner approximation[a,b]

Range	Function	Max. error in $P_{FO}(E)$
Plane	$A = 4/(1.61593 - \ell n(\Sigma\ell)) - \Sigma\ell - 0.225\,(\Sigma\ell)^2$	0.4%
$0 \le \Sigma\ell \le 1.36$	$A = 1 + 1.2978(\Sigma\ell)^{-1} - 1.8241(\Sigma\ell)^{-2}$	0.75%
$1.36 < \Sigma\ell \le \infty$	$+ 0.75275(\Sigma\ell)^{-3}$	
Infinite Cylinder		
$0 \le \Sigma\ell < 2$	$A = 1.5013 + 0.14879(\Sigma\ell)^{1/2} - 0.17226\,\Sigma\ell$	0.5%
$2 \le \Sigma\ell \le \infty$	$A = 1 + (\Sigma\ell)^{-1} - (\Sigma\ell)^{-3}$	0.5%
Sphere		
$0 \le \Sigma\ell < 1.36$	$A = 16/9 - 0.2625\,\Sigma\ell + 0.0258(\Sigma\ell)^3$	0.2%
$1.36 \le \Sigma\ell \le \infty$	$A = 1 + 1.09(\Sigma\ell)^{-1} - 0.591(\Sigma\ell)^{-2}$	0.3%

[a]This table was taken directly from ref. 14 by J. M. Otter.
[b]For an isolated fuel lump (where $C \equiv 0$), the fitted parameter (a) used in the Modified Wigner Approximation is given by $a = 1/A$; in general, "a" is defined by Eq. (M7.A.32).

M7.A.4 THE NARROW-RESONANCE APPROXIMATION FOR THE FLUX, AS DERIVED FROM A GENERALIZED FORM OF THE NORDHEIM INTEGRAL EQUATION

For the sake of argument, let the Nordheim integral equation be written as

$$\Sigma_{tF}(E)\,\phi_F(E) + \left[1 - P^{o}_{F\to M}(E)\right] \int_E^{E/\alpha_F^{25}} \phi_F(E')\Sigma_{sF}^{25}(E')\left(\frac{1}{1-\alpha_F^{25}}\right)\left(\frac{1}{E'}\right) dE'$$

$$+ \int_E^{E/\alpha_F^{28}} \phi_F(E')\Sigma_{sF}^{28}(E')\left(\frac{1}{1-\alpha_F^{28}}\right)\left(\frac{1}{E'}\right) dE'$$

$$+ \int_E^{E/\alpha_F^{16}} \phi_F(E')\Sigma_{sF}^{16}(E')\left(\frac{1}{1-\alpha_F^{16}}\right)\left(\frac{1}{E'}\right) dE'$$

$$+ \frac{P^{o}_{F\to M}(E)\Sigma_{tF}(E)}{\bar{\xi}\bar{\Sigma}_s E} \qquad \text{(M7.A.35)}$$

where the slowing down due to the ^{235}U, ^{238}U, and oxygen have all been represented explicitly. Other nuclides present in the fuel could be represented in like fashion.

The most common way to proceed is to assume that the NR approximation applies to each of the nuclides in the fuel (^{235}U, ^{238}U, O).

If the average energy loss in an elastic collision with a particular fuel nuclide [$\frac{1}{2}(1 - \alpha_F^i)E_{res}$] is much larger than the practical width of the response (Γ_p), then it is very unlikely that a neutron will have a second collision within the resonance. Under these conditions, the contribution to $\Sigma_{tF}(E)\phi_F(E)$ due to the integration of $\phi_F(E')\,\Sigma^i_{sF}(E')$ over the narrow energy range associated with the resonance will be negligible compared to the contribution due to the integration of $\phi_F(E')\,\Sigma^i_{sF}(E')$ over the rest of the range (from just above the resonance [$E' = E_2 \approx E$] to $E' = E/\alpha$). Figure M7.A.4 is an attempt to illustrate this situation. For energies just above the resonance we will, wittingly or not, assume that there is very little absorption such that the flux there may be replaced by its asymptotic form:

$$\phi_F(E') = \phi_F^{\infty} = \frac{1}{\bar{\xi}\bar{\Sigma}_s E'} . \qquad \text{(M7.A.36)}$$

(If indeed there is very little absorption between E and E/α, then $\Sigma_{tF}(E) = \Sigma_{sF}(E)$ = *constant potential scattering cross section* at energies above the resonance. Under these conditions, direct substitution of Eq. (M7.A.36) into Eq. (M7.A.35) will show it to be the solution for any and all energies *above* the resonance). While Eq. (M7.A.8) may be valid for the flux in a nonabsorbing external moderator, Eq. (M7.A.36) is valid for the flux in the fuel only if the resonances are widely spaced. In this particular example, this "widely spaced" assumption would require that neither ^{235}U nor ^{238}U have another resonance in the range E to E/α^{25}, E to E/α^{28}, or E to E/α^{16}. While this last condition is never met and the first two are met only rarely, use of the asymptotic flux [Eq. (M7.A.36)] for energies above the resonance remains a common assumption.

Using the narrow resonance approximation (see Fig. M7.A.4) and invoking Eq. (M7.A.36) for the flux at energies just above the resonance, we may write

$$\int_E^{E/\alpha^i} \phi_F(E')\Sigma^i_{sF}(E')\left(\frac{1}{1-\alpha^i_F}\right)\left(\frac{1}{E'}\right)dE'$$

$$= \int_E^{E_2=E+\epsilon} [\ ]dE' + \int_{E_2=E+\epsilon}^{E/\alpha^i_F} \frac{1}{\bar{\xi}\bar{\Sigma}_s E'}\Sigma^i_{sF}(E')\left(\frac{1}{1-\alpha^i_F}\right)\left(\frac{1}{E'}\right)dE'$$

0 (first integral) ; constant (second integral)

$$= \left(\frac{\Sigma^i_{sF}}{\bar{\xi}\bar{\Sigma}_s}\right)\left(\frac{1}{1-\alpha^i_F}\right)\int_E^{E/\alpha^i_F}\frac{1}{x^2}dx = \left(\frac{\Sigma^i_{sF}}{\bar{\xi}\bar{\Sigma}_s}\right)\left(\frac{1}{E}\right) \qquad \text{(M7.A.37)}$$

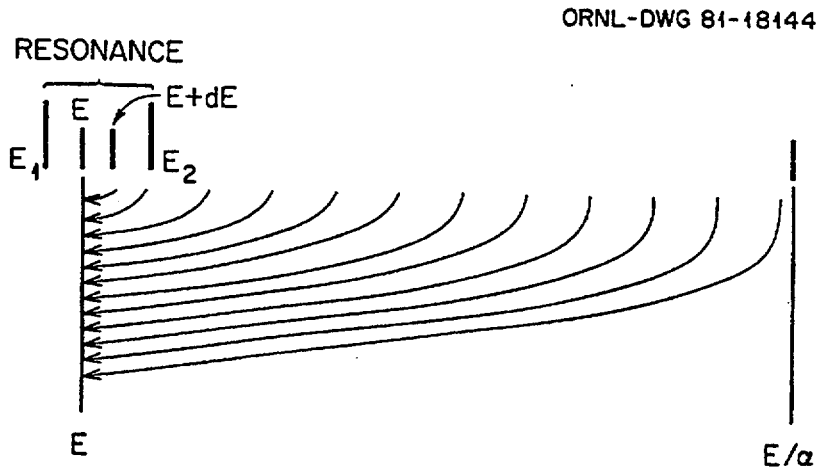

Figure M7.A.4 Elastic scattering into dE about E when E lies inside a narrow resonance

Substituting this result (for ^{235}U, ^{238}U, and O) into Eq. (M7.A.35), and recognizing that

$$1 - P^{o}_{F\to M}(E) = 1 - \left[\frac{\Sigma_{esc}}{\Sigma_{esc} + \Sigma_{tF}(E)}\right] = \frac{\Sigma_{tF}(E)}{\Sigma_{esc} + \Sigma_{tF}(E)} \qquad \text{(M7.A.38)}$$

yields

$$\Sigma_{tF}(E)\,\phi_F(E) = \left(\frac{\Sigma_{tF}(E)}{\Sigma_{esc} + \Sigma_{tF}(E)}\right)\left(\frac{\Sigma^{25}_{sF} + \Sigma^{28}_{sF} + \Sigma^{16}_{sF}}{\bar{\xi}\bar{\Sigma}_s E}\right)$$

$$+ \left(\frac{\Sigma_{esc}}{\Sigma_{esc} + \Sigma_{tF}(E)}\right)\left(\frac{\Sigma_{tF}(E)}{\bar{\xi}\bar{\Sigma}_s E}\right) \qquad \text{(M7.A.39)}$$

$$\Rightarrow \quad \phi_F(E) = \left(\frac{\Sigma_{sF} + \Sigma_{esc}}{\bar{\xi}\bar{\Sigma}_s}\right)\left(\frac{1}{\Sigma_{tF}(E) + \Sigma_{esc}}\right)\left(\frac{1}{E}\right) . \qquad \text{(M7.A.40)}$$

constant

To the extent that one has a sequence of widely spaced narrow resonances, this expression accurately described the flux underneath any given resonance and in the region between resonances. Between resonances, for example, $\Sigma_{tF}(E) = \Sigma_{sF}(E) = \Sigma_{sF}$ = *constant potential scattering cross section* and Eq. (M7.A.40) reduces to the asymptotic solution. As a result, this expression may be used for the flux over an entire energy group.

When $\phi_F(E)$ is used as a weighting function to produce group-averaged cross-section data, it appears in both the numerator and the denominator [cf. Eq. (M7.A.1)], such that the leading constant cancels and is of no consequence. For that reason, people frequently write $\phi_F(E)$ as simply

$$\phi_F(E) = \left(\frac{1}{\Sigma_{tF}(E) + \Sigma_{esc}}\right)\left(\frac{1}{E}\right) . \qquad \text{(M7.A.41)}$$

Expressing the flux as a function of lethargy [$u = \ell n(E_o/E)$], Eq. (M7.A.41) would be equivalent to saying that $\phi_F(u)$ is constant between resonances, and that $\phi_F(u)\Sigma_{tF}(u)$ is constant underneath a resonance (where Σ_{esc} = 0 for an infinite system).

M7.A.5 THE NARROW-RESONANCE/INFINITE-MASS APPROXIMATION FOR THE FLUX, AS DERIVED FROM THE NORDHEIM INTEGRAL EQUATION

Before proceeding further, it is necessary to point out that there are instances in which the NR approximation is *not* valid, that is, instances where

$$\Gamma_P << \left[\frac{1}{2}(1-\alpha_F^i)E_{res}\right] \qquad \text{(M7.A.42)}$$

is *not* true, and where Fig. M7.A.4 does *not* depict the real situation. In the present example (UO_2), the upper limit of integration (E/α_F^i) for the oxygen may lie well outside the resonance where the upper limit for the ^{235}U and ^{238}U integrals may actually lie inside the resonance. (At E = 10 eV, for example, E/α^{16} = 12.8 eV, whereas $E/\alpha^{25} = E/\alpha^{28}$ = 10.2 eV). Before showing how such situations may be handled, let us diverge for a moment to define the practical width (Γ_P) and to identify key instances where the NR approximation is not valid.

The practical width of a resonance in a given mixture (Γ_P) is defined as the difference between those energies at which the anomalous cross section given by the single-level Breit-Wigner formula is equal to the potential scattering cross section for the mixture

$$\frac{N^i\sigma_{res}}{1+\left(\frac{2}{\Gamma}\right)^2(E-E_{res})^2} = \Sigma_{pF} = N^{25}\sigma_p^{25} + N^{28}\sigma_p^{28} + N^{16}\sigma_s^{16} \qquad \text{(M7.A.43)}$$

where N^i is the number density of the resonance nuclide (^{25}N or ^{28}N) and σ_{res}, the maximum value of the anomalous cross section, is defined by

$$\sigma_{res} = 4\pi\left(\frac{2.0722\times10^5 \text{ eV barns}}{E_{res}}\right)\left(\frac{A+1}{A}\right)^2\left(\frac{g\Gamma_n}{\Gamma}\right) \qquad \text{(M7.A.44)}$$

where the resonance parameters (E_{res}, Γ, and $g\Gamma_n$) may be found in BNL-325.[15] [The natural width (Γ), of course, is defined as the difference between those energies at which the anomalous cross section is equal to half of its maximum value.] Substituting $E = E_{res} \pm (\frac{1}{2})\Gamma_P$ into Eq. (M7.A.43) and solving for Γ_P yields

$$\Gamma_P = \Gamma\sqrt{\left(\frac{N^i\sigma_{res}}{\Sigma_{pF}}\right) - 1}\,. \qquad \text{(M7.A.45)}$$

As a specific example, consider the 6.67-eV resonance in ^{238}U where Γ = 0.0275 eV and $g\Gamma_n$ = 0.00152 eV. Equation (M7.A.44) yields σ_{res} = 21760 barns. Noting that $\sigma_p^{25} \approx \sigma_p^{28} \approx$ 10 barns and that $\sigma_s^{16} \approx$ 3.8 barns yields

$$\Gamma_P = (0.0275\ \text{eV})\sqrt{\frac{21760}{10 + 2(3.8)} - 1} = 0.97\ \text{eV} . \qquad \text{(M7.A.46)}$$

Thus, Γ_P is considerably larger than Γ, making the narrow resonance criterion

$$\Gamma_P << \left[\tfrac{1}{2}(1 - \alpha_F^i)E_{res}\right] \qquad \text{(M7.A.47)}$$

even more difficult to satisfy. Generally speaking, the practical width (Γ_P) is about 10 to 30 times larger than the natural width (Γ).[12]

Using Eqs. (M7.A.44), (M7.A.45), and (M7.A.47) in conjunction with the resonance parameters found in the third edition of BNL-325, one can determine when and where the narrow resonance approximation is applicable. As might be shown by such an exercise, it is quite good for all but the very low-energy resonances. Even then, it is usually applicable for all but the heaviest nuclides where $\alpha_F^i \rightarrow 1$. Some of the more outstanding examples of where the narrow resonance approximation is not applicable would include the 21.78- and 23.43-eV resonances in ^{232}Th, the 1.79- and 10.37-eV resonances in ^{233}U, the 6.67-, the 20.9-, and the 36.8-eV resonances in ^{238}U, and the 1.056- and 20.46-eV resonances in ^{240}Pu.

As noted above, many of the heavy nuclides have broad low-energy resonances for which Eq. (M7.A.47) cannot be satisfied. In many of those cases, just the reverse is true (i.e., the average energy loss in an elastic collision with a heavy fuel nuclide is much smaller than the practical width):

$$\left[\tfrac{1}{2}(1 - \alpha_F^i)E_{res}\right] << \Gamma_P . \qquad \text{(M7.A.48)}$$

Fortunately, this type of situation occurs only with the heavy nuclides where $\alpha_F^i \rightarrow 1$, as illustrated in Fig. M7.A.5. Under such conditions, the range of integration, E to E/α_F^i, becomes so small that $E' \approx E$ over the entire range, and

$$\lim_{\alpha \rightarrow 1} \int_E^{E/\alpha} \phi_F(E')\Sigma_{sF}(E')\left(\frac{1}{1-\alpha}\right)\left(\frac{1}{E'}\right) dE'$$

$$= \phi_F(E)\Sigma_{sF}(E)\left(\frac{1}{E}\right) \lim_{\alpha \rightarrow 1}\left(\frac{1}{1-\alpha}\right)\int_E^{E/\alpha} dE'$$

$$= \phi_F(E)\Sigma_{sF}(E) \lim_{\alpha \rightarrow 1}\left(\frac{\frac{1}{\alpha} - 1}{1-\alpha}\right) = \phi_F(E)\Sigma_{sF}(E) \qquad \text{(M7.A.49)}$$

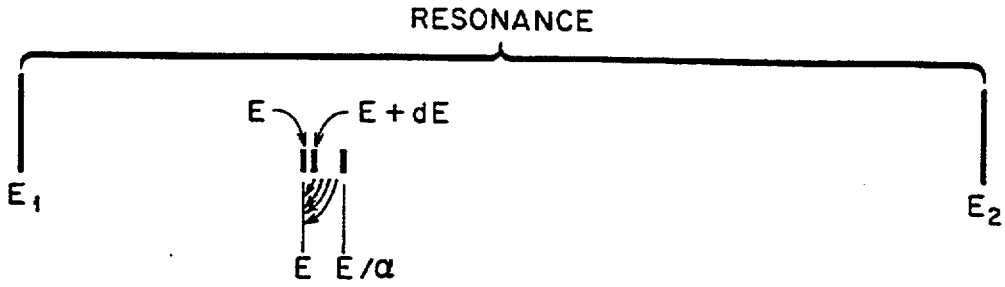

Figure M7.A.5 Elastic scattering into dE about E when E lies inside a broad resonance or $\alpha \to 1$

Alternatively, one may take $\phi_F(E')\Sigma_{sF}(E') \approx$ constant over the narrow range from E to E/α_F^i, and leave the (1/E') term inside the integral, in which case

$$\lim_{\alpha\to 1}\left(\frac{1}{1-\alpha}\right)\int_{E}^{E/\alpha}\left(\frac{1}{E'}\right)dE' = \lim_{\alpha\to 1}\frac{\ell n\left(\frac{1}{\alpha}\right)}{1-\alpha} = 1 \ . \qquad \text{(M7.A.50)}$$

Equation (M7.A.49) is commonly known as the infinite mass (IM) approximation. Substituting this expression into Eq. (M7.A.35), but retaining the narrow resonance approximation for the oxygen term, yields:

$$\Sigma_{tF}(E)\phi_F(E) = \left(\frac{\Sigma_{tF}(E)}{\Sigma_{esc}+\Sigma_{tF}(E)}\right)\left[\phi_F(E)\Sigma_{sF}^{25}(E) + \phi_F(E)\Sigma_{sF}^{28}(E) + \left(\frac{\Sigma_{sF}^{16}}{\bar{\xi}\bar{\Sigma}_s}\right)\left(\frac{1}{E}\right)\right]$$

$$+ \left(\frac{\Sigma_{esc}}{\Sigma_{esc}+\Sigma_{tF}(E)}\right)\left(\frac{\Sigma_{tF}(E)}{\bar{\xi}\bar{\Sigma}_s}\right)\left(\frac{1}{E}\right) \qquad \text{(M7.A.51)}$$

$$\Rightarrow \left[\Sigma_{esc} + \Sigma_{tF}(E) - \Sigma_{sF}^{25}(E) - \Sigma_{sF}^{28}(E)\right]\phi_F(E) = \left(\frac{\Sigma_{sF}^{16}+\Sigma_{esc}}{\bar{\xi}\bar{\Sigma}_s}\right)\left(\frac{1}{E}\right) \qquad \text{(M7.A.52)}$$

$$\Rightarrow \phi_F(E) = \left(\frac{\Sigma_{sF}^{16}+\Sigma_{esc}}{\bar{\xi}\bar{\Sigma}_s}\right)\left[\frac{1}{\Sigma_{AF}^{25}(E)+\Sigma_{AF}^{28}(E)+\Sigma_{tF}^{16}(E)+\Sigma_{esc}}\right]\left(\frac{1}{E}\right) \ . \qquad \text{(M7.A.53)}$$

constant

Except for the leading constant which cancels out when $\phi_F(E)$ is used to produce group-averaged cross-section data, this expression differs from Eq. (M7.A.40) only insofar as the denominator here contains the absorption cross section (rather than the total cross section) for the heavy nuclides in the fuel. Whereas Eq. (M7.A.40) should be used for the flux underneath a narrow resonance, Eq. (M7.A.53) should be used for the flux underneath a broad resonance. Because the narrow resonance approximation was (justifiably) retained for the oxygen term, Eq. (M7.A.53) also assumes that the resonances are widely separated relative to the average energy lost in an elastic collision with the oxygen.

M7.A.6 THEORETICAL BASIS FOR THE BASIC BONDARENKO METHOD IN THE ABSENCE OF OVERLAPPING RESONANCES

Having used the narrow resonance approximation to derive an expression for the flux which is valid underneath any given resonance and in the region between resonances [cf. Eq. (M7.A.41)] the group-averaged absorption cross section for resonance nuclide i may be written as

$$\sigma_A^{i,g} = \frac{\displaystyle\int_{E^g}^{E^{g-1}} \sigma_A^i(E)\left(\frac{1}{\Sigma_{tF}(E)+\Sigma_{esc}}\right)\left(\frac{1}{E}\right) dE}{\displaystyle\int_{E^g}^{E^{g-1}} \left(\frac{1}{\Sigma_{tF}(E)+\Sigma_{esc}}\right)\left(\frac{1}{E}\right) dE} . \qquad \text{(M7.A.54)}$$

Since $\alpha_A^i(E) \to 0$ between resonances, the numerator may be replaced by a sum of integrals over the individual resonances of nuclide i lying in group g. In the denominator, the integrand vanishes in the vicinity of a resonance such that one need only evaluate the integral between resonances where $\Sigma_{tF}(E) = \Sigma_{sF}(E) = \Sigma_{sF} =$ *constant potential scattering cross section.* Provided the resonances are very narrow compared to the width of the energy group, the original limits of integration may be retained with little error. To illustrate, consider the expression for $\sigma_A^{25,g}$ in a mixture of UO_2 where, for simplicity, we assume the ^{235}U has only two resonances in group g (cf. Fig. M7.A.6):

$$\sigma_A^{25,g} = \left[\frac{\Sigma_{sF}+\Sigma_{esc}}{\ell n(E^{g-1}/E^g)}\right] \left\{\int_{\substack{res\\ \#1}} \left(\frac{\sigma_A^{25}(E)}{\Sigma_{tF}(E)+\Sigma_{esc}}\right)\frac{dE}{E} + \int_{\substack{res\\ \#2}} \left(\frac{\sigma_A^{25}(E)}{\Sigma_{tF}(E)+\Sigma_{esc}}\right)\frac{dE}{E}\right\} \cdot \text{(M7.A.55)}$$

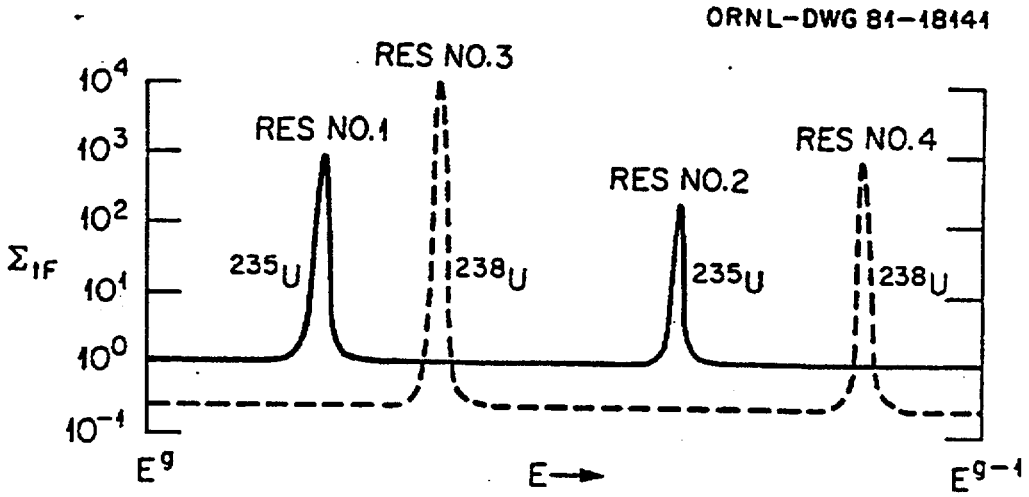

Figure M7.A.6 Well-separated resonances in a mixture of UO_2

If the resonances for the mixture are well separated (as required for the narrow resonance approximation to be valid), then $\Sigma_{tF}^{28}(E) \approx$ *constant* underneath resonance 1, and $\Sigma_{tF}^{28} \approx$ *constant* underneath resonance 2. [Indeed, under each of the ^{235}U resonances, $\Sigma_{tF}^{28}(E) = \Sigma_{sF}^{28}(E) = \Sigma_{sF}^{28}$ = *constant potential scattering cross section.*] Under each of the ^{235}U resonances, we may then write

$$\Sigma_{tF}(E) = \Sigma_{tF}^{25}(E) + \Sigma_{tF}^{28}(E) + \Sigma_{tF}^{16}(E) = \Sigma_{tF}^{25}(E) + \Sigma_{sF}^{28} + \Sigma_{sF}^{16} \qquad \text{(M7.A.56)}$$

or, more generally,

$$\Sigma_{tF}(E) = \Sigma_{tF}^{i}(E) + \Sigma_{sF} - \Sigma_{sF}^{i} \, . \qquad \text{(M7.A.57)}$$

Substituting Eq. (M7.A.57) into each term of Eq. (M7.A.55) (and again noting that $\sigma_A^i(E) \to 0$ between resonances) allows us to recombine the integrals as:

$$\sigma_A^{i,g} = \left[\frac{\Sigma_{sF} + \Sigma_{esc}}{\ell n(E^{g-1}/E^{g})}\right] \int_{E^{g}}^{E^{g-1}} \left[\frac{\sigma_A^i(E)}{\Sigma_{tF}^i(E) + (\Sigma_{sF} - \Sigma_{sF}^i + \Sigma_{esc})}\right] \frac{dE}{E} \, . \qquad \text{(M7.A.58)}$$

If the concentration of the resonance nuclide (N^i) is so small that

$$\Sigma_{tF}^{i}(E) << \Sigma_{sF} + \Sigma_{esc} \quad \text{at} \quad E = E_{res} \qquad \text{(M7.A.59)}$$

then Eq. (M7.A.58) yields the "infinitely dilute" cross section, $\sigma_A^{i,g}(\infty)$:

$$\sigma_A^{i,g}(\infty) = \frac{1}{\ell n(E^{g-1}/E^{g})} \int_{E^{g}}^{E^{g-1}} \sigma_A^i(E) \frac{dE}{E} = \frac{1}{\Delta u_g} \left\langle \sigma_A^i(u) \right\rangle \qquad \text{(M7.A.60)}$$

where $u = \ell n(E_0/E)$, and $\langle\rangle$ designates the integral over lethargy. If the resonance nuclide is not infinitely dilute, its very presence affects the way the group-averaged value should be calculated [cf. Eq. (M7.A.58)]. Defining σ_o^i as a constant "background" cross section which is independent of energy,

$$\sigma_o^i = \left(\frac{1}{N^i} \right) \left(\Sigma_{sF} - \Sigma_{sF}^i + \Sigma_{esc} \right) = \text{constant} \qquad \text{(M7.A.61)}$$

and substituting this into Eq. (M7.A.58) allows the group-averaged value of the absorption cross section to be written as

$$\sigma_A^{i,g} = \left[\frac{\sigma_{sF}^i + \sigma_o^i}{\ell n(E^{g-1}/E^{g})} \right] \int_{E^{g}}^{E^{g-1}} \left[\frac{\sigma_A^i(E)}{\sigma_{tF}^i(E) + \sigma_o^i} \right] \frac{dE}{E} . \qquad \text{(M7.A.62)}$$

The point to be made is that the self-shielded, group-averaged cross sections for a resonance nuclide can be tabulated as a function of a single variable (σ_o^i), even though that nuclide may be in a mixture with other nuclides. Indeed, extensive tables of these group-averaged values do exist for various group structures. Knowing the composition of a given mixture, the user may calculate σ_o^i and then go to the appropriate table to find the self-shielded group-averaged value of $\sigma_A^{i,g}$ for that particular mixture.

The procedure described above forms the basis of the Bondarenko method which is described in more detail below. The approach, however, is certainly not new. Users of the KENO 16-group cross-section library[16] will recall, for example, that it contains over 55 different sets of data for ^{238}U — each based on a different value of σ_o (ranging from $\sigma_o = 12$ barns to $\sigma_o = 100{,}000$ barns). After calculating σ_o^i for the mixture at hand, one would then have to specify the ID number for the appropriate set of data.

The use of precalculated self-shielded cross-section data tabulated as a function of σ_o has also proved to be an attractive alternative to the Nordheim integral method when performing space-time depletion analyses for certain types of reactors (LMFBR's in particular). Even though relatively inexpensive depletion calculations may be performed on a zone-averaged basis using ultra-fine time steps, it is periodically necessary to use the updated number densities to recalculate the power distribution throughout the core and blanket. Prior to performing the spatial flux calculation, it is desirable to produce new self-shielded cross-section data for each zone. The Bondarenko method described above provides a very fast (and therefore very attractive) alternative to solving the Nordheim integral equation on a point-wise basis in energy for each of the (many) spatial zones.

While the self-shielded group-averaged cross-section data for a given resonance nuclide may be tabulated as a function of the background cross section, $\sigma_A^{i,g}$ is usually expressed as the infinitely dilute value times a self-shielding factor:

$$\sigma_A^{i,g} = f_A^{i,g}(T,\sigma_o)\sigma_A^{i,g}(\infty) \qquad \text{(M7.A.63)}$$

where the form of the f-factor (or "Bondarenko factor") may be deduced by dividing Eq. (M7.A.62) by Eq. (M7.A.60). The explicit appearance of temperature in the self-shielding factor is in recognition of the fact that the cross sections in Eq. (M7.A.62) [$\sigma_A^i(E)$ and $\sigma_{tF}^i(E)$] should be Doppler broadened to the appropriate temperature. In his 1964 book on the subject,[2] Bondarenko has compiled extensive tables of various self-shielding factors [$f_A^{i,g}(T,\sigma_o)$, $f_C^{i,g}(T,\sigma_o)$, $f_F^{i,g}(T,\sigma_o)$, $f_T^{i,g}(T,\sigma_o)$, $f_{\ell\ell}^{i,g}(T,\sigma_o)$, etc.] for most of the important resonance nuclides. In that particular work, 25 fast or epithermal groups were used in conjunction with one thermal (sink) group. A more complete discussion of these resonance self-shielding factors will be presented after some additional comments have been made regarding the limitations of the basic method and the evolution of the "Iterative Bondarenko Method" used in most current computer codes.

M7.A.7 THE EFFECT OF RESONANCE OVERLAP ON THE GROUP-AVERAGED CROSS SECTIONS

The procedure wherein one uses the potential scattering cross section of the various nuclides to calculate the background cross section (σ_o) for the mixture, and then applies the appropriate f-factor to obtain the self-shielded group-averaged cross section for the resonance nuclide of interest, might be described as the "Non-Iterative Bondarenko Method." Whereas, Eq. (M7.A.54) or Eq. (M7.A.55) show $\sigma_A^{i,g}$ to be dependent on both the number density and the energy-dependent cross section of all other nuclides in the fuel, the assumption that the resonances were "well separated" allowed $\sigma_A^{i,g}$ (or $f_A^{i,g}$) to be tabulated as a function of a single variable, σ_o^i. The effect of that assumption may be seen by writing Eqs. (M7.A.55) and (M7.A.58) in a similar format and comparing the results in a more realistic case where some resonance overlap is possible. Equation (M7.A.55), which uses the narrow resonance approximation for the flux, may be written as

$$\sigma_A^{25,g}\Big|_{\substack{\text{as in}\\ \text{Eq. M7.A.55}}} = \left[\frac{\Sigma_{sF}+\Sigma_{esc}}{\ell n\left(\frac{E^{g-1}}{E^g}\right)}\right]\int_{E^g}^{E^{g-1}} \frac{\sigma_A^{25}(E)}{\Sigma_{tF}^{25}(E)+\Sigma_{tF}^{28}(E)+\Sigma_{tF}^{16}+\Sigma_{esc}}\,\frac{dE}{E}\,. \qquad \text{(M7.A.64)}$$

Equation (M7.A.58), which further assumes that the resonances are "well separated," may be written as

$$\sigma_A^{25,g}\Big|_{\substack{\text{as in}\\ \text{Eq. M7.A.55}}} \doteq \left[\frac{\Sigma_{sF}+\Sigma_{esc}}{\ell n\left(\frac{E^{g-1}}{E^g}\right)}\right]\int_{E^g}^{E^{g-1}} \frac{\sigma_A^{25}(E)}{\Sigma_{tF}^{25}(E)+\Sigma_{sF}^{28}+\Sigma_{sF}^{16}+\Sigma_{esc}}\,\frac{dE}{E}\,. \qquad \text{(M7.A.65)}$$

In the case where the resonances are well separated, we have shown these equations to yield the same result. To qualitatively illustrate the effect of resonance overlap, consider the extreme case depicted in Fig. M7.A.7 where one resonance of nuclide A directly overlaps another resonance of nuclide B. In this case, $\Sigma_{sF}^{28} << \Sigma_{tF}^{28}(E)$ underneath the ^{235}U resonance and the subsequent use of the potential scattering cross section

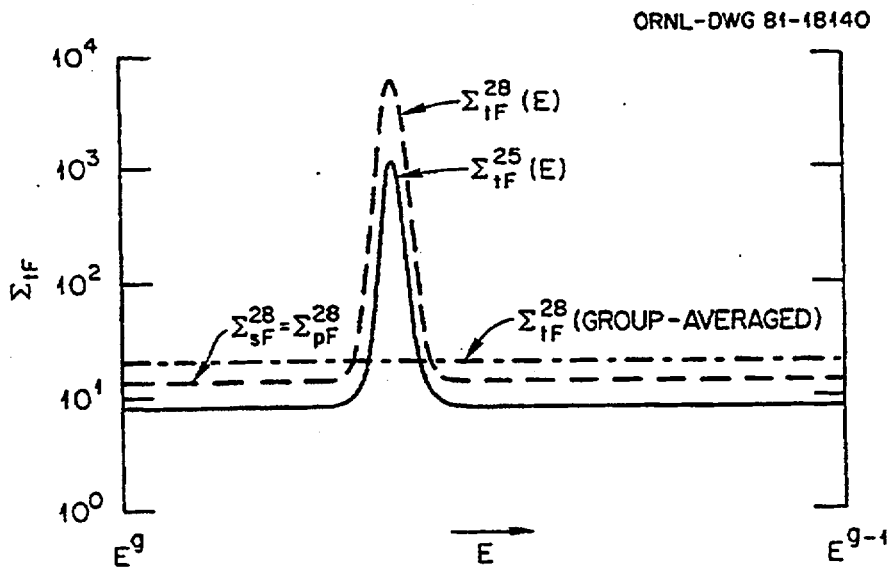

Figure M7.A.7 Hypothetical case of resonance overlap in UO_2

(Σ_{sF}^{28}) in Eq. (M7.A.65) will cause it to overestimate $\sigma_A^{25,g}$. Moreover, such a procedure will overestimate $\sigma_A^{i,g}$, $\sigma_F^{i,g}$, $\sigma_s^{i,g}$, etc., whenever the resonances of one nuclide overlap the resonances of another.* Figures (M7.A.8a–d) illustrate a few classic examples of resonance overlap in some common fuel mixtures. With the fissile isotopes, the reactivity effect of overestimating $\sigma_A^{i,g}$ is partially offset by the fact that $\sigma_F^{i,g}$ is also overestimated. Fertile isotopes on the other hand do not fission at resonance energies, and the effect of overestimating $\sigma_A^{i,g}$ can be fairly serious. (More will be said of this later.) From this example, it is also clear that such resonance overlap effects will be more important in concentrated systems where

$$\Sigma_{tF}(E)\Big|_{\substack{\text{resonance}\\ \text{nuclides}}} \quad \Sigma_{esc} + \Sigma_{tF}\Big|_{\substack{\text{nonresonance}\\ \text{nuclides}}} \qquad \text{(M7.A.66)}$$

(i.e., where σ_o^i is small), and less important in dilute systems (where σ_o^i is large). As a final point, we parenthetically note that the above conclusions were based on the NR approximation for the flux, but that one could have started with the NRIM approximation for the flux [cf. Eq. (M7.A.53)] and arrived at the same conclusions.

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*Whereas ^{235}U and ^{238}U have overlapping (or partially overlapping) resonances only at 21 and 6.4 eV, ^{235}U ^{238}U ^{239}Pu systems have a number of overlapping resonances (cf. 6.4, 12, 15, 21, 66, 75, 102, 165, 190, and 275 eV, etc.). Also, ^{232}Th ^{233}U ^{235}U ^{238}U systems, typical of advanced thorium converters, have a number of overlapping resonances (cf. 3.6, 6.4, 16, 19, 21, 23.5, 37, and 462 eV, etc.). Likewise, ^{235}U ^{238}U ^{239}Pu ^{240}Pu ^{241}Pu ^{242}Pu systems typical of LMFBRs have a larger number of overlapping resonances (cf. 0.28, 6.4, 8.8, 14.5, 18, 21, 26, 42, 66, 75, 92, 103, and 275 eV, etc.).

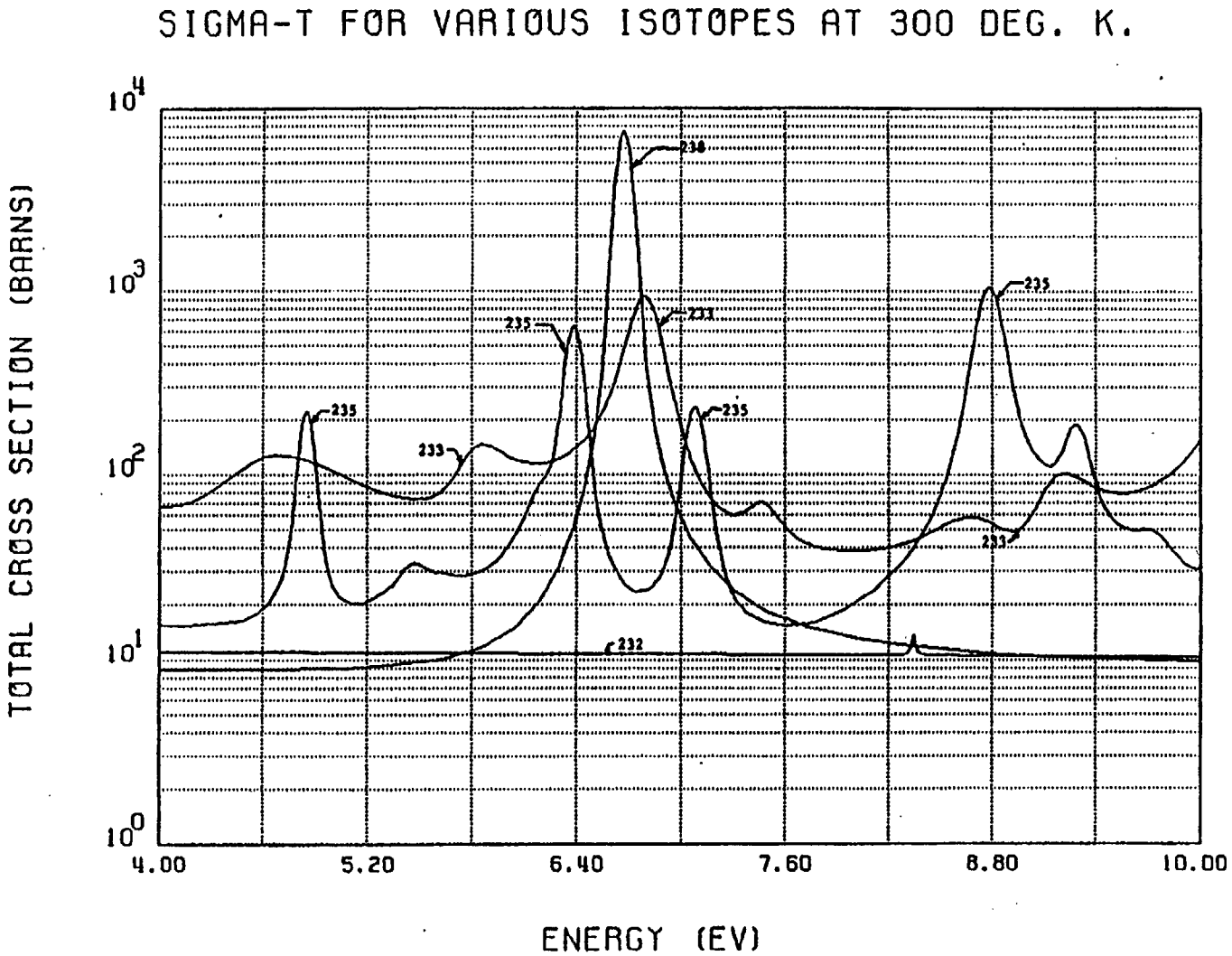

Figure M7.A.8a Resonance overlap for ^{232}Th, ^{233}U, and ^{238}U in the 4- to 10-eV energy range

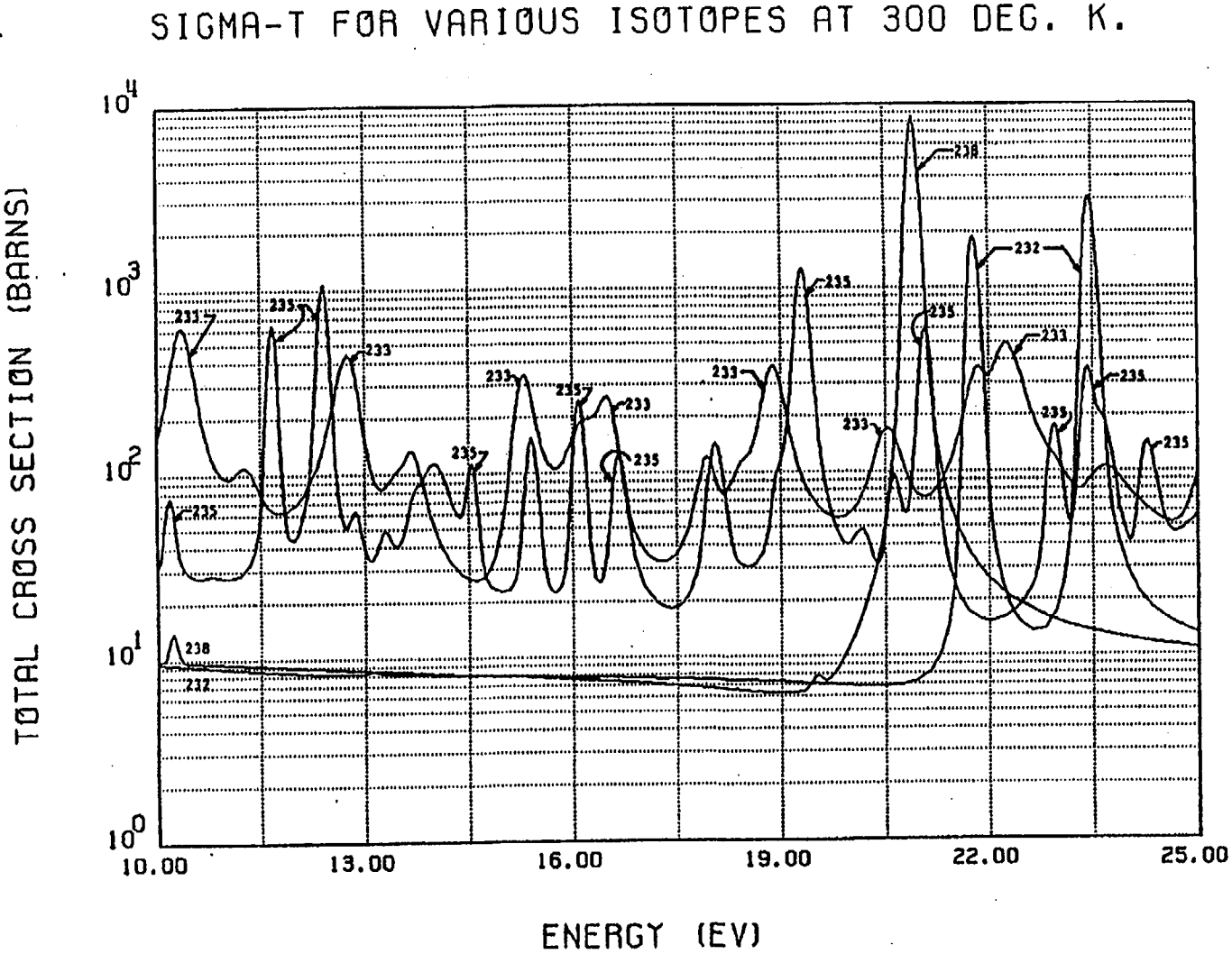

Figure M7.A.8b Resonance overlap for ^{232}Th, ^{232}U, ^{235}U, and ^{238}U in the 10- to 25-eV energy range

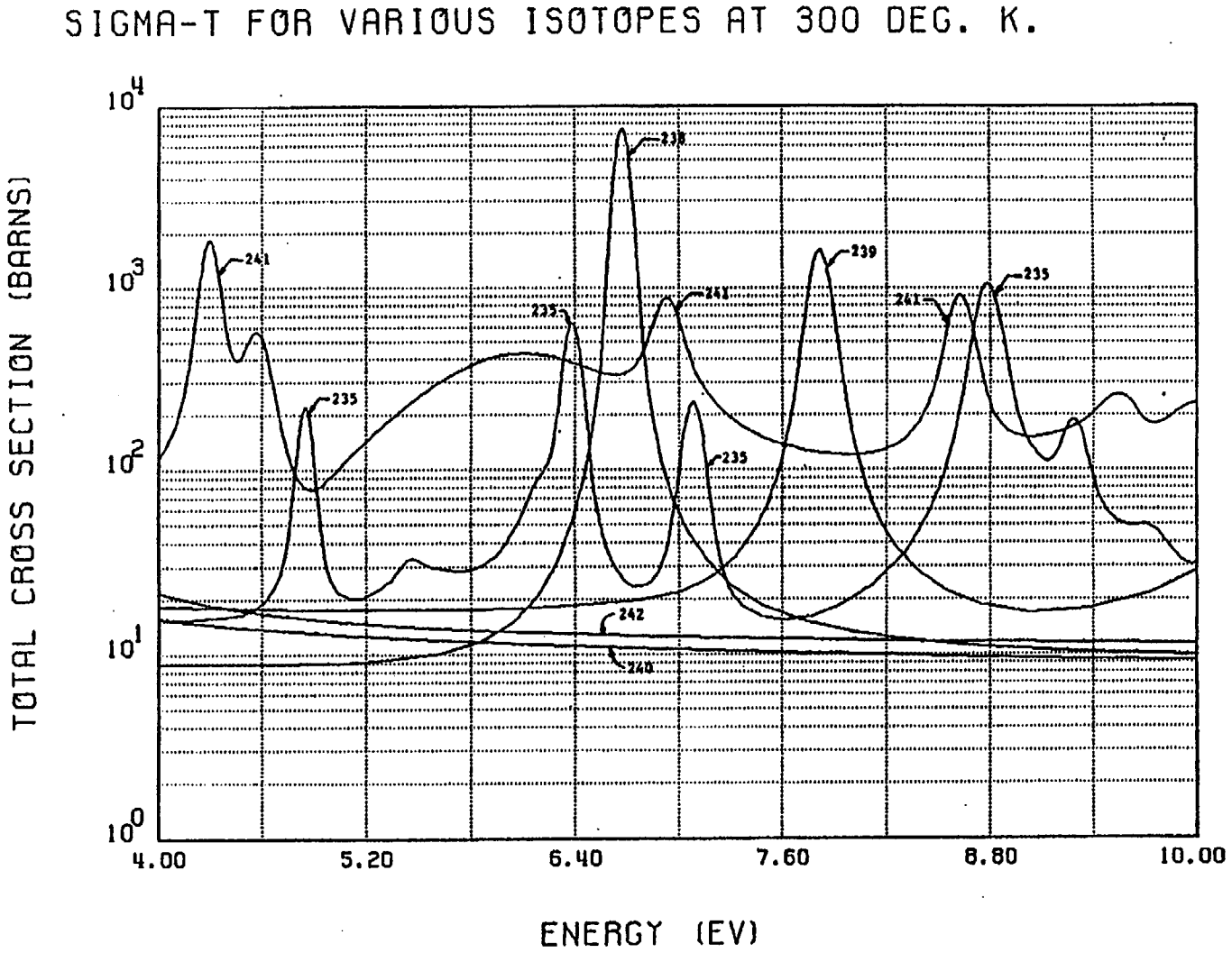

Figure M7.A.8c Resonance overlap for ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu, and ^{242}Pu in the 4- to 10-eV energy range

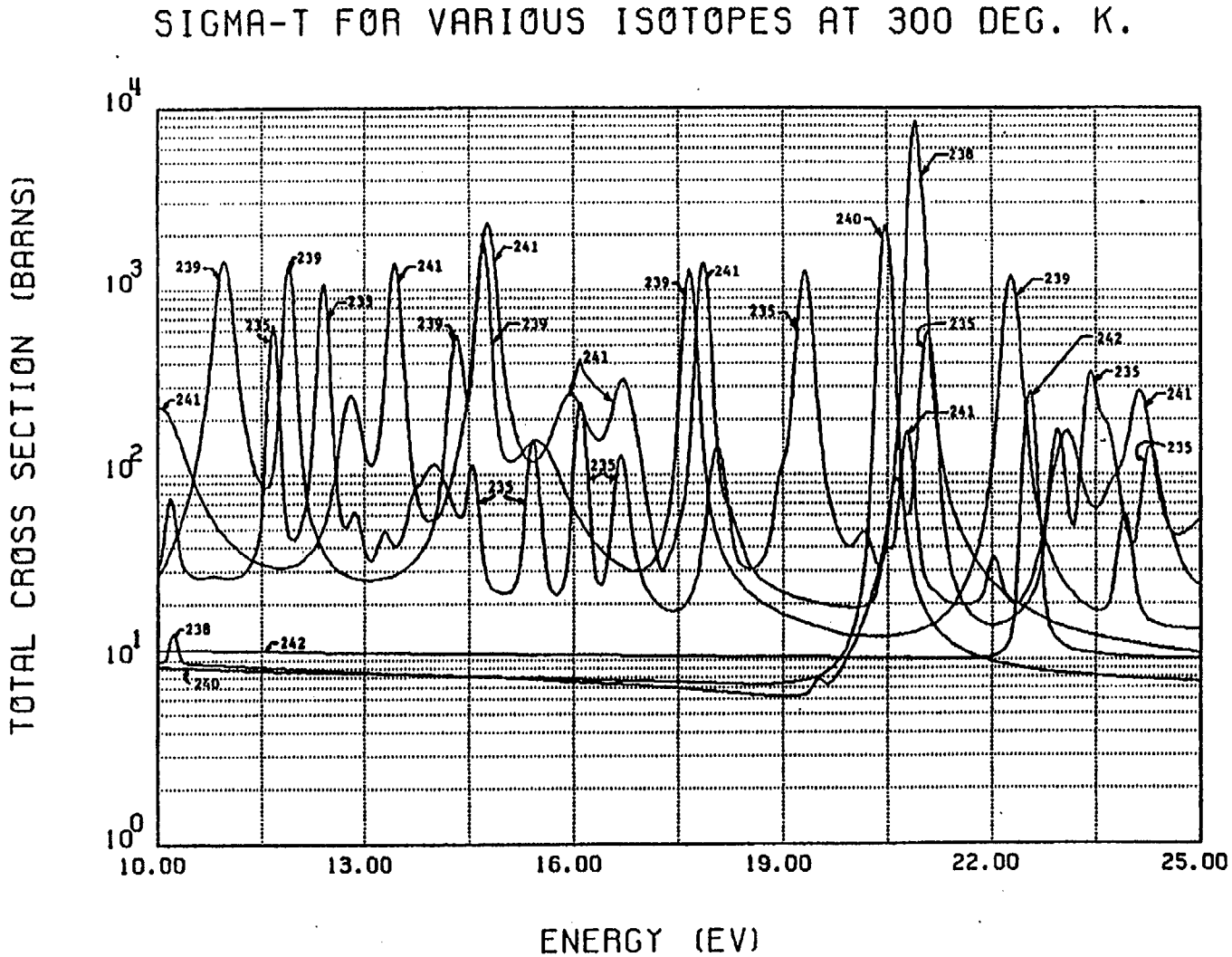

Figure M7.A.8d Resonance overlap for ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu, and ^{242}Pu in the 10- to 25-eV energy range

M7.A.8 THE ITERATIVE BONDARENKO METHOD AND HOW IT PARTIALLY ACCOUNTS FOR RESONANCE OVERLAP USING A MODIFIED DEFINITION OF THE BACKGROUND CROSS SECTION

Having used the narrow resonance approximation to derive an expression for the flux which is valid underneath any given resonance and in the region between responses [cf. Eq. (M7.A.41)], the group-averaged absorption cross section for resonance nuclide i may be written as

$$\sigma_A^{i,g} = \frac{\int_{E^g}^{E^{g-1}} \sigma_A^i(E)\left(\frac{1}{\Sigma_{tf}(E)+\Sigma_{esc}}\right)\left(\frac{1}{E}\right)dE}{\int_{E^g}^{E^{g-1}} \left(\frac{1}{\Sigma_{tF}(E)+\Sigma_{esc}}\right)\left(\frac{1}{E}\right)dE} . \qquad \text{(M7.A.67)}$$

If the resonances are narrow compared with the width of the energy group, if the resonances for the mixture are well separated, and if $\sigma_A^i(E) \to 0$ between resonances such that $\Sigma_{tf}^i(E) = \Sigma_{sF}^i(E) = \Sigma_{sF}^i$ = *constant potential scattering cross section* (between resonances), then the arguments presented in Sect. M7.A.6 are completely valid, the denominator of Eq. (M7.A.67) may be evaluated analytically, and the group-averaged value of the absorption cross section may be written as

$$\sigma_A^{i,g} = \left[\frac{\sigma_{sF}^i + \sigma_o^i}{\ell n\left(\frac{E^{g-1}}{E^g}\right)}\right]\int_{E^g}^{E^{g-1}} \left[\frac{\sigma_A^i(E)}{\sigma_{tF}^i(E)+\sigma_o^i}\right]\frac{dE}{E} \qquad \text{(M7.A.68)}$$

where

$$\sigma_o^i = \left(\frac{1}{N^i}\right)\left(\Sigma_{sF} - \Sigma_{sF}^i + \Sigma_{esc}\right) = \text{constant} \quad . \qquad \text{(M7.A.69)}$$

This was, in fact, a matter of great calculational convenience insofar as it permitted the resonance self-shielded cross sections for a resonance nuclide to be tabulated as a function of a single variable (σ_o^i), even though that nuclide may be in a mixture with other nuclides.

Starting with Eq. (M7.A.67), it is possible to derive expressions similar to Eqs. (M7.A.68) and (M7.A.69) which relax the assumption that $\sigma_A^i(E) \rightarrow 0$ between resonances and which replace the potential scattering cross section (Σ_{sF}^i) with a constant group-averaged value of the total cross section ($\Sigma_{tF}^{i,g}$).* Defining the background cross section for a particular energy group as

$$\sigma_o^{i,g} \equiv \left(\frac{1}{N^i}\right)\left(\Sigma_{tF}^g - \Sigma_{tF}^{i,g} + \Sigma_{esc}\right) \qquad \text{(M7.A.70)}$$

Eq. (M7.A.67) can then be written as

$$\sigma_A^{i,g} = \frac{\int_{E^g}^{E^{g-1}} \left(\frac{\sigma_A^i(E)}{\sigma_{tF}^i(E)+\sigma_o^{i,g}}\right)\left(\frac{1}{E}\right) dE}{\int_{E^g}^{E^{g-1}} \left(\frac{1}{\sigma_{tf}^i(E)+\sigma_o^{i,g}}\right)\left(\frac{1}{E}\right) dE} = \frac{\left\langle \frac{\sigma_A^i(u)}{\sigma_{tF}^i(u)+\sigma_o^{i,g}} \right\rangle_g}{\left\langle \frac{1}{\sigma_{tF}^i(u)+\sigma_o^{i,g}} \right\rangle_g} \qquad \text{(M7.A.71)}$$

where $u \equiv \ell n(E_o/E)$ and $\langle\rangle_g$ designates the integral over lethargy. In the case of the simple UO_2 system used for illustration purposes,

$$\sigma_o^{25,g} = \left(\frac{1}{N^{25}}\right)\left(\Sigma_{tF}^{28,g} + \Sigma_{tF}^{16,g} + \Sigma_{esc}\right) \qquad \text{(M7.A.72)}$$

and

$$\sigma_o^{28,g} = \left(\frac{1}{N^{28}}\right)\left(\Sigma_{tF}^{25,g} + \Sigma_{tF}^{16,g} + \Sigma_{esc}\right) . \qquad \text{(M7.A.73)}$$

Formulating $\sigma_o^{i,g}$ in terms of the group-averaged total cross section for the other nuclides in the fuel allows one to partially account for the fact that the absorption cross section in those nuclides may not be negligible compared to their potential scattering cross section. While $\sigma_A^i(E)$ is often negligible with respect to σ_s^i for

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*Even though such expressions can be derived and applied as shown in this section, such a feeble attempt to account for the absorption cross section of the other nuclides in the mixture is only partially satisfying. Apart from the obvious shortcoming of having to ignore the detailed energy dependence of $\sigma_A^j(E)$ for the other nuclides (j) in the mixture [i.e., assuming that $\sigma_A^j(E) = \sigma_A^{j,g} = constant$], the validity of Eq. (M7.A.67) itself may be questioned when/if the resulting absorption rates are not negligible. Recall, for example, that the narrow resonance approximation for the flux as given by Eq. (M7.A.40) was derived by replacing the flux [$\phi_F(E')$] in Eqs. (M7.A.35) and (M7.A.37) with its asymptotic approximation [cf. Eq. (M7.A.36)] for $E < E' < E/\alpha^1$. The asymptotic expression given by Eq. (M7.A.36) is, of course, rigorously valid only if the absorption in this range is completely negligible.

many of the light nuclides, this is not the case with many of the uranium and plutonium isotopes where the wings of adjacent resonances frequently overlap. Indeed, the group-averaged value of the absorption cross section ($\sigma_A^{i,g}$) may be several times the potential scattering cross section (σ_s^i) for some of the resonance nuclides, thus making the present definition of $\sigma_o^{i,g}$ much more attractive than that used in Sect. M7.A.6.

While the definition of the background cross section ($\sigma_o^{i,g}$) has been modified to partially account for absorption by other nuclides, the key point to be made here is that the self-shielded group-averaged cross sections for a resonance nuclide [cf. Eq. (M7.A.71)] can still be tabulated as a function of a single variable ($\sigma_o^{i,g}$). Indeed, this data does exist for many multigroup libraries. Typically, $\sigma_A^{i,g}$ is expressed as the infinitely dilute value [cf. Eq. (M7.A.60)] times a self-shielding factor:

$$\sigma_A^{i,g} = f_A^{i,g}(T,\sigma_o^{i,g})\sigma_A^{i,g}(\infty) \qquad \text{(M7.A.74)}$$

where the form of the f-factor (or "Bondarenko factor") may be deduced by dividing Eq. (M7.A.71) by Eq. (M7.A.60). The explicit appearance of temperature in the self-shielding factor is in recognition of the fact that the cross sections in Eq. (M7.A.71) [$\sigma_A^i(E)$ and $\sigma_{tF}^i(E)$] should be Doppler broadened to the appropriate temperature. Even though expressions for $\sigma_A^{i,g}$ have been used thus far for illustrative purposes, similar expressions may also be written for $\sigma_t^{i,g}$, $\sigma_c^{i,g}$, $\sigma_f^{i,g}$, $\sigma_\ell^{i,g}$, etc. Thus, for example, $\sigma_t^{i,g}$ may be written* as:

$$\sigma_t^{i,g} = \frac{\displaystyle\int_{E_g}^{E_{g-1}} \left(\frac{\sigma_t^i(E)}{\sigma_{tF}^i(E)+\sigma_o^{i,g}}\right)\left(\frac{1}{E}\right) dE}{\displaystyle\int_{E_g}^{E_{g-1}} \left(\frac{1}{\sigma_{tF}^i(E)+\sigma_o^{i,g}}\right)\left(\frac{1}{E}\right) dE} = \frac{\left\langle \dfrac{\sigma_t^i(u)}{\sigma_{tF}^i(u)+\sigma_o^{i,g}} \right\rangle_g}{\left\langle \dfrac{1}{\sigma_{tF}^i(u)+\sigma_o^{i,g}} \right\rangle_g} \qquad \text{(M7.A.75)}$$

or alternatively:

$$\sigma_t^{i,g} = f_t^{i,g}(T,\sigma_o^{i,g})\sigma_t^{i,g}(\infty) \qquad \text{(M7.A.76)}$$

Using expressions similar to Eq. (M7.A.71) or Eq. (M7.A.75), multigroup Bondarenko f-factors have been tabulated for each of the various resonance reactions as a function of T and σ_o. Given a library of pretabulated data, one need only apply the various f-factors (evaluated at the appropriate value of $\sigma_o^{i,g}$) to obtain the necessary self-shielded cross-section data characteristic of the particular fuel lump. [Note that the size of the fuel lump ($\bar{\ell}$) and the transparency of the external moderator (as measured by the Dancoff factor) are represented by the escape cross section (Σ_{esc}), which factors into the background cross section ($\sigma_o^{i,g}$)]. For systems containing more than one resonance nuclide, Eqs. (M7.A.70) and (M7.A.76) must be evaluated in an iterative fashion for each energy group. For a simple mixture of enriched UO_2, the iterative procedure would proceed as follows:

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*This definition of $\sigma_t^{i,g}$ preserves the total reaction rate per unit volume, such that $\sigma_t^{i,g}\,\phi^g = \sigma_t^{i,g}\langle\phi(u)\rangle = \langle\sigma_t^i(u)\phi(u)\rangle$.

$$\begin{bmatrix} \sigma_t^{25,g} = f_t^{25,g}(T,\sigma_o^{25,g})\sigma_t^{25,g}(\infty) \\ \sigma_t^{28,g} = f_t^{28,g}(T,\sigma_o^{28,g})\sigma_t^{28,g}(\infty) \end{bmatrix}$$

$$\begin{bmatrix} \sigma_o^{25,g} = \left(\frac{1}{N^{25}}\right)\left(\Sigma_{tF}^{28,g} + \Sigma_{tF}^{16,g} + \Sigma_{esc}\right) \\ \sigma_o^{28,g} = \left(\frac{1}{N^{28}}\right)\left(\Sigma_{tF}^{25,g} + \Sigma_{tF}^{16,g} + \Sigma_{esc}\right) \end{bmatrix} \qquad \text{(M7.A.77)}$$

Since the multigroup self-shielding factors, $f^g(T,\sigma_o)$ are typically tabulated at only a few discrete values of T and σ_o, numerical codes employing the Iterative Bondarenko Method must interpolate to determine the f-factors at the end of each iteration. Simple interpolation formulas such as

$$f^g(T,\sigma_o) = \alpha + \beta \ell nT \quad T_j < T < T_{j+1} \qquad \text{(M7.A.78)}$$

and

$$f^g(T,\sigma_o) = \alpha' + \beta' \ell n\sigma_o \quad \sigma_k < \sigma_o < \sigma_{k+1} \qquad \text{(M7.A.79)}$$

are still used in some codes. Proceeding in this fashion, the background cross section(s) can be converged to any desired degree of accuracy. Adequate convergence is typically achieved after several iterations. Once the background cross sections are fully converged, the resonance self-shielded values of $\sigma_t^{i,g}$, $\sigma_c^{i,g}$, $\sigma_f^{i,g}$, $\sigma_\ell^{i,g}$, etc., may be calculated by multiplying the appropriate f-factors by the infinitely dilute values of the respective cross sections. Because the Iterative Bondarenko Method makes use of pretabulated self-shielding factors and requires only a few iterations involving a limited number of algebraic steps, it is very fast and provides an attractive alternative to the Nordheim Integral Method. Even though neither method can properly account for overlapping resonances found in many fuel mixtures, the applicability of the Bondarenko Method is somewhat more limited due to the fact that the self-shielding factors are usually generated using the narrow resonance approximation for the flux [cf. Eq. (M7.A.41)].

M7.A.9 SOME GENERAL COMMENTS ON THE GENERATION OF BONDARENKO SELF-SHIELDING FACTORS

The generation of Bondarenko self-shielding factors by codes such as ETOX, MINX, ENDRUN, or TABU is a separate calculational step completely divorced from the use and application of that data in codes such as XSRES, SPHINX, TDOWN, or BONAMI which actually generate the resonance self-shielded cross sections for a particular set of mixtures in a particular application. As we have seen in the previous section, however, the approximations that go into the generation of these f-factors ultimately limit the applicability of the method. For completeness, therefore, let us make a few additional remarks concerning the definition of the various f-factors.

Many nuclear processes involve resonance reactions; the ones of greatest importance in neutronic calculations are fission, radiative capture, and elastic scattering. In multigroup calculations, the corresponding

resonance self-shielded cross sections ($\sigma_f^{i,g}$, $\sigma_c^{i,g}$, $\sigma_\ell^{i,g}$) should be defined so as to reproduce the integrated reaction rate that one would obtain if he performed the calculation on a point-wise energy basis. Since those reaction rates are given by the product of the scalar flux times, the respective cross sections, the multigroup cross sections should be defined such that

$$\sigma_f^{i,g}\phi^g = \sigma_f^{i,g}\int_{E^g}^{E^{g-1}} \phi(E)dE = \int_{E^g}^{E^{g-1}} \sigma_f^i(E)\,\phi(E)dE \qquad \text{(M7.A.80)}$$

Using the narrow resonance approximation for the flux,

$$\phi(E) = \left(\frac{1}{\Sigma_{tF}(E)+\Sigma_{esc}}\right)\left(\frac{1}{E}\right) \qquad \text{(M7.A.81)}$$

and writing the above expression in terms of lethargy, where

$$u \equiv \ell n\ (E_o/E), \qquad du = -\left(\frac{1}{E}\right)dE \qquad \text{(M7.A.82a,b)}$$

and $\langle\rangle_g$ denotes the integral over lethargy, we obtain

$$\sigma_f^{i,g}\phi^g = \sigma_f^{i,g}\langle\phi(u)\rangle_g = \langle\sigma_f^i(u)\,\phi(u)\rangle, \qquad \text{or} \qquad \text{(M7.A.83)}$$

$$\sigma_f^{i,g} = \frac{\langle\sigma_f^i(u)\,\phi(u)\rangle_g}{\langle\phi(u)\rangle_g} = \frac{\left\langle\dfrac{\sigma_f^i(u)}{\sigma_{tF}^i(u)+\sigma_o^{i,g}}\right\rangle}{\left\langle\dfrac{1}{\sigma_{tF}^i(u)+\sigma_o^{i,g}}\right\rangle_g} \qquad \text{(M7.A.84)}$$

where $\sigma_o^{i,g}$ is the (constant) background cross section defined by Eq. (M7.A.70). Since the Bondarenko factor is defined as the resonance self-shielded cross section divided by the infinitely dilute value [cf. Eq. (M7.A.60)], the corresponding f-factor would be defined as

$$f_f(T,\sigma_o) = \frac{\Delta u_g}{\langle\sigma_f^i(T,u)\rangle_g}\,\frac{\left\langle\dfrac{\sigma_f^i(T,u)}{\sigma_t^i(T,u)+\sigma_o}\right\rangle_g}{\left\langle\dfrac{1}{\sigma_t^i(T,u)+\sigma_o}\right\rangle_g}. \qquad \text{(M7.A.85)}$$

Expressions for $f_c(T,\sigma_o)$ and $f_\ell(T,\sigma_o)$ may be derived in a similar fashion, yielding

$$f_c(T,\sigma_o) = \frac{\Delta u_g}{\langle \sigma_c(T,u) \rangle_g} \frac{\left\langle \frac{\sigma_c^i(T,u)}{\sigma_t^i(T,u)+\sigma_o} \right\rangle_g}{\left\langle \frac{1}{\sigma_t^i(T,u)+\sigma_o} \right\rangle_g} \qquad \text{(M7.A.86)}$$

and

$$f_{e\ell}(T,\sigma_o) = \frac{\Delta u_g}{\langle \sigma_{e\ell}(T,u) \rangle_g} \frac{\left\langle \frac{\sigma_{e\ell}(T,u)}{\sigma_t^i(T,u)+\sigma_o} \right\rangle_g}{\left\langle \frac{1}{\sigma_t^i(T,u)+\sigma_o} \right\rangle_g} \qquad \text{(M7.A.87)}$$

Although a similar expression may be written for $f_A(T,\sigma_o)$, these (superfluous) values are not typically stored in the cross-section data file since, by definition, $\sigma_A^{i,g} = \sigma_f^{i,g} + \sigma_c^{i,g}$.

The Bondarenko factor for the total cross section $f_t(T,\sigma_o)$ is defined differently by different codes, depending on whether $\sigma_t^{i,g}$ is ultimately to be used in a multigroup transport-theory calculation or a multigroup diffusion-theory calculation. If it is ultimately to be used in a multigroup transport-theory calculation, one should define the resonance self-shielded cross section so that the multigroup calculation accurately reproduces the total collision density per unit path length. If $\psi(\Omega)$ denotes the angular flux, $\sigma_t^{i,g}$ should be defined such that

$$\sigma_t^{i,g}\psi^g(\Omega) = \sigma_t^{i,g}\langle \psi(u,\Omega) \rangle_g = \left\langle \sigma_t^i(u)\psi(u,\Omega) \right\rangle_g \qquad \text{(M7.A.88)}$$

Integrating over all solid angles and interchanging the order of integration, this again reduces to

$$\sigma_t^{i,g} = \frac{\left\langle \sigma_t^i(u)\phi(u) \right\rangle_g}{\langle \phi(u) \rangle_g} = \frac{\left\langle \frac{\sigma_t^i(u)}{\sigma_{tF}^i(u)+\sigma_o^{i,g}} \right\rangle_g}{\left\langle \frac{1}{\sigma_{tF}^i(u)+\sigma_o^{i,g}} \right\rangle_g} \qquad \text{(M7.A.89)}$$

and the corresponding Bondarenko factor is given by

$$f_t^i(T,\sigma_o) = \frac{\Delta u_g}{\left\langle \sigma_t^i(T,u) \right\rangle} \frac{\left\langle \dfrac{\sigma_t^i(T,u)}{\sigma_t^i(T,u)+\sigma_o} \right\rangle_g}{\left\langle \dfrac{1}{\sigma_t^i(T,u)+\sigma_o} \right\rangle_g} \qquad \text{(M7.A.90)}$$

Indeed, the Bondarenko factors used by BONAMI in the iterative process described by Eqs. (M7.A.77) are defined in exactly this fashion. In point of fact, Bondarenko factors as defined by Eq. (M7.A.90) are somewhat superfluous since $\sigma_t^{i,g}$ may be defined in terms of the other resonance self-shielded cross sections. Noting, for example, that

$$\sigma_t^{i,g}\phi^g = \sigma_f^{i,g}\phi^g + \sigma_c^{i,g}\phi^g + \sigma_{el}^{i,g}\phi^g + \sigma^{i,g}\ \phi^g \qquad \text{(M7.A.91)}$$

all other nonresonance processes

one can write

$$\sigma_t^{i,g} = \sigma_f^{i,g} + \sigma_c^{i,g} + \sigma_{el}^{i,g} + \sigma^{i,g} \qquad \text{(M7.A.92)}$$

all other nonresonance processes

Noting that the infinitely dilute total cross section is defined as

$$\sigma_t^{i,g}(\infty) = \sigma_f^{i,g}(\infty) + \sigma_c^{i,g}(\infty) + \sigma_{el}^{i,g}(\infty) + \sigma^{i,g}(\infty) \qquad \text{(M7.A.93)}$$

all other nonresonance processes

one can combine Eqs. (M7.A.92) and (M7.A.93), and express $\sigma_t^{i,g}$ as

$$\sigma_t^{i,g} = \sigma_t^{i,g}(\infty) - \sigma_f^{i,g}(\infty) - \sigma_c^{i,g}(\infty) - \sigma_{el}^{i,g}(\infty) - \sigma^{i,g}(\infty)$$

all other nonresonance processes

$$+ \sigma_f^{i,g} + \sigma_c^{i,g} + \sigma_{e\ell}^{i,g} + \sigma^{i,g} \Big|_{\substack{\text{all other} \\ \text{nonresonance} \\ \text{processes}}} \qquad \text{(M7.A.94)}$$

Noting that

$$\sigma^{i,g} \Big|_{\substack{\text{all other} \\ \text{nonresonance} \\ \text{processes}}} = \sigma^{i,g}(\infty) \Big|_{\substack{\text{all other} \\ \text{nonresonance} \\ \text{processes}}} \qquad \text{(M7.A.95)}$$

$\sigma_t^{i,g}$ can then be written as simply

$$\sigma_t^{i,g} = \sigma_t^{i,g}(\infty) + \left[\sigma_f^{i,g} - \sigma_f^{i,g}(\infty)\right] + \left[\sigma_c^{i,g} - \sigma_c^{i,g}(\infty)\right] + \left[\sigma_{e\ell}^{i,g} - \sigma_{e\ell}^{i,g}(\infty)\right] \qquad \text{(M7.A.96)}$$

For that reason, retention of $f_t^i(T,\sigma_o)$ in the cross-section data file is somewhat superfluous. As a matter of calculational convenience, however, $f_t^i(T,\sigma_o)$ as defined by Eq. (M7.A.90) is retained in the input data file for BONAMI and used in the iterative procedure described above. Once the background cross section(s) has been adequately converged and the resonance self-shielded values of $\sigma_f^{i,g}$, $\sigma_c^{i,g}$, and $\sigma^{i,g}$ have been determined, the code actually calculates $\sigma_t^{i,g}$ using Eq. (M7.A.96). Even though this gives essentially the same value that is obtained by multiplying $f_t^i(T,\sigma_o)$ by the infinitely dilute cross section, the code uses Eq. (M7.A.96) in order to eliminate round-off discrepancies in the output data file.

If, on the other hand, the resonance self-shielding calculation is being performed in order to prepare multigroup cross-section data for use in a diffusion-theory calculation where absorption is negligible and the diffusion coefficient is defined as

$$D^{g,MIX} = \frac{1}{3\Sigma_t^{g,MIX}} \qquad \text{(M7.A.97)}$$

the f-factor, $f_t^i(T,\sigma_o)$, must be defined in a somewhat different fashion. In such a situation, the quantity to be preserved is the net leakage of particles into or out of the system boundary (i.e., the multigroup calculation should reproduce the leakage rate that one would obtain if the calculation were done on a point-wise energy basis). Mathematically, this requires that

$$D^{g,MIX}\nabla^2\phi^g(r) = \left\langle D^{MIX}(u)\nabla^2\phi(u,r)\right\rangle \qquad \text{(M7.A.98)}$$

$$\frac{1}{3\Sigma_t^{MIX}(u)}\left\langle -B^2\phi(u,r)\right\rangle = \left\langle \frac{1}{3\Sigma_t^{MIX}(u)}(-B^2)\phi(u,r)\right\rangle \qquad \text{(M7.A.99a)}$$

$$\frac{B^2}{3}\frac{\langle\phi(u)\rangle}{\Sigma_t^{MIX}(u)} = \frac{B^2}{3}\left\langle\frac{\phi(u)}{\Sigma_t^{MIX}(u)}\right\rangle \qquad \text{(M7.A.99b)}$$

$$\Sigma_t^{MIX}(u) = \frac{\langle\phi(u)\rangle}{\left\langle\frac{\phi(u)}{\Sigma_t^{MIX}(u)}\right\rangle} \qquad \text{(M7.A.99c)}$$

and

$$\Sigma_t^i(u) + \Sigma_o = \frac{\langle\phi(u)\rangle}{\left\langle\frac{\phi(u)}{\Sigma_t^i(u)+\Sigma_o}\right\rangle} \qquad \text{(M7.A.99d)}$$

Using the narrow resonance approximation for the flux, this becomes

$$\Sigma_t^i(u) + \Sigma_o = \frac{\left\langle\frac{1}{\Sigma_t^i(u)+\Sigma_o}\right\rangle}{\left\langle\frac{1}{\left(\Sigma_t^i(u)+\Sigma_o\right)^2}\right\rangle} \qquad \text{(M7.A.100)}$$

and

$$\sigma_t^{i,g} = \frac{\left\langle\frac{1}{\sigma_t^i(u)+\sigma_o}\right\rangle}{\left\langle\frac{1}{\left(\sigma_t^i(u)+\sigma_o\right)^2}\right\rangle} - \sigma_o \qquad \text{(M7.A.101)}$$

Dividing $\sigma_t^{i,g}$ by the infinitely dilute value, we then obtain the appropriate expression for $f_t^i(T,\sigma_o)$:

$$f_t^i(T,\sigma_o) = \frac{\Delta u_g}{\left\langle \sigma_t^i(T,u) \right\rangle_g} \left[\frac{\left\langle \frac{1}{\sigma_t^i(T,u)+\sigma_o} \right\rangle_g}{\left\langle \frac{1}{(\sigma_t^i(T,u)+\sigma_o)^2} \right\rangle_g} - \sigma_o \right] \qquad \text{(M7.A.102)}$$

This, in fact, is the expression originally given by Bondarenko in his classic book on the subject.[17] Indeed, it is the expression still used in many codes.

Since Bondarenko self-shielding factors have been generated for numerous multigroup libraries using various cross-section processing codes, the user should be careful to make sure that the Bondarenko factors contained in a given library were generated in a fashion that is consistent with his intended application.

M7.A.10 DERIVATION OF THE SELF-SHIELDING FACTORS FOUND IN THE ORIGINAL HANSEN-ROACH CROSS-SECTION LIBRARY (0°K)

One of the oldest and most useful multigroup libraries used in the United States for criticality analysis is the 16-group Hansen-Roach cross-section library.[18] Originally developed as a six-group library for criticality analysis of fast, heavy-metal systems, the lowest energy group was later divided into ten epithermal energy groups and one thermal energy group so that critical assemblies having an intermediate neutron flux spectrum could be analyzed. Of particular interest here is the fact that the original report (December 1961) contained plots of the resonance self-shielded, group-averaged values of σ_f^g as a function of the background cross section (σ_o) for ^{233}U, ^{235}U, and ^{239}Pu, and resonance self-shielded values of σ_c^g (the radiative capture cross section) as a function of the background cross section (σ_o) for ^{232}Th, ^{233}U, ^{235}U, ^{238}U, ^{239}Pu, and ^{240}Pu. Because modified versions of this 16-group library are still in wide use today, the determination of these constants is of historical interest. The determination of the original resonance self-shielded data will be presented in this section. The Knight-Modified Hansen-Roach data currently being disseminated with the SCALE system will be discussed in Sect. M7.A.13.

While the resonance self-shielded, group-averaged constants reported by Hansen and Roach were calculated in a fashion consistent with Eqs. M7.A.85 or M7.A.86, the closed-form algebraic expression they actually used appears, at first glance, to be significantly different. To arrive at that expression, it is necessary to consider the single-level Breit-Wigner expression for an unbroadened (T=0°K) isolated resonance, insert those expressions for $\sigma_c(E)$, $\sigma_f(E)$, and $\sigma_t(E)$ into Eq. M7.A.71, and carry out the required integration over the particular energy group. In this particular case, the integration is most conveniently carried out in the energy domain rather than lethargy. Before pursuing the details of that integration, however, it is convenient to review some of the simplifying assumptions first introduced in Sect. M7.A.6.

Using the narrow resonance approximation for the flux, the resonance self-shielded value of $\sigma_f^{i,g}$ may be written as

$$\sigma_f^{i,g} = \frac{\int_{E^g}^{E^{g-1}} \left(\frac{\sigma_f^i(E)}{\sigma_t^i(E) + \sigma_o^i} \right) \left(\frac{1}{E} \right) dE}{\int_{E^g}^{E^{g-1}} \left(\frac{1}{\sigma_t^i(E) + \sigma_o^i} \right) \left(\frac{1}{E} \right) dE} \qquad \text{(M7.A.103)}$$

In the denominator, the integrand vanishes in the vicinity of a resonance such that one need only evaluate that integral between resonances where $\sigma_t^i(E) \rightarrow \sigma_p^i$, the potential scattering cross section of nuclide i. Assuming that the resonances are very narrow compared with the width of the energy group such that one can retain the original limits of integration, the denominator can then be written as

$$\int_{E^g}^{E^{g-1}} \left(\frac{1}{\sigma_t^i(E) + \sigma_o^i} \right) \left(\frac{1}{E} \right) dE \doteq \left(\frac{1}{\sigma_p^i + \sigma_o^i} \right) \int_{E^g}^{E^{g-1}} \left(\frac{1}{E} \right) dE = \left(\frac{1}{\sigma_o} \right) \ell n \left(\frac{E^{g-1}}{E^g} \right) = \left(\frac{\Delta u_g}{\sigma_o} \right) \qquad \text{(M7.A.104)}$$

where

$$\sigma_o \equiv \sigma_p^i + \sigma_o^i \qquad \text{(M7.A.105)}$$

Assuming that the resonances are narrow compared with the width of the energy group and widely spaced such that $\sigma_f^i(E) \rightarrow 0$ between resonances, the numerator of Eq. (M7.A.103) may be replaced by a sum of integrals over the individual resonances of nuclide i in group g. Thus, Eq. (M7.A.103) may be written as

$$\sigma_f^{i,g} = \left(\frac{\sigma_o}{\Delta u_g} \right) \sum_{\substack{\text{res} \\ j \in g}} \int_{E_{min}^{res(j)}}^{E_{max}^{res(j)}} \left(\frac{\sigma_f^i(E)}{\sigma_t^i(E) + \sigma_o^i} \right) \left(\frac{1}{E} \right) dE \qquad \text{(M7.A.106)}$$

Use of the single-level Breit-Wigner equation for an unbroadened (T=0 K) isolated resonance then permits an analytic evaluation of each of the resonance integrals appearing in Eq. (M7.A.106). Specifically, we note that $\sigma_f^i(E)$ is given by

$$\sigma_f^i(E_c) = \pi \lambda_{res}^2 g \left(\frac{E_{res}}{E_c} \right)^{1/2} \frac{\Gamma_n \Gamma_f}{(E_c - E_{res})^2 + (\Gamma^2/4)} \qquad \text{(M7.A.107)}$$

where

E_{res} denotes a resonance centered about $E = E_{res}$,

E_c denotes the energy of the neutron in the center-of-mass system,

Γ denotes the total width of the resonance,

Γ_n denotes the neutron width,

Γ_f denotes the fission width,

λ_{res} denotes the reduced wavelength of a neutron at $E = E_{res}$; that is, $\lambda_1 = \bar{h}/\sqrt{2\mu E_1}$ where μ is the reduced mass of the neutron, or
$\lambda_1 \doteq 4.55 \times 10^{-10}\ \text{cm}/\sqrt{E_1}$, where E_1 is in eV,

g denotes the statistical spin factor.

Likewise, the single-level Breit-Wigner formula for radiative capture (n,γ) is given as

$$\sigma_c^i(E_c) = \pi\lambda_{res}^2 g\left(\frac{E_{res}}{E_c}\right)^{1/2} \frac{\Gamma_n\Gamma_\gamma}{(E_c - E_{res})^2 + (\Gamma^2/4)} \qquad \text{(M7.A.108)}$$

At $E_c = E_{res}$, one obtains the maximum cross section for each of these reactions types, denoted here as $\sigma_f^{i,o}$ and $\sigma_c^{i,o}$:

$$\sigma_f^{i,o} = \sigma_f^i(E_{res}) = 4\pi\lambda_{res}^2 g\left(\frac{\Gamma_n}{\Gamma}\right)\left(\frac{\Gamma_f}{\Gamma}\right) \qquad \text{(M7.A.109)}$$

and

$$\sigma_c^{i,o} = \sigma_c^i(E_{res}) = 4\pi\lambda_{res}^2 g\left(\frac{\Gamma_n}{\Gamma}\right)\left(\frac{\Gamma_\gamma}{\Gamma}\right) \qquad \text{(M7.A.110)}$$

Although the Breit-Wigner formula for s-wave scattering does have an additional term that produces an asymmetric dip in $\sigma_{e\ell}(E_c)$ at energies just below E_{res}, the maximum value of $\sigma_{e\ell}(E_c)$ (not including the potential scattering term) is given by

$$\sigma_{e\ell}^{i,o} = \sigma_{e\ell}^i(E_{res}) = 4\pi\lambda_{res}^2 g\left(\frac{\Gamma_n}{\Gamma}\right)\left(\frac{\Gamma_n}{\Gamma}\right) \qquad \text{(M7.A.111)}$$

Noting that

$$\Gamma \equiv \Gamma_n + \Gamma_\gamma + \Gamma_f \qquad \text{(M7.A.112)}$$

the maximum value of the total cross section is given by

$$\sigma_t^{i,o} = \sigma_t^i(E_{res}) = 4\pi\lambda_{res}^2 g\left(\frac{\Gamma_n}{\Gamma}\right) \qquad \text{(M7.A.113)}$$

and $\sigma_t^i(E_c)$ may (for all practical purposes) be approximated as

$$\sigma_t^i(E_c) \doteq \pi\lambda_{res}^2 g\left(\frac{E_{res}}{E_c}\right)^{1/2} \frac{\Gamma_n\Gamma}{(E_c - E_{res})^2 + (\Gamma^2/4)} + \sigma_p^i \qquad \text{(M7.A.114)}$$

where σ_p^i is the potential scattering cross section for nuclide i. Before substituting the various cross sections into Eq. (M7.A.106) and evaluating the various resonance integrals, two additional simplifications can be made: (1) for collisions with intermediate and heavy nuclides, the energy of the neutron in the center-of-mass system E_c is essentially the same as the energy in the laboratory system (E); and (2) at energies underneath the (narrow) resonance and in the immediate vicinity of the narrow resonance,

$$\frac{E_{res}}{E_c} \doteq \frac{E_{res}}{E} \doteq 1.0 \qquad \text{(M7.A.115)}$$

Using these simplifications along with the definitions of $\sigma_f^{i,o}$, $\sigma_c^{i,o}$, and $\sigma_t^{i,o}$, the energy-dependent cross sections needed in Eq. (M7.A.106) may be written as

$$\sigma_f^i(E) = \frac{\sigma_f^{i,o}}{\left[\left(\frac{2}{\Gamma}\right)(E - E_{res})\right]^2 + 1} \qquad E_{min}^{res(j)} \le E \le E_{max}^{res(j)} \qquad \text{(M7.A.116a)}$$

$$\sigma_c^i(E) = \frac{\sigma_c^{i,o}}{\left[\left(\frac{2}{\Gamma}\right)(E - E_{res})\right]^2 + 1} \qquad E_{min}^{res(j)} \le E \le E_{max}^{res(j)} \qquad \text{(M7.A.116b)}$$

and

$$\sigma_t^i(E) = \frac{\sigma_t^{i,o}}{\left[\left(\frac{2}{\Gamma}\right)(E - E_{res})\right]^2 + 1} + \sigma_p^i \qquad E_{min}^{res(j)} \le E \le E_{max}^{res(j)} \qquad \text{(M7.A.116c)}$$

Returning to Eq. (M7.A.106), we need to make one more approximation. Since the integration is over a very narrow band of energies where $E = E_{res}$, the (1/E) term appearing in Eq. (M7.A.106) may be replaced by $(1/E_{res})$. The integrand may then be written as

$$\left(\frac{\sigma_f^i(E)}{\sigma_t^i(E)+\sigma_o^i}\right)\left(\frac{1}{E}\right)dE = \left(\frac{\sigma_f^{i,o}}{\sigma_t^{i,o}+(\sigma_p^i+\sigma_o^i)[x^2+1]}\right)\left(\frac{1}{E_{res}}\right)dE$$

$$= \left(\frac{\sigma_f^{i,o}}{\sigma_t^{i,o}+\sigma_o+\sigma_o x^2}\right)\left(\frac{1}{E_{res}}\right)dE = \left(\frac{1}{E_{res}}\right)\left(\frac{\sigma_f^{i,o}}{\sigma_o}\right)\left(\frac{1}{a^2+x^2}\right)dE \qquad \text{(M7.A.117a)}$$

where

$$x = \left(\frac{2}{\Gamma}\right)(E - E_{res}) \qquad \text{(M7.A.117b)}$$

$$\sigma_o = \sigma_p^i + \sigma_o^i \qquad \text{(M7.A.117c)}$$

and

$$a^2 = 1 + \left(\frac{\sigma_t^{i,o}}{\sigma_o}\right) \qquad \text{(M7.A.117d)}$$

The resonance integral may then be written as

$$\int_{E_{min}^{res(j)}}^{E_{max}^{res(j)}}\left(\frac{\sigma_f^i(E)}{\sigma_t^i(E)+\sigma_o^i}\right)\left(\frac{1}{E}\right)dE \doteq \left(\frac{1}{E_{res}}\right)\left(\frac{\sigma_f^{i,o}}{\sigma_o}\right)\int_{E_{min}^{res(j)}}^{E_{max}^{res(j)}}\frac{1}{\left(\frac{\sigma_t^{i,o}+\sigma_o}{\sigma_o}\right)+\left[\left(\frac{2}{\Gamma}\right)(E-E_{res})\right]^2}dE \qquad \text{(M7.A.118)}$$

To the extent that the integrand vanishes whenever

$$\left(\frac{\sigma_t^{i,o}+\sigma_o}{\sigma_o}\right) + \left[\left(\frac{2}{\Gamma}\right)(E-E_{res})\right]^2 >> 1 \qquad \text{(M7.A.119)}$$

the limits of integration may be replaced by $+\infty$ and $-\infty$ with very little residual error. This is certainly true at energies more than a few half-widths away from E_{res}, that is, whenever

$$\left[\left(\frac{2}{\Gamma}\right)(E-E_{res})\right]^2 >> 1 \qquad \text{(M7.A.120)}$$

Thus, in addition to being widely spaced, the (narrow) resonances are assumed to lie well inside the group boundaries. Defining $x = \left(\frac{2}{\Gamma}\right)(E - E_{res})$, such that $dE = \left(\frac{\Gamma}{2}\right)dx$, the integral is then of the form

$$\int_{-\infty}^{\infty} \frac{1}{a^2+x^2}dx = \frac{\pi}{a}, \quad \text{where } a^2 = 1 + \left(\frac{\sigma_t^{i,o}}{\sigma_o}\right) \qquad \text{(M7.A.121a,b)}$$

The resonance integral may then be expressed as

$$\int_{E_{min}^{res(j)}}^{E_{max}^{res(j)}} \left(\frac{\sigma_f^i(E)}{\sigma_t^i(E)+\sigma_o^i}\right)\left(\frac{1}{E}\right) dE = \left(\frac{1}{E_{res}}\right)\left(\frac{\sigma_f^{i,o}}{\sigma_o}\right)\left(\frac{\Gamma}{2}\right)\frac{\pi}{\sqrt{1+\left(\frac{\sigma_t^{i,o}}{\sigma_o}\right)}} \qquad \text{(M7.A.122)}$$

Substituting this result into Eq. (M7.A.106), the resonance self-shielded group-averaged value of $\sigma_f^{i,g}$ is then given by

$$\sigma_f^{i,g} = \left(\frac{1}{\Delta u_g}\right)\left(\frac{\pi}{2}\right)\sum_{\substack{res \\ j\epsilon g}} \frac{\left(\frac{\Gamma}{E_{res}}\right)\sigma_f^{i,o}}{\sqrt{1+\left(\frac{\sigma_t^{i,o}}{\sigma_o}\right)}} \qquad \text{(M7.A.123)}$$

Likewise, the resonance self-shielded, group-averaged value of $\sigma_c^{i,g}$ is given by

$$\sigma_c^{i,g} = \left(\frac{1}{\Delta u_g}\right)\left(\frac{\pi}{2}\right)\sum_{\substack{res \\ j\epsilon g}} \frac{\left(\frac{\Gamma}{E_{res}}\right)\sigma_c^{i,o}}{\sqrt{1+\left(\frac{\sigma_t^{i,o}}{\sigma_o}\right)}} \qquad \text{(M7.A.124)}$$

Using the resonance data available at that time (1961), Hansen and Roach used Eqs. (M7.A.123) and M7.A.124 to tabulate the resonance self-shielded, group-averaged values of $\sigma_f^{i,g}$ and $\sigma_c^{i,g}$ as a function of σ_o.

Despite the fact that Hansen and Roach ignored the effects of Doppler broadening, resonance scattering, and resonance overlap, their simplified approach did provide a useful set of multigroup cross-section data which accounted for the gross spectral effects of resonance self-shielding. Figure M7.A.9 shows the resonance self-shielded values of the capture cross section ($\sigma_c^{28,g}$, g = 8, 9, 10, 11, 12) for ^{238}U as a function of σ_o. Note that the effect of the resonance self-shielding can be quite significant in certain energy groups. Whereas the group-12 cross section may have a value of 110 barns in an infinitely dilute mixture such as an aqueous solution of uranylfluoride, its value in an undermoderated UO_2 lattice would be considerably less, and its value in a thick uranium-metal shield may be as little as 6 barns.

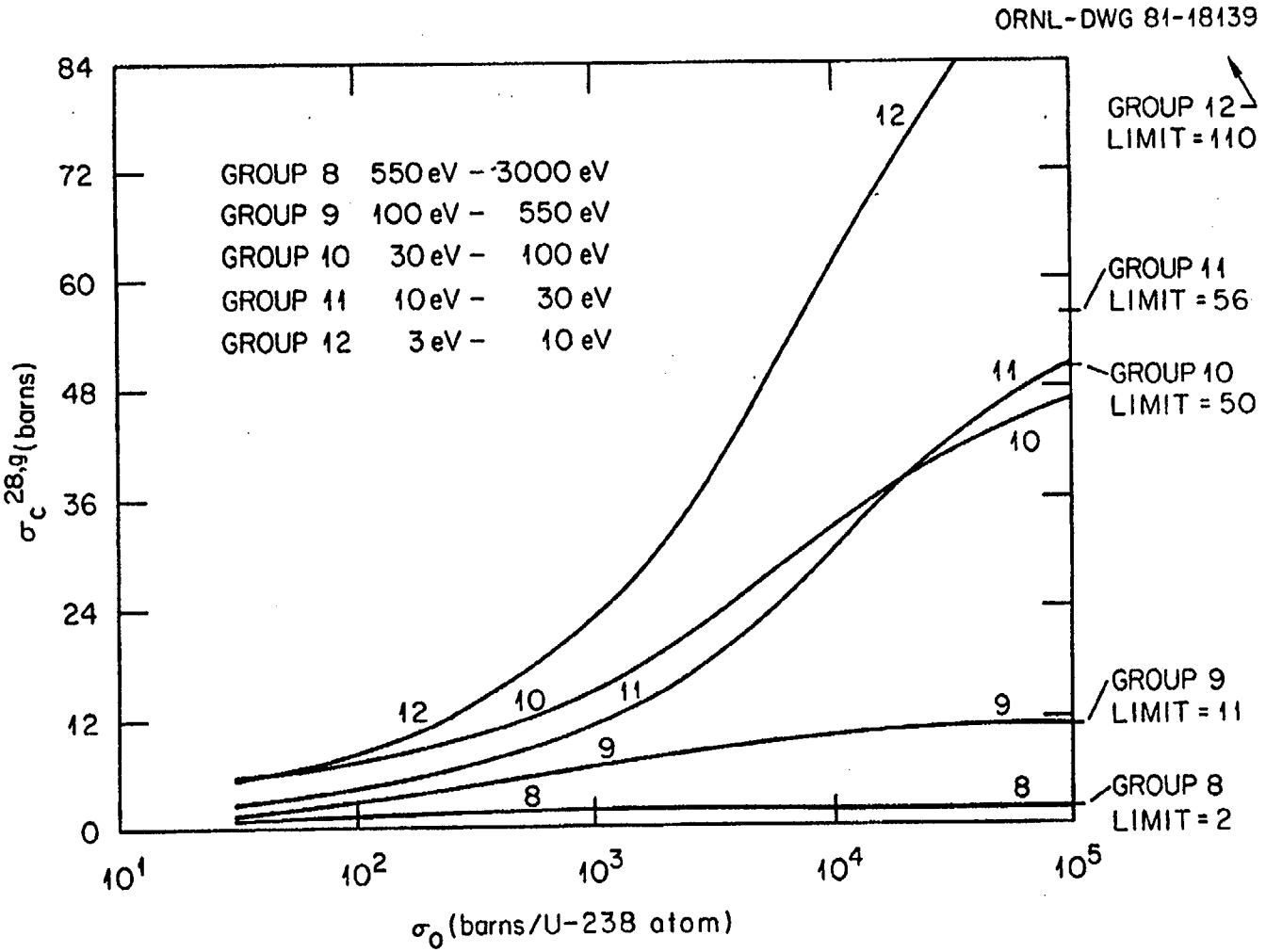

Figure M7.A.9 Resonance self-shielded group-averaged (η,γ) capture cross section for ^{238}U as a function of the background cross section (σ_0)

M7.A.11 THE EFFECT OF RESONANCE SCATTERING ON THE GROUP-AVERAGED CROSS SECTIONS

Somewhat distressing in the derivation of Eqs. (M7.A.123) and (M7.A.124) is the fact that Hansen and Roach ignored the effect of resonance scattering. Indeed, for an unbroadened resonance, its inclusion would have been trivial. Using the Breit-Wigner formula for s-wave scattering, $\sigma_{e\ell}(E_c)$ may be written as

$$\sigma^i_{e\ell}(E_c) = \pi\lambda^2_{res}\, g\left(\frac{E_{res}}{E_c}\right)^{1/2}\left[\frac{\Gamma_n^2}{(E_c - E_{res})^2 + (\Gamma^2/4)}\right]$$

$$+ 4\pi\lambda_{res}\, g R\Gamma_n\left[\frac{(E_c - E_{res})}{(E_c - E_{res})^2 + (\Gamma^2/4)}\right] + \sigma^i_p \qquad \text{(M7.A.125)}$$

where R is the effective radius of the nucleus, and

$$\sigma^i_p = 4\pi R^2 \qquad \text{(M7.A.126)}$$

Incorporating the asymmetric term into the total cross section, we may write

$$\sigma^i_t(E_c) = \frac{\sigma^{i,o}_t}{1+x^2} + \frac{\sigma^{i,o}_t x d}{1+x^2} + \sigma^i_p \qquad \text{(M7.A.127a)}$$

where

$$d \equiv \left(\frac{1}{\lambda_{res}}\right)\sqrt{\frac{\sigma^i_p}{\pi}} \qquad \text{(M7.A.127b)}$$

and

$$x = \left(\frac{2}{\Gamma}\right)(E_c - E_{res}) \qquad \text{(M7.A.127c)}$$

Proceeding as before, the integrand in the resonance integral [cf. Eq. (M7.A.106)] may be written as

$$\left(\frac{\sigma_f^i(E)}{\sigma_t^i(E)+\sigma_o^i}\right)\left(\frac{1}{E}\right)dE = \left(\frac{\Gamma}{2E_{res}}\right)\left(\frac{\sigma_f^{i,o}}{\sigma_t^{i,o}+\sigma_t^{i,o}xd+(\sigma_p^i+\sigma_o^i)(1+x^2)}\right)dx$$

$$= \left(\frac{1}{2}\right)\left(\frac{\Gamma}{E_{res}}\right)\left(\frac{1}{x^2+bx+c}\right)dx \qquad \text{(M7.A.128a)}$$

where

$$\sigma_o \equiv \sigma_p^i + \sigma_o^i, \quad b \equiv \left(\frac{\sigma_t^{i,o}}{\sigma_o}\right)d, \quad \text{and} \quad c \equiv 1 + \left(\frac{\sigma_t^{i,o}}{\sigma_o}\right) \qquad \text{(M7.A.128b,c,d)}$$

By "completing the square" in the denominator, the resonance integral may be put in the same standard form as the previous case. To illustrate, consider the following:

$$x^2 + bx + c = \left[x^2 + 2\left(\frac{b}{2}\right)x + \left(\frac{b}{2}\right)^2\right] + \left[c - \left(\frac{b}{2}\right)^2\right] = y^2 + a^2 \qquad \text{(M7.A.129a)}$$

where

$$y = x + \left(\frac{b}{2}\right) \quad \text{and} \quad a^2 = c - \left(\frac{b}{2}\right)^2 \qquad \text{(M7.A.129b,c)}$$

Using Eq. (M7.A.128c) for "b," Eq. (M7.A.127b) for "d," and Eq. (M7.A.113) for $\sigma_t^{i,o}$, the quantity $\left(\frac{b}{2}\right)^2$ may be written as

$$\left(\frac{b}{2}\right)^2 = \left(\frac{\sigma_t^{i,o}d}{2\sigma_o}\right)^2 = \left(\frac{\sigma_t^{i,o}}{\sigma_o}\right)^2\left(\frac{1}{4}\right)\left(\frac{1}{\lambda_{res}^2}\right)\left(\frac{\sigma_p^i}{\pi}\right) \qquad \text{(M7.A.130)}$$

Since $g \le 1$, $\Gamma n \le \Gamma$, and $\sigma_p^i \le \sigma_o$, it follows that

$$\left(\frac{b}{2}\right)^2 \le \left(\frac{\sigma_t^{i,o}}{\sigma_o}\right) < \left(\frac{\sigma_t^{i,o}}{\sigma_o}\right) + 1 \equiv c \qquad \text{(M7.A.131)}$$

Hence, the parameter a^2, defined here as $a^2 = c - \left(\frac{b}{2}\right)^2$, is always positive and

$$\int_{-\infty}^{\infty} \frac{1}{\left[x+\frac{b}{2}\right]^2 + \left[c-\left(\frac{b}{2}\right)^2\right]} dx = \int_{-\infty}^{\infty} \frac{1}{y^2+a^2} dy = \frac{\pi}{a} \qquad \text{(M7.A.132a)}$$

where

$$a = \sqrt{1+\left(\frac{\sigma_t^{i,o}}{\sigma_o}\right)\left[1-\left(\frac{g\Gamma_n}{\Gamma}\right)\frac{\sigma_p^i}{\sigma_o}\right]} \qquad \text{(M7.A.132b)}$$

Thus, the resonance integral found in Eq. (M7.A.106) may be written as

$$\int_{E_{min}^{res(j)}}^{E_{max}^{res(j)}} \left(\frac{\sigma_f^i(E)}{\sigma_t^i(E)+\sigma_o^i}\right)\left(\frac{1}{E}\right) dE = \frac{1}{2}\left(\frac{\Gamma}{E_{res}}\right)\left(\frac{\sigma_f^{i,o}}{\sigma_o}\right) \frac{\pi}{\sqrt{1+\left(\frac{\sigma_t^{i,o}}{\sigma_o}\right)\left[1-\left(\frac{g\Gamma_n}{\Gamma}\right)\left(\frac{\epsilon}{\epsilon}\right.\right.}} \qquad \text{(M7.A.133)}$$

Indeed, this form of the resonance integral (for an unbroadened resonance at T = 0 K) was noted by Dresner[19] some time prior to the release of the original Hansen-Roach cross-section library. Denoting the two forms of the resonance integral as I_D and I_{HR}, we see that they give essentially the same result whenever the resonance scattering is negligible ($g\Gamma_n << \Gamma$), or whenever the resonance nuclide is reasonably dilute ($\sigma_p^i << \sigma_o$). In a concentrated system, such as a thick uranium-metal shield (where $\sigma_o \approx \sigma_p^i$), the more correct form proposed by Dresner [Eq. (M7.A.133)] will yield resonance self-shielded, group-averaged cross sections which are consistently larger than those obtained using Eq. (M7.A.122). Table M7.A.2 shows the ratio of the capture integrals (I_D/I_{HR}) for the first few low-energy resonances in ^{238}U. In the first case (σ_o = 45 b, σ_p^i = 10.7 b), the resonance integrals are within a few percent of each other; in the second case ($\sigma_o = \sigma_p^i$ = 10.7 b), the resonance integrals are seen to be significantly different. The saving feature, of course, is that many of these low-energy resonances are reasonably broad such that one should in fact use the narrow-resonance/infinite-mass approximation for the flux underneath the resonance (cf. Sect. M7.A.5). Unlike the NR approximation for the flux which has $\sigma_t^i(E)$ in the denominator, the NRIM approximation for the flux has only the absorption cross section $\sigma_A^i(E)$ in the denominator [cf. Eq. (M7.A.40) and (M7.A.53)]. For broad resonances, therefore, the interference term in the resonance scattering cross section is completely negligible.

Table M7.A.2 Comparison of the Dresner and Hansen-Roach resonance integrals (I_D and I_{HR}) for ^{238}U

				σ_o=45 b	σ_o=10.7 b
E_{res}(eV)	$\sigma_t^{i,o}$(barns)	$g\Gamma_n$(MeV)	Γ(MeV)	I_D/I_{HR}	I_D/I_{HR}
6.67	21,700	1.52	27.5	1.01	1.03
20.9	32,600	8.7	34.0	1.03	1.16
36.8	39,500	32.0	57.0	1.08	2.27
66.1	20,900	26.0	48.0	1.08	1.47
102.5	19,500	70.0	96.0	1.10	1.92
116.8	10,300	30.0	52.0	1.08	1.54

M7.A.12 THE EFFECT OF DOPPLER BROADENING ON THE GROUP-AVERAGED CROSS SECTIONS

M7.A.12.1 Temperature Dependence of the Doppler-Broadened, Energy-Dependent, Cross-Section Data: A Qualitative Explanation and a Mathematical Description in Terms of the ψ and χ Functions

Somewhat more distressing in the derivation of Eqs. (M7.A.123) and (M7.A.124) is the fact that Hansen and Roach ignored the Doppler broadening of the energy-dependent cross sections at elevated temperatures (T > 0 K). While the single-level Breit-Wigner equation does accurately describe the energy-dependent cross sections at 0 K, and while the energy of the neutron in the center-of-mass and laboratory systems may be taken as essentially equal, the vibratory energy associated with the thermal motion of the target nuclide (E=kT) cannot be ignored relative to the width of a narrow resonance (Γ). At room temperature, for example, the vibratory energy associated with a ^{238}U nucleus is 0.0253 eV. By comparison, the width of the (relatively broad) 6.67-eV resonance is only 0.0275 eV. To qualitatively assess the impact of that vibratory motion on the "effective" energy-dependent cross section [$\sigma_c(E)$, $\sigma_f(E)$, $\sigma_t(E)$, etc.], let us consider the following analogy:

> "Assume that a marksman is consistently firing a steady stream of bullets into a very small bull's-eye painted on a stationary target. Next, assume that the target starts vibrating back and forth with some small amplitude. While the amplitude of the vibratory motion may be very small compared with the trajectory of the bullets (i.e., $\Delta E <<< E_{res}$), it may not be negligible compared with the size of the bull's-eye ($\Delta E \approx \Gamma$). As the amplitude of that vibratory motion increases, fewer and fewer bullets traveling along the fixed trajectory (E_{res}) will end up in the bulls-eye. (In the analogy, this would correspond to a decreased absorption probability at $E = E_{res}$). On the other hand, some of the bullets which would have been 'near misses' for the stationary target now land in the bull's-eye (i.e., the absorption probability at $E = E_{res} \pm \epsilon$ tends to increase)."

Indeed, the behavior described in the analogy is characteristic of all resonance reactions. Figure M7.A.10 shows the "effective" energy-dependent capture cross section for the 6.67-eV resonance in ^{238}U as a function of temperature. Note that the effective (Doppler-broadened) cross section, $\sigma_c^{28}(E,T)$, is

substantially lower and substantially wider at elevated temperatures. Note also that it is this Doppler-broadened, energy-dependent cross section (not the Breit-Wigner energy-dependent cross section at T=0 K) that should be used in Eq. (M7.A.103) when preparing resonance self-shielded, group-averaged cross-section data for a particular application.

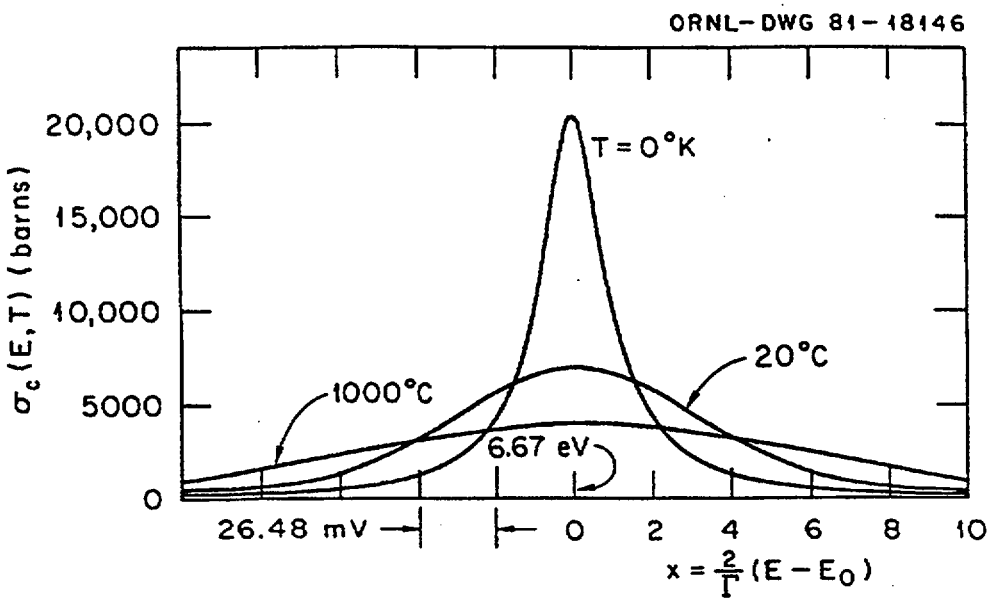

Figure M7.A.10 Doppler broadening of the ^{238}U capture cross section near the 6.67 eV resonance

To obtain an expression for the Doppler-broadened energy-dependent cross section, we note that it [$\sigma(E,T)$] should be defined so as to yield the same overall reaction rate (for neutrons of energy E) that one would obtain if he explicitly integrated over the velocity distribution [N(V)] of all the atoms in the target at temperature T. That is, $\sigma(E,T)$ should be defined such that

$$nvN\sigma(E,T) = \int n|\bar{v} - \bar{V}|N(\bar{V})\sigma(E_c)d\bar{V} = \int nv_r N(V_z)\sigma(E_c)dV_z \qquad \text{(M7.A.134)}$$

where $V_z = \bar{v}\cdot\bar{V}$ is the component of the target velocity parallel to the flight of the neutron, where the relative speed $v_r = |\bar{v} - \bar{V}|$ of the neutron with respect to the target nuclide is essentially the same* as the speed of the neutron (v) in the lab system (such that $nv_r = nv = \phi$), and where $\sigma(E_c)$ is the energy-dependent cross section as given by the single-level Breit-Wigner equation. Assuming that the velocity distribution of the atoms in the target is Maxwellian

*For a ^{238}U nucleus in thermal equilibrium at room temperature (293 K), its vibrational speed $|\bar{V}|$ is ~143 m/s, whereas the speed $|\bar{v}|$ of a 6.67-eV neutron is ~35,700 m/s.

$$N(V_z) = N\left(\frac{M}{2\pi kT}\right)^{1/2} e^{-\left(\frac{MV_z^2}{2kT}\right)} \qquad \text{(M7.A.135)}$$

the Doppler-broadened cross section for neutrons of energy E may be written as

$$\sigma(E,T) = \left(\frac{M}{2\pi kT}\right)^{1/2} \int_{-\infty}^{\infty} \sigma(E_c) e^{-\left(\frac{MV_z^2}{2kT}\right)} dV_z \qquad \text{(M7.A.136)}$$

or

$$\sigma_c(E,T) = \sigma_c^{i,o} \int_{-\infty}^{\infty} \frac{e^{-\left(\frac{MV_z^2}{2kT}\right)}}{\left[\left(\frac{2}{\Gamma}\right)(E_c - E_{res})\right]^2 + 1} \left(\frac{M}{2\pi kT}\right)^{1/2} dV_z \qquad \text{(M7.A.137)}$$

Although it is usually presented in a somewhat different format and tabulated in terms of two dimensionless variables, the integral on the right is the well-known ψ function. When evaluated at a number of different temperatures, the resulting profile of $\sigma_c(E,T)$ as a function of E behaves exactly as shown in Fig. M7.A.10. Furthermore, it can be shown that the area under these curves

$$A = \int_{-\infty}^{\infty} \sigma_c(E,T)\, dE = \sigma_c^{i,o} \pi \qquad \text{(M7.A.138)}$$

is independent of temperature. From this result, we will later show that the resonance self-shielded, group-averaged value of $\sigma_c^{i,g}$, $\sigma_f^{i,g}$, $\sigma_t^{i,g}$, etc., will *increase* with temperature. Before proceeding along those lines, however, it is convenient to put the ψ function of Eq. (M7.A.137) into its standard form. The first step is to write V_z in terms of E and E_c. If E and E_A represent the energy of the neutron in the lab system and the vibrational energy of the target nuclide in the lab system ($\frac{1}{2}MV^2$), then the energy of the neutron in the center-of-mass system (E_c) may be written as

$$E_c = \left(\frac{M}{m+M}\right) E + \left(\frac{m}{m+M}\right) E_A - \left(\frac{mM}{m+M}\right) \bar{v} \cdot \bar{V} \qquad \text{(M7.A.139)}$$

Since $m << M$ and $E_A << E$, this may be written as

$$E_c = E - mvV_z \quad \text{where} \quad v = \sqrt{\frac{2E}{m}} \doteq \sqrt{\frac{2E_{res}}{m}} \qquad \text{(M7.A.140a,b)}$$

from which we conclude

$$dE_c = -mvdV_z \quad \text{and} \quad dV_z = -\frac{1}{mv}dE_c = -\left(\frac{1}{2mE_{res}}\right)^{1/2} dE_c \qquad \text{(M7.A.141a,b)}$$

Equation (M7.A.140a) may also be rearranged and written as

$$V_z = \left(\frac{1}{mv}\right)(E - E_c) = \left(\frac{1}{mv}\right)\left[(E - E_{res}) - (E_c - E_{res})\right] \qquad \text{(M7.A.142)}$$

from which we conclude that

$$V_z^2 = \left(\frac{1}{2mE_{res}}\right)\left(\frac{\Gamma^2}{4}\right)(x-y)^2 \,, \qquad \text{(M7.A.143a)}$$

where

$$x \equiv \left(\frac{2}{\Gamma}\right)(E - E_{res}) \quad \text{and} \quad y \equiv \left(\frac{2}{\Gamma}\right)(E_c - E_{res}) \,. \qquad \text{(M7.A.143b,c)}$$

Noting that

$$dy = \frac{2}{\Gamma}dE_c \Rightarrow dE_c = \left(\frac{\Gamma}{2}\right)dy \,, \qquad \text{(M7.A.144a,b)}$$

Eq. (M7.A.141b) may be written as

$$dV_z = -\left(\frac{\Gamma}{2}\right)\left(\frac{1}{2mE_{res}}\right)^{1/2} dy \,. \qquad \text{(M7.A.145)}$$

Substituting Eqs. (M7.A.143) and (M7.A.145) into (M7.A.137) yields

$$\sigma_c^i(E,T) = \sigma_c^{i,o}\int_{-\infty}^{\infty} \frac{\exp\left[-\left(\frac{M}{2kT}\right)\left(\frac{1}{2mE_{res}}\right)\left(\frac{\Gamma^2}{4}\right)(x-y)^2\right]}{y^2+1}\left(\frac{\Gamma}{2}\right)\left(\frac{M}{4\pi mE_{res}kT}\right)^{1/2} dy \,. \qquad \text{(M7.A.146)}$$

Noting that

$$A = (M/m) , \qquad \text{(M7.A.147a)}$$

and defining

$$\Gamma_D \equiv \sqrt{\frac{4kTE_{res}}{A}} \quad \text{and} \quad \xi \equiv \frac{\Gamma}{\Gamma_D} , \qquad \text{(M7.A.147b,c)}$$

Eq. (M7.A.146) can then be written as

$$\sigma_c(E,T) = \sigma_c^{i,o}\psi(\xi,x) , \qquad \text{(M7.A.148)}$$

where the ψ function is formally defined as

$$\psi(\xi,x) = \frac{\xi}{2\sqrt{\pi}}\int_{-\infty}^{\infty} \frac{e^{-[\xi^2(x-y)^2/4]}}{1+y^2}dy . \qquad \text{(M7.A.149)}$$

Likewise, the Doppler-broadened, energy-dependent fission cross section may be written as

$$\sigma_f^i(E,T) = \sigma_f^{i,o}\psi(\xi,x) , \qquad \text{(M7.A.150)}$$

where

$$\xi = \left(\frac{\Gamma}{2}\right)\sqrt{\frac{A}{kTE_{res}}} \quad \text{and} \quad x = \left(\frac{2}{\Gamma}\right)(E - E_{res}) . \qquad \text{(M7.A.151a,b)}$$

Proceeding in the same fashion, the Doppler-broadened, energy-dependent, elastic-scattering cross section may be written as

$$\sigma_{el}^i(E,T) = \left(\frac{\sigma_t^{i,o}\Gamma_n}{\Gamma}\right)\psi(\xi,x) + \sigma_t^{i,o}d\chi(\xi,x) + \sigma_p^i , \qquad \text{(M7.A.152)}$$

where $\sigma_t^{i,o}$ and d are given by Eqs. (M7.A.113) and (M7.A.127b), respectively, and the χ function is defined as

$$\chi(\xi,x) = \frac{\xi}{\sqrt{\pi}}\int_{-\infty}^{\infty} \frac{ye^{-[\xi^2(x-y)^2/4]}}{1+y^2}dy , \qquad \text{(M7.A.153)}$$

Depending upon whether or not one wishes to account for the asymmetric interference term introduced by the possible presence of resonance scattering, the Doppler-broadened, energy-dependent total cross section may then be written as

$$\sigma_t^i(E,T) = \sigma_t^{i,o}\psi(\xi,x) + \sigma_p^i \qquad \text{(M7.A.154)}$$

or

$$\sigma_t^i(E,T) = \sigma_t^{i,o}\psi(\xi,x) + \sigma_t^{i,o}d\chi(\xi,x) + \sigma_p^i \ . \qquad \text{(M7.A.155)}$$

Tables of the ψ and χ functions have been around since the mid-1950's and their properties are well known.[12,19,20]

M7.A.12.2 Temperature Dependence of the Resonance-Self-Shielded Group-Averaged Cross Sections: A Mathematical Description in Terms of the J Functions, a Qualitative Explanation Using a Simplified Model, and a Quantitative Assessment with Numerical Examples

Resonance self-shielded, group-averaged cross sections for a material at some elevated temperature may then be evaluated as in Sect. M7.A.10, except that now the energy-dependent cross sections appearing in Eq. (M7.A.106) should be the Doppler-broadened cross sections. That is,

$$\sigma_c^{i,g}(T) = \left(\frac{\sigma_o}{\Delta u_g}\right)\sum_{\substack{\text{res}\\ j\in g}}\int_{E_{min}^{res(j)}}^{E_{max}^{res(j)}}\left(\frac{\sigma_c^i(E,T)}{\sigma_t^i(E,T)+\sigma_o^i}\right)\left(\frac{1}{E}\right)dE \ . \qquad \text{(M7.A.156)}$$

Ignoring the interference term caused by resonance scattering, the resonance integral may then be written as

$$\int_{E_{min}^{res(j)}}^{E_{max}^{res(j)}}\left(\frac{\sigma_c^i(E,T)}{\sigma_t^i(E,T)+\sigma_o^i}\right)\left(\frac{1}{E}\right)dE = \left(\frac{1}{E_{res}}\right)\left(\frac{\Gamma}{2}\right)\int_{-\infty}^{\infty}\frac{\sigma_c^{i,o}\psi(\xi,x)}{\sigma_t^{i,o}\psi(\xi,x)+(\sigma_p^i+\sigma_o^i)}dx$$

$$= \left(\frac{1}{E_{res}}\right)\left(\frac{\Gamma}{2}\right)\left(\frac{\sigma_c^{i,o}}{\sigma_t^{i,o}}\right)2\int_0^{\infty}\frac{\psi(\xi,x)}{\psi(\xi,x)+\left(\frac{\sigma_p^i+\sigma_o^i}{\sigma_t^{i,o}}\right)}dx$$

$$= \left(\frac{\Gamma_c}{E_{res}}\right)J(\xi,\beta) \ , \qquad \text{(M7.A.157a)}$$

where

$$\beta \equiv \left(\frac{\sigma_o}{\sigma_t^{i,o}}\right) = \left(\frac{\sigma_p^i + \sigma_o^i}{\sigma_t^{i,o}}\right) , \qquad \text{(M7.A.157b)}$$

and $J(\xi,\beta)$ is defined as

$$J(\xi,\beta) \equiv \int_o^\infty \frac{\psi(\xi,x)}{\psi(\xi,x)+\beta} dx . \qquad \text{(M7.A.158)}$$

Note, of course, that ξ and β vary from resonance to resonance, and that ξ also depends on the temperature (T). Thus,

$$\sigma_c^{i,g}(T_k) = \left(\frac{\sigma_o}{\Delta u_g}\right) \sum_{\substack{res \\ j\epsilon g}} \left(\frac{\Gamma_c^j}{E_{res}^j}\right) J(\xi_k^j, \beta^j) . \qquad \text{(M7.A.159)}$$

As with the ψ and χ functions, tables of the J-function have been around since the mid-1950's and its properties are well known.[19,20]

While Eqs. (M7.A.157a,b) are based on the narrow resonance approximation for the flux, a similar expression could be developed for those (low-energy) resonances where the narrow-resonance infinite-mass (NRIM) approximation is more appropriate. Indeed, the only real difference lies in the leading constant and the definition of β. Using the NRIM approximation for the flux, the resonance self-shielded group-averaged value of $\sigma_c^{i,g}(T)$ may be written as

$$\sigma_c^{i,g}(T) = \left(\frac{\sigma_o^i}{\Delta u_g}\right) \sum_{\substack{res \\ j\epsilon g}} \int_{E_{min}^{res(j)}}^{E_{max}^{res(j)}} \left(\frac{\sigma_c^i(E,T)}{\sigma_A^i(E,T)+\sigma_o^i}\right)\left(\frac{1}{E}\right) dE , \qquad \text{(M7.A.160)}$$

and the resonance integral may be written as

$$\int_{E_{min}^{res(j)}}^{E_{max}^{res(j)}} \left(\frac{\sigma_c^i(E,T)}{\sigma_A^i(E,T)+\sigma_o^i}\right)\left(\frac{1}{E}\right) dE = \left(\frac{1}{E_{res}}\right)\left(\frac{\Gamma}{2}\right) \int_{-\infty}^{\infty} \frac{\sigma_c^{i,o}\psi(\xi,x)}{\sigma_A^{i,o}\psi(\xi,x)+\sigma_o^i} dx$$

$$= \left(\frac{1}{E_{res}}\right)\left(\frac{\Gamma}{2}\right)\left(\frac{\sigma_c^{i,o}}{\sigma_A^{i,o}}\right) 2\int_o^{\infty} \frac{\psi(\xi,x)}{\psi(\xi,x)+\left(\frac{\sigma_o^i}{\sigma_A^{i,o}}\right)} dx$$

$$= \left(\frac{1}{E_{res}}\right)\left(\frac{\Gamma\Gamma_c}{\Gamma_f+\Gamma_c}\right) J(\xi,\beta) \ , \qquad \text{(M7.A.161a)}$$

where β is now defined as

$$\beta = \frac{\sigma_o^i}{\sigma_A^{i,o}} = \left(\frac{\sigma_o - \sigma_p^i}{\sigma_t^{i,o}}\right)\left(\frac{\Gamma}{\Gamma_f+\Gamma_c}\right) \ . \qquad \text{(M7.A.161b)}$$

Without dwelling on the details, it should be pointed out for the sake of completeness that one can simultaneously account for resonance scattering and Doppler broadening with the tools already developed. Using the narrow resonance approximation for the flux, the resonance integral may then be written as

$$\int_{E_{min}^{res(j)}}^{E_{max}^{res(j)}} \left(\frac{\sigma_c^i(E,T)}{\sigma_t^i(E,T)+\sigma_o^i}\right)\left(\frac{1}{E}\right) dE$$

$$= \left(\frac{1}{E_{res}}\right)\left(\frac{\Gamma}{2}\right)\int_{-\infty}^{\infty} \frac{\sigma_c^{i,o}\psi(\xi,x)}{\sigma_t^{i,o}\psi(\xi,x)+\sigma_t^{i,o} d\,\chi(\xi,x)+(\sigma_p^i+\sigma_o^i)} dx$$

$$= \left(\frac{\Gamma_c}{E_{res}}\right) J(\xi,\beta,d) \ , \qquad \text{(M7.A.162a)}$$

where

$$\beta \equiv \left(\frac{\sigma_o}{\sigma_t^{i,o}}\right) = \left(\frac{\sigma_p^i+\sigma_o^i}{\sigma_t^{i,o}}\right) \ , \qquad \text{(M7.A.162b)}$$

and the modified J-function, $J(\xi,\beta,d)$, is defined as

$$J(\xi,\beta,d) \equiv \frac{1}{2}\int_{-\infty}^{\infty} \frac{\psi(\xi,x)}{\psi(\xi,x)+d\,\chi(\xi,x)+\beta}dx\ , \qquad \text{(M7.A.163)}$$

where

$$d = \left(\frac{1}{\lambda_{res}}\right)\sqrt{\frac{\sigma_p^i}{\pi}}\ . \qquad \text{(M7.A.164)}$$

In an early treatise on the subject, Dresner[19] has shown that

$$J(\xi,\beta,d) \doteq J(\xi\rightarrow\infty,\beta,d) + J(\xi,\beta) - J(\xi\rightarrow\infty,\beta)$$

$$= j(\xi,\beta) + \left(\frac{\pi}{2}\right)\left[\left(\frac{1}{\beta^2+\beta\left[1-\left(\frac{g\Gamma_n}{\Gamma}\right)\left(\frac{\sigma^{i_p}}{\sigma_o}\right)\right]}\right)^{1/2} - \left(\frac{1}{\beta^2+\beta}\right)^{1/2}\right] \text{ for } \beta << \xi^2/6\ , \qquad \text{(M7.A.165)}$$

and

$$J(\xi,\beta,d) \doteq J(\xi,\beta) \quad \text{for } \xi << 1 \text{ and } \beta >> \xi^2/6\ . \qquad \text{(M7.A.166)}$$

Other approximations for $J(\xi,\beta,d)$ have been developed by Rothenstein.[21] The key facet to be noted, however, is that the effect of resonance scattering becomes less and less important at higher temperatures where the Doppler-broadening effect tends to dominate.

To assess the impact of Doppler broadening on the resonance self-shielded, group-averaged cross sections, it is necessary to examine the behavior of $J(\xi,\beta)$. In the infinitely dilute case where σ_o is very large [such that $\beta \equiv \left(\frac{\sigma_o}{\sigma_t^{i,o}}\right) >> \psi(\xi,x=0)$],

$$J(\xi,\beta) = \underset{\beta\rightarrow\infty}{\text{limit}}\int_o^{\infty} \frac{\psi(\xi,x)}{\psi(\xi,x)+\beta}dx = \frac{1}{\beta}\int_o^{\infty}\psi(\xi,x)\,dx$$

$$= \frac{\xi}{2\beta\sqrt{\pi}} \int_o^\infty \left[\int_{-\infty}^\infty \frac{e^{-\left[\frac{\xi}{2}(x-y)\right]^2}}{1+y^2} dy \right] dx \ . \qquad \text{(M7.A.167)}$$

Interchanging the order of integration and defining

$$u = \frac{\xi}{2}(x-y) \ , \qquad \text{(M7.A.168)}$$

we have

$$J(\xi,\beta\to\infty) = \frac{1}{2\beta} \int_{-\infty}^\infty \frac{1}{1+y^2} \left[\underset{v\to\infty}{\text{limit}} \frac{2}{\sqrt{\pi}} \int_o^v e^{-u^2} du \right] dy$$

$$= \frac{1}{\beta} \int_o^\infty \frac{1}{1+y^2} \left[\underset{v\to\infty}{\text{limit}} \text{erf}(v) \right] dy = \frac{1}{\beta} \int_o^\infty \frac{1}{1+y^2} dy$$

$$= \left(\frac{1}{\beta}\right)\left(\frac{\pi}{2}\right) = \left(\frac{\sigma_t^{i,o}}{\sigma_o}\right)\left(\frac{\pi}{2}\right) \ . \qquad \text{(M7.A.169)}$$

Note that $J(\xi,\beta\to\infty)$ is independent of ξ, which was defined as

$$\xi = \left(\frac{\Gamma}{2}\right)\sqrt{\frac{A}{kTE_{res}}} \ . \qquad \text{(M7.A.170)}$$

Thus, in an infinitely dilute system, the resonance self-shielded, group-averaged cross sections given by Eq. (M7.A.159) will be independent of temperature. Indeed, if we substitute Eq. (M7.A.169) into Eq. (M7.A.159), we obtain

$$\sigma_c^{i,g} = \left(\frac{1}{\Delta u_g}\right)\left(\frac{\pi}{2}\right)\sum_{\substack{res \\ j\in g}}\left(\frac{\Gamma_c}{E_{res}}\right)\sigma_t^{i,o} = \left(\frac{1}{\Delta u_g}\right)\left(\frac{\pi}{2}\right)\sum_{\substack{res \\ j\in g}}\left(\frac{\Gamma}{E_{res}}\right)\sigma_c^{i,o} , \qquad \text{(M7.A.171)}$$

which is identical to the result obtained by Hansen and Roach [cf. Eq. (M7.A.124)] as $\sigma_o \to \infty$. For all practical purposes, the numerical value thus obtained will be identical to the unshielded, infinitely dilute value given by

$$\sigma_c^{i,g}(\infty) \equiv \frac{1}{\ell n(E^{g-1}/E^{g})}\int_{E^{g}}^{E^{g-1}} \sigma_c^{i}(E)\frac{dE}{E} = \left(\frac{1}{\Delta u_g}\right)\left\langle\sigma_c^{i}(u)\right\rangle . \qquad \text{(M7.A.172)}$$

Note that this temperature independence will be characteristic of the fission cross section as well as the radiative capture cross section.

In more concentrated mixtures of practical interest, the resonance self-shielded, group-averaged cross sections will be slightly higher at elevated temperatures than at lower temperatures. Note that this is true for the group-averaged values of $\sigma_f^{i,g}(T)$, $\sigma_c^{i,g}(T)$, and $\sigma_t^{i,g}(T)$, despite the fact that $\sigma_f^{i}(E_{res},T)$, $\sigma_c^{i}(E_{res},T)$, and $\sigma_t^{i}(E_{res},T)$ will be considerably lower (cf. Fig. M7.A.9). Even though the point may be proven mathematically, it is probably more instructive to resort to a simplified model of an isolated resonance as a function of temperature (cf. Fig. M7.A.11). As shown in Fig. M7.A.11a, the profile of the "effective" energy-dependent cross section [$\sigma(E,T)$] is substantially flatter at elevated temperatures (i.e., the resonance becomes much wider and the peak value at $E = E_{res}$ is substantially reduced). In the simplified model (cf. Fig. M7.A.11b), we shall approximate $\sigma(E,T)$ by a series of rectangular profiles, each becoming shorter and wider as the temperature increases. While the shape of the rectangular profile tends to flatten out at higher temperatures, the area under each profile remains constant and is independent of temperature. That is,

$$\left[E_{max}^{res(j)} - E_{min}^{res(j)}\right]\sigma_c^{\square}(T) = \int_{E_{min}^{res(j)}}^{E_{max}^{res(j)}} \sigma_c(E,T)dE = \int_{-\infty}^{\infty}\left[\sigma_c^{i,o}\psi(\xi,x)\right]dx = \pi\sigma_c^{i,o} . \qquad \text{(M7.A.173)}$$

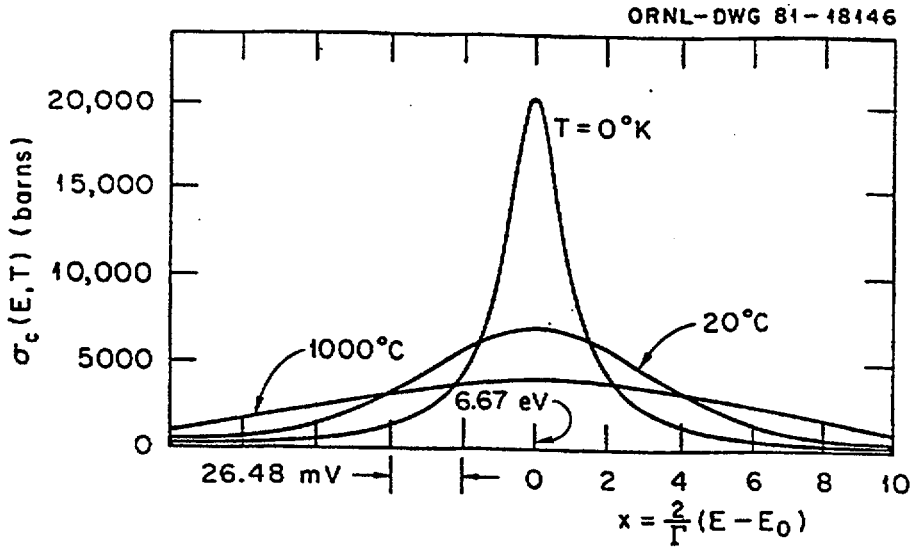

Figure M7.A.11a Actual profiles of the Doppler-broadened ^{238}U capture cross section near the 6.67-eV resonance

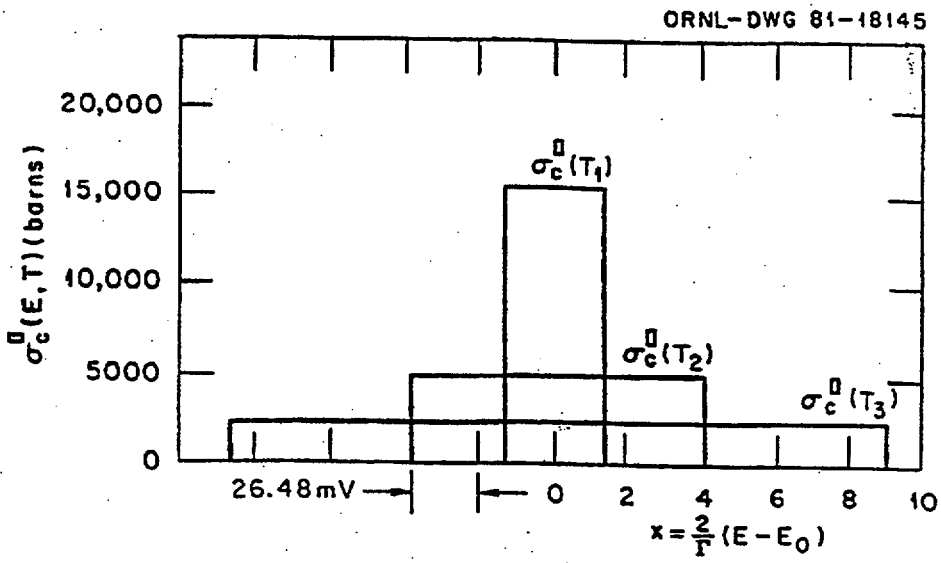

Figure M7.A.11b Idealized rectangular profiles for the Doppler-broadened ^{238}U capture cross section near the 6.67-eV resonance

Since this characteristic is crucial to the arguments that follow, it may be worthwhile to prove the point. Using Eqs. (M7.A.148) and (M7.A.149),

$$\int_{E_{min}^{res(j)}}^{E_{max}^{res(j)}} \sigma_c(E,T)dE = \int_{-\infty}^{\infty} \left[\sigma_c^{i,o}\psi(\xi,x)\right]dx$$

$$= \sigma_c^{i,o}\frac{\xi}{2\sqrt{\pi}}\int_{-\infty}^{\infty}\left[\int_{-\infty}^{\infty}\frac{e^{-[\xi^2(x-y)^2/4]}}{1+y^2}dy\right]dx \ . \qquad \text{(M7.A.174)}$$

Interchanging the order of integration and defining

$$u = \frac{\xi}{2}(x-y) \ , \qquad \text{(M7.A.175)}$$

we have

$$\int_{E_{min}^{res(j)}}^{E_{max}^{res(j)}} \sigma_c(E,T)dE = \sigma_c^{i,o}\int_{-\infty}^{\infty}\frac{1}{1+y^2}\left[\lim_{v\to\infty}\frac{2}{\sqrt{\pi}}\int_o^v e^{-u^2}du\right]dy$$

$$= \sigma_c^{i,o}\int_{-\infty}^{\infty}\frac{1}{1+y^2}\left[\lim_{v\to\infty}\text{erf}(v)\right]dy$$

$$= \sigma_c^{i,o}\int_{-\infty}^{\infty}\frac{1}{1+y^2}[1]dy = \pi\sigma_c^{i,o} \ . \qquad \text{(M7.A.176)}$$

Using the narrow resonance approximation for the flux and the rectangular cross-section profiles shown in Fig. M7.A.10b, the resonance integral may then be written as

$$\int_{E_{min}^{res(j)}}^{E_{max}^{res(j)}}\left(\frac{\sigma_c^i(E,T)}{\sigma_t^i(E,T)+\sigma_o}\right)\left(\frac{1}{E}\right)dE = \frac{1}{E_{res}}\int_{E_{min}^{res(j)}}^{E_{max}^{res(j)}}\frac{\sigma_c^{\square}(T)}{\sigma_t^{\square}(T)+\sigma_o}dE$$

$$\int_{E_{min}^{res(j)}}^{E_{max}^{res(j)}} \left(\frac{\sigma_c^i(E,T)}{\sigma_t^i(E,T)+\sigma_o} \right) \left(\frac{1}{E} \right) dE = \frac{1}{E_{res}} \int_{E_{min}^{res(j)}}^{E_{max}^{res(j)}} \frac{\sigma_c^{\square}(T)}{\sigma_t^{\square}(T)+\sigma_o} dE$$

$$= \left(\frac{1}{E_{res}} \right) \frac{\sigma_c^{\square}(T) \left[E_{max}^{res(j)} - E_{min}^{res(j)} \right]}{\sigma_t^{\square}(T)+\sigma_o} = \frac{1}{E_{res}} \frac{\pi \sigma_c^{i,o}}{\sigma_t^{\square}(T)+\sigma_o} . \qquad \text{(M7.A.177)}$$

Since $\sigma_t^{\square}(T)$ gets smaller and smaller at higher temperatures, the resonance integral tends to increase as the temperature increases. Since the resonance self-shielded, group-averaged value of $\sigma_c^{i,g}(T)$ is defined as

$$\sigma_c^{i,g}(T) = \frac{\sigma_o}{\Delta u_g} \sum_{\substack{res \\ j \in g}} \int_{E_{min}^{res(j)}}^{E_{max}^{res(j)}} \left(\frac{\sigma_c^i(E,T)}{\sigma_t^i(E,T)+\sigma_o} \right) \left(\frac{1}{E} \right) dE , \qquad \text{(M7.A.178)}$$

the resonance self-shielded, group-averaged value of $\sigma_c^{i,g}(T)$ tends to increase as the temperature increases. Likewise, the same is also true for $\sigma_f^{i,g}(T)$, $\sigma_t^{i,g}(T)$, etc. The reactivity of a fissile mixture may, of course, increase, decrease, or remain constant, depending on the relative change in the capture-to-fission ratio. In low-enriched thermal systems where there is a preponderance of fertile nuclides relative to fissile nuclides, the reactivity typically goes down as the temperature increases.

Having examined the effect of Doppler broadening mathematically, and having used some simplifying assumptions to gain a qualitative feel for the processes involved, it is (at last) necessary to consider some numerical results so that the magnitude of these effects may be kept in proper perspective. As noted above, the resonance self-shielded, group-averaged cross sections for capture, fission, etc., tend to increase as the temperature increases. In his book on resonance absorption[19] (cf. Tables 4–8, page 106), Dresner indicates that the total capture integral for UO_2 at 300 K may be 10–15% higher than at 0 K when σ_o is $\leq$ 200 barns. At temperatures found near the center of a fuel pellet in an operating reactor, the difference may be larger still. In his original book on the subject, Bondarenko[17] lists his 26-group self-shielding factors for capture, fission, etc., as a function of both temperature (T) and the background cross section (σ_o) given in Table M7.A.3a. Tables M7A.3b and M7.A.3c show the corresponding f-factors for ^{235}U and ^{238}U at 300 K, 900 K, and 2100 K. In many of the groups the self-shielding factors at 900 K are 5–10% higher than at 300 K, and another 5–10% higher at 2100 K than at 900 K. This is particularly noticeable for the ^{238}U data in groups 12–18 when σ_o is < 1000 barns. Obviously in the infinitely dilute case, the f-factors will be independent of temperature. In the more concentrated systems where σ_o is small, the Doppler effect will be more noticeable. Lastly, we note that while the Doppler effect is very important (increasing $\sigma_c^{i,g}(T)$, $\sigma_f^{i,g}(T)$, etc., by several percent), it may still be regarded as a second-order effect when compared with the rather large adjustment that must be made for σ_o.

Table M7.A.3a Energy group structure used by Bondarenko, and some infinitely dilute data for ^{235}U and ^{238}U

			Uranium (U-235)						Uranium (U-238)					
Group	E_n													
1	6.5-10.5 MeV	0.48	6.30	1.75	3.40	0.02	1.03	3.50	6.30	1.00	3.48	0.00	1.80	3.50
2	4.0-6.5 MeV	0.48	7.40	1.15	3.04	0.03	1.92	4.30	7.50	0.58	3.09	0.01	2.51	4.40
3	2.5-4.0 MeV	0.48	7.70	1.25	2.79	0.04	1.91	4.50	7.70	0.58	2.87	0.02	2.60	4.50
4	1.4-2.5 MeV	0.57	7.00	1.28	2.63	0.06	1.76	3.90	7.10	0.49	2.67	0.06	2.25	4.30
5	0.8-1.4 MeV	0.57	6.60	1.25	2.52	0.12	1.38	3.85	6.90	0.02	2.58	0.13	2.15	4.60
6	0.4-0.8 MeV	0.69	7.40	1.23	2.46	0.17	1.20	4.80	7.80	-	-	0.13	1.65	6.02
7	0.2-0.4 MeV	0.69	9.20	1.41	2.47	0.25	1.00	6.54	9.60	-	-	0.15	1.05	8.40
8	0.1-0.2 MeV	0.69	11.2	1.70	2.45	0.40	0.60	8.50	11.5	-	-	0.22	0.55	10.7
9	46.5-100 keV	0.77	12.5	2.10	2.44	0.60	0.18	9.62	12.8	-	-	0.35	0.19	12.3
10	21.5-46.5 keV	0.77	14.0	2.65	2.43	1.00	0.06	10.3	13.5	-	-	0.46	-	13.0
11	10.0-21.5 keV	0.77	16.0	3.40	2.42	1.50	-	11.1	14.0	-	-	0.60	-	13.4
12	4.65-10.0 keV	0.77	19.0	4.40	2.42	2.10	-	12.5	15.5	-	-	0.78	-	14.7
13	2.15-4.65 keV	0.77	23.0	5.40	2.42	2.75	-	14.8	16.5	-	-	1.20	-	15.3
14	1.0-2.15 keV	0.77	27.0	7.30	2.42	3.80	-	15.9	18.0	-	-	2.10	-	15.9
15	465-1000 eV	0.77	32.0	11.0	2.42	6.3	-	14.7	23.0	-	-	3.60	-	19.4
16	215-465 eV	0.77	38.0	16.0	2.42	9.5	-	12.5	18.5	-	-	4.50	-	14.0
17	100-215 eV	0.77	47.7	22	2.42	13.5	-	12.2	80.0	-	-	17.0	-	63.0
18	46.5-100 eV	0.77	69.0	35	2.42	22	-	12	40.0	-	-	15.0	-	25.0
19	21.5-46.5 eV	0.77	88.0	45	2.42	31	-	12	140	-	-	58.0	-	82.0
20	10.0-21.5 eV	0.77	111	45	2.42	54	-	12	120	-	-	82.0	-	38.0
21	4.65-10.0 eV	0.77	93.0	37	2.42	44	-	12	190	-	-	171	-	19.0
22	2.15-4.65 eV	0.77	39.0	20	2.42	7	-	12	9.54	-	-	0.54	-	9.00
23	1.0-2.15 eV	0.77	61.0	35	2.42	13	-	13	9.47	-	-	0.47	-	9.00
24	0.465-1.0 eV	0.77	88.0	64	2.42	10	-	14	9.58	-	-	0.58	-	9.00
25	0.215-0.465 eV	0.77	205	155	2.42	35	-	15	9.90	-	-	0.90	-	9.00
T	0.0252 eV	-	698	582	2.42	101	-	15	11.7	-	-	2.71	-	9.00

Table M7.A.3b Bondarenko self-shielding factors for ^{235}U

Group	T K	f_f at σ_o equal to				f_c at σ_o equal to				f_i at σ_o equal to			f_e at σ_o equal to		
		10^3	10^2	10	0	10^3	10^2	10	0	10^2	10	0	10^2	10	0
	300	1.00	1.00	0.98	0.97	1.00	1.00	0.98	0.97	1.00	0.99	0.98	1.00	1.00	1.00
11	900	1.00	1.00	1.00	0.99	1.00	1.00	1.00	0.99	1.00	1.00	1.00	1.00	1.00	1.00
	2100	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
	300	1.00	0.99	0.96	0.94	1.00	0.99	0.96	0.94	1.00	0.98	0.96	1.00	1.00	0.99
12	900	1.00	1.00	0.98	0.97	1.00	1.00	0.98	0.97	1.00	0.99	0.98	1.00	1.00	1.00
	2100	1.00	1.00	1.00	0.99	1.00	1.00	1.00	0.99	1.00	1.00	0.99	1.00	1.00	1.00
	300	1.00	0.99	0.93	0.89	1.00	0.99	0.93	0.89	0.99	0.96	0.93	1.00	0.99	0.98
13	900	1.00	1.00	0.97	0.94	1.00	1.00	0.97	0.94	1.00	0.99	0.97	1.00	1.00	0.99
	2100	1.00	1.00	0.99	0.98	1.00	1.00	0.99	0.98	1.00	1.00	0.99	1.00	1.00	1.00
	300	1.00	0.97	0.88	0.82	1.00	0.97	0.88	0.82	0.96	0.92	0.88	1.00	0.98	0.96
14	900	1.00	0.99	0.95	0.91	1.00	0.99	0.95	0.91	0.99	0.97	0.94	1.00	0.99	0.97
	2100	1.00	1.00	0.98	0.97	1.00	1.00	0.98	0.97	1.00	0.99	0.97	1.00	1.00	0.98
	300	1.00	0.94	0.82	0.75	1.00	0.94	0.81	0.74	0.93	0.88	0.82	0.99	0.97	0.95
15	900	1.00	0.97	0.92	0.86	1.00	0.97	0.92	0.85	0.97	0.95	0.93	1.00	0.99	0.97
	2100	1.00	0.99	0.97	0.93	1.00	0.99	0.97	0.93	0.99	0.98	0.97	1.00	1.00	0.99
	300	0.99	0.90	0.75	0.67	0.99	0.89	0.74	0.65	0.85	0.78	0.73	1.00	1.00	1.00
16	900	1.00	0.95	0.87	0.81	1.00	0.95	0.86	0.80	0.94	0.89	0.86	1.00	1.00	1.00
	2100	1.00	0.98	0.93	0.89	1.00	0.98	0.93	0.88	0.98	0.95	0.93	1.00	1.00	1.00
	300	0.97	0.83	0.67	0.60	0.97	0.81	0.64	0.56	0.80	0.70	0.62	1.00	1.00	1.00
17	900	0.99	0.90	0.81	0.75	0.99	0.89	0.79	0.72	0.87	0.83	0.77	1.00	1.00	1.00
	2100	1.00	0.97	0.93	0.88	1.00	0.97	0.92	0.86	0.94	0.91	0.90	1.00	1.00	1.00
	300	0.95	0.77	0.61	0.55	0.94	0.74	0.56	0.48	0.70	0.56	0.50	1.00	1.00	1.00
18	900	0.97	0.82	0.71	0.64	0.96	0.80	0.68	0.59	0.75	0.64	0.58	1.00	1.00	1.00
	2100	0.99	0.87	0.80	0.73	0.98	0.86	0.78	0.70	0.80	0.72	0.66	1.00	1.00	1.00
	300	0.91	0.70	0.56	0.52	0.90	0.65	0.48	0.43	0.57	0.42	0.39	1.00	1.00	1.00
19	900	0.93	0.73	0.60	0.56	0.92	0.67	0.52	0.47	0.59	0.45	0.42	1.00	1.00	1.00
	2100	0.95	0.76	0.64	0.60	0.94	0.70	0.56	0.51	0.61	0.48	0.45	1.00	1.00	1.00
	300	0.88	0.64	0.52	0.49	0.86	0.58	0.42	0.38	0.46	0.36	0.32	1.00	1.00	1.00
20	900	0.90	0.66	0.53	0.50	0.88	0.60	0.43	0.39	0.47	0.37	0.33	1.00	1.00	1.00
	2100	0.91	0.67	0.53	0.51	0.90	0.62	0.44	0.40	0.48	0.38	0.34	1.00	1.00	1.00
	300	0.86	0.62	0.50	0.47	0.83	0.55	0.40	0.35	0.42	0.31	0.29	1.00	1.00	1.00
21	900	0.87	0.63	0.50	0.47	0.84	0.56	0.41	0.36	0.43	0.32	0.29	1.00	1.00	1.00
	2100	0.88	0.64	0.51	0.48	0.85	0.57	0.42	0.37	0.44	0.32	0.30	1.00	1.00	1.00
	300	1.00	0.90	0.79	0.74	0.97	0.81	0.62	0.56	0.82	0.68	0.64	1.00	1.00	1.00
22	900	1.00	0.90	0.79	0.74	0.97	0.81	0.62	0.56	0.82	0.68	0.64	1.00	1.00	1.00
	2100	1.00	0.90	0.79	0.74	0.97	0.81	0.62	0.56	0.82	0.68	0.64	1.00	1.00	1.00
	300	1.00	0.87	0.74	0.70	1.00	0.86	0.69	0.64	0.80	0.65	0.63	1.00	1.00	1.00
23	900	1.00	0.87	0.74	0.70	1.00	0.87	0.74	0.70	0.80	0.65	0.63	1.00	1.00	1.00
	2100	1.00	0.87	0.74	0.70	1.00	0.87	0.74	0.70	0.80	0.65	0.63	1.00	1.00	1.00

Table M7.A.3c Bondarenko self-shielding factors for ^{238}U

Group	T K	f_c at σ_o equal to						f_i at σ_o equal to				f_e at σ_o equal to			
		∞	10^4	10^3	10^2	10	0	10^3	10^2	10	0	10^3	10^2	10	0
10	300	1.00	1.00	1.00	0.99	0.98	0.93	1.00	1.00	0.98	0.97	1.00	1.00	0.99	0.98
	900	1.00	1.00	1.00	0.99	0.98	0.96	1.00	1.00	1.00	0.98	1.00	1.00	0.99	0.98
	2100	1.00	1.00	1.00	1.00	1.00	0.99	1.00	1.00	1.00	0.99	1.00	1.00	1.00	1.00
11	300	1.00	1.00	1.00	0.98	0.89	0.80	1.00	0.99	0.96	0.92	1.00	1.00	0.97	0.93
	900	1.00	1.00	1.00	0.99	0.95	0.90	1.00	1.00	0.98	0.93	1.00	1.00	0.97	0.95
	2100	1.00	1.00	1.00	1.00	0.99	0.97	1.00	1.00	0.99	0.94	1.00	1.00	0.99	0.98
12	300	1.00	1.00	0.99	0.92	0.75	0.63	0.99	0.98	0.87	0.73	0.99	0.98	0.91	0.85
	900	1.00	1.00	0.99	0.95	0.86	0.77	1.00	0.99	0.89	0.73	1.00	0.98	0.93	0.87
	2100	1.00	1.00	1.00	0.98	0.93	0.87	1.00	1.00	0.93	0.73	1.00	1.00	0.95	0.88
13	300	1.00	1.00	0.96	0.82	0.56	0.46	0.95	0.88	0.75	0.60	0.98	0.94	0.84	0.70
	900	1.00	1.00	0.98	0.89	0.66	0.55	0.96	0.90	0.78	0.61	0.99	0.95	0.87	0.73
	2100	1.00	1.00	1.00	0.95	0.79	0.67	0.97	0.94	0.82	0.62	1.00	0.99	0.92	0.76
14	300	1.00	0.99	0.89	0.63	0.34	0.29	0.91	0.74	0.64	0.50	0.95	0.84	0.74	0.60
	900	1.00	1.00	0.93	0.74	0.43	0.36	0.92	0.78	0.65	0.51	0.97	0.86	0.77	0.63
	2100	1.00	0.99	0.97	0.82	0.51	0.42	0.93	0.82	0.68	0.53	0.99	0.91	0.82	0.66
15	300	0.99	0.97	0.81	0.42	0.23	0.17	0.84	0.60	0.53	0.43	0.86	0.66	0.56	0.48
	900	1.00	0.98	0.87	0.52	0.29	0.21	0.85	0.64	0.54	0.43	0.90	0.70	0.58	0.49
	2100	1.00	1.00	0.93	0.60	0.34	0.26	0.87	0.68	0.55	0.44	0.90	0.70	0.60	0.50
16	300	0.97	0.94	0.65	0.27	0.136	0.106	0.87	0.60	0.50	0.46	0.84	0.73	0.68	0.63
	900	0.99	0.95	0.74	0.35	0.18	0.132	0.92	0.63	0.51	0.46	0.88	0.75	0.70	0.64
	2100	1.00	0.97	0.83	0.45	0.23	0.17	0.95	0.66	0.52	0.46	0.92	0.78	0.72	0.65
17	300	0.95	0.83	0.35	0.13	0.063	0.049	0.38	0.17	0.14	0.070	0.37	0.23	0.19	0.12
	900	0.97	0.86	0.38	0.15	0.071	0.053	0.45	0.17	0.15	0.070	0.38	0.24	0.20	0.12
	2100	0.99	0.89	0.44	0.17	0.081	0.063	0.51	0.18	0.16	0.070	0.40	0.25	0.21	0.12
18	300	0.91	0.81	0.30	0.108	0.052	0.042	0.39	0.29	0.25	0.22	0.54	0.45	0.42	0.38
	900	0.93	0.87	0.33	0.12	0.055	0.044	0.44	0.30	0.25	0.22	0.54	0.45	0.42	0.38
	2100	0.95	0.94	0.37	0.13	0.061	0.049	0.48	0.30	0.26	0.22	0.54	0.45	0.42	0.38
19	300	0.88	0.60	0.19	0.058	0.029	0.023	0.15	0.096	0.078	0.047	0.29	0.17	0.14	0.10
	900	0.90	0.67	0.23	0.060	0.029	0.023	0.16	0.096	0.078	0.047	0.33	0.18	0.14	0.10
	2100	0.91	0.75	0.28	0.070	0.029	0.023	0.17	0.096	0.078	0.047	0.37	0.19	0.15	0.10
20	300	0.86	0.66	0.23	0.065	0.030	0.023	0.17	0.11	0.087	0.075	0.43	0.31	0.28	0.24
	900	0.87	0.73	0.28	0.073	0.030	0.023	0.20	0.11	0.087	0.075	0.47	0.31	0.28	0.24
	2100	0.88	0.82	0.36	0.080	0.030	0.023	0.23	0.11	0.087	0.075	0.51	0.32	0.28	0.24
21	300	1.00	0.71	0.27	0.084	0.041	0.034	0.16	0.093	0.072	0.059	0.64	0.54	0.52	0.49
	900	1.00	0.78	0.33	0.089	0.041	0.034	0.18	0.094	0.072	0.059	0.66	0.55	0.52	0.49
	2100	1.00	0.86	0.40	0.105	0.041	0.034	0.21	0.095	0.072	0.059	0.69	0.56	0.52	0.49

M7.A.13 THE KNIGHT-MODIFIED HANSEN-ROACH CROSS-SECTION LIBRARY

M7.A.13.1 Modifications Made by J. R. Knight to the ^{238}U Capture Cross Section for Concentrated Systems ($\sigma_o < 400$ barns)

The original Hansen-Roach library was one of the first multigroup libraries used in the United States for criticality analyses. It was deemed quite useful insofar as it did account for the gross spectral effects of resonance self-shielding (cf. Sect. M7.A.10). Unfortunately, many of the resonance parameters available at that time had not yet been fully refined and, indeed, the methodology used by Hansen and Roach did not account for Doppler broadening, interference effects in resonance scattering, or resonance overlap. When used to analyze well-thermalized critical experiments at room temperature, it was not uncommon to calculate k-effective's between 0.8 and 0.9. Raffety and Mihalczo[22] report one case involving a 2% enriched mixture of UF_4 in paraffin ($H/^{235}U = 195$; $\sigma_o^{28} \approx 120$) where the measured value of k_∞ was 1.195 ± 0.015, but the calculated value using the original Hansen-Roach data was 1.114. Characteristically, the original Hansen-Roach data have been found to overestimate the resonance capture in ^{238}U.* Obviously, in fast systems where the resonance escape probability is less important and the amount of ^{238}U is somewhat reduced, this difficulty is not so apparent.

To develop a set of data that could be used with good results in the analysis of thermal systems, J. R. Knight and G. E. Whitesides modified the resonance-self-shielded, group-averaged cross sections given by Hansen and Roach as a function of σ_o (cf. Fig. M7.A.9). Given that uncertainties in the resonance parameters or improvements in the calculation of the resonance integrals would affect both the fission and capture cross sections in the same way, and the fact that the resulting changes in the calculated reactivity would tend to cancel, they decided not to modify the reported data for any of the fissile isotopes. This decision was also justified on the grounds that the Hansen-Roach data were known to give fairly good results whenever the background cross σ_o^1 was greater than several hundred barns. Obviously in a low-enriched system where $N^{25}/N^U < 3\%$, the background cross section for the ^{235}U self-shielding calculation is quite large. That is,

$$\sigma_o^{25} \equiv \frac{1}{N^{25}}(N^{25}\sigma_p^{25} + N^{28}\sigma_p^{28} + ...) = (12)\left[1 + \left(\frac{N^{28}}{N^{25}}\right) + ...\right]. \qquad \text{(M7.A.179)}$$

In a 3% enriched system σ_o^{25} will be $\gtrsim 400$ barns, and the need for better self-shielding factors for $\sigma_o^{25} \lesssim 400$ barns was viewed as academic. Consequently, they focused their attention solely on the resonance-self-shielded capture data for ^{238}U ($\sigma_c^{28,g}$, g = 8,9,10,11,12). Noting the good agreement between the Hansen-Roach data for ^{238}U (at 0 K) and Dresner's data for ^{238}U (at 300 K) whenever σ_o^{28} was $\gtrsim 200$ barns, and noting that calculated values of k_∞ using the Hansen-Roach data were in good agreement with a number of critical experiments whenever σ_o^{28} was $\gtrsim 400$ barns, they then decided to modify the capture data only for those cases where the background cross section (σ_o^{28}) was less than 400 barns.

To modify the Hansen-Roach data in a systematic way, Knight et al. relied on a series of experiments[23,24] in which k-infinity (k_∞) was measured for several different fissile mixtures as a function of the H/U ratio. The first set of experimental measurements involved relatively dry mixtures of UO_3 and water having H/U ratios between 3.7 and 7.5. The second set of measurements involved homogeneous mixtures of UO_3 and paraffin having H/U ratios between 3.6 and 30.2. The final set of measurements involved

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*Interestingly, if one modifies the original Hansen-Roach data to account for Doppler broadening and/or resonance scattering, the capture cross sections for ^{238}U would tend to increase, thus making the calculated values for k_∞ even worse. The difficulty, therefore, was assumed to lie in the resonance parameters that were used at the time the original library was compiled.

homogeneous mixtures of $UO_2(NO_3)_2$ and paraffin having H/U ratios between 6.1 and 31.0. In the first set of experiments, the uranium was enriched to ~1 wt % ^{235}U, while in the other two it was enriched to ~3 wt % ^{235}U. Table M7.A.4 shows the explicit H/U ratios that were present in each mixture and the corresponding value of the background cross section (σ_o^{28}) that should be used to determine the resonance-self-shielded, group-averaged cross sections for the ^{238}U in each case. Attention was eventually focused on just a handful of these experiments (σ_o^{28} = 109b, 157b, 182b, 216b, 267b, 321b, and 366b). In each case, the Hansen-Roach capture data for ^{238}U was numerically scaled up or down until the calculated value of k_∞ agreed with the measured value of k_∞. To be more precise, these adjusted data (commonly referred to as the Knight-Modified Hansen-Roach data) were defined by multiplying the original Hansen-Roach data by a fudge factor [$x(\sigma_o)$] which was assumed to be the same for each energy group:

$$\sigma_{KM}^{28,g}(\sigma_o) = x(\sigma_o)\sigma_{HR}^{28,g}(\sigma_o) \quad g = 8,9,10,11,12 \qquad \text{(M7.A.180)}$$

The corresponding fudge factors [$x(\sigma_o)$, σ_o = 109b, 157b, 182b, 216b, 267b, 321b, and 366b] were then determined by trial and error for each of the seven different experiments, and plotted as a function of σ_o. Interestingly, simple extrapolation of $x(\sigma_o)$ to σ_o = 45b yielded a fudge factor very close to that required (0.77) to bring the original Hansen-Roach data into agreement with that obtained using the Doppler-broadened resonance integrals computed by Dresner. That value (0.77 at σ_o = 45b) was therefore taken as an additional anchor point. For values of $\sigma_o \gtrsim$ 400b, $x(\sigma_o)$ was assumed to be 1.0.

Knowing $x(\sigma_o)$ as a function of σ_o, Knight et al. then made plots of the resonance self-shielded, group-averaged capture cross sections for ^{238}U, similar to those shown in Fig. M7.A.9 [$\sigma_{c,KM}^{28,g}(\sigma_o)$, g = 8,9,10,11,12]. Based on that, they later prepared multigroup cross-section sets for many different values of σ_o(σ_o = 12; 15,20,25,...100; 110,120,130,140; 160,180,...,300; 330,360,etc). This Knight-Modified Hansen-Roach data were then released as part of the standard 16-group cross-section library packaged with the KENO IV Monte Carlo code[16] for criticality analysis. Owing to the wide popularity of the code itself, the availability of the cross-section data and instructions for its use, and the good agreement that people subsequently obtained with still other experiments,[22] the Knight-Modified Hansen-Roach data became even more popular and were subsequently adopted for use as one of the libraries in the SCALE system for Standardized Computer Analyses for Licensing Evaluation. At the time that it was adopted for use in the SCALE system, the infinitely dilute cross sections in each energy group were used to reduce the various background-dependent libraries to Bondarenko factors so that the appropriate resonance-self-shielded, group-averaged cross sections for a given mixture could be obtained automatically by application of the Iterative Bondarenko Method as embodied in the BONAMI code (cf. Sect. M7.A.8). Since that time, results using this library have been benchmarked against dozens of critical experiments, with excellent agreement in each case.[25]

M7.A.13.2 Brief Description of the Experiments Upon Which the Knight Modifications Were Based

The original experiments upon which the Knight modifications were based are well documented in refs. 23 and 24. All three sets of experiments described in the two reports were performed at the Physical Constants Testing Reactor in Hanford, Washington. Because the experimental results were reported in terms of k_∞ (rather than k_{eff} for a finite system), the corresponding 0-dimensional spectral calculations performed by Knight were straightforward and free of geometric approximation. To achieve such a measurement, a relatively large sample of the given material was placed in the central cavity of the test reactor. The PCTR was a graphite-moderated assembly driven by highly enriched fuel. It measured 7 ft × 7 ft × 7 ft and had a central

Table M7.A.4Values of the background cross section (σ_0^{28}) for several different experiments in which k_∞ of the homogeneous mixture was measured as a function of the H/U ratio (shown here in parentheses)

UO_3/H_2O	UO_3/C_2H_2	$UO_2(NO_3)_2/C_2H_2$
109 (3.73)[a]	110 (3.58)	---
139 (5.00)	---	---
157 (5.78)[a]	---	---
166 (6.16)	165 (5.86)	---
---	177 (6.38)	---
182 (6.88)[a]	---	---
196 (7.50)	---	---
---	---	210 (6.10)
---	216 (8.01)[a]	---
---	230 (8.60)	---
---	267 (10.12)[a]	---
---	---	275 (8.81)
---	321 (12.36)[a]	---
---	---	366 (13.02)[a]
---	749 (30.20)	---
---	---	808 (31.00)

[a] Used in generating the Knight-Modified Hansen Roach data.

cavity measuring 2 ft × 2 ft × 3 ft. Near the center of the reactor the flux was spatially flat, as it would be in an infinite sample of the test material. The sample section(s) consisted of a central test sample surrounded by a relatively thick "buffer" region which was a layer of material identical to that used in the central test sample. The purpose of the buffer region was to provide a medium in which the neutron spectrum could come into equilibrium with the central test sample. By making the buffer region thick enough, the resulting spectrum in the central test sample would be essentially identical to that which would exist in an infinite system. Measurements of the (infinite) multiplication factor for the central test sample were then made by comparing the behavior of the reactor with the central test sample in place and with a void in the same region. [Since a neutron entering the central void must simply pass through it and come out again, the multiplication factor of the void (k_∞) is exactly 1.0.] The actual measurements were then made in the following fashion:

1. Adjust the reactor so that it is critical with the buffer and central test sample removed.

2. For a given test sample with a known H/U ratio, calculate the amount of poison that is required to yield $k_\infty^P = 1.0$ [where k_∞^P denotes the infinite multiplication factor for the poisoned system (central test sample and buffer)]. Note that a nonfissile 1/v thermal absorber was used for this purpose.

3. Insert the buffer only, and make minor adjustments in the reactor so that it is again critical with only the buffer in place.

4. Insert control rods to shut down the reactor, and insert the central test sample.

5. Make the reactor slightly supercritical to build up the observable flux, then slowly return the control rods to position (3) and measure the resulting period.

6. If the resulting period is not infinite (i.e., if the reactor is not critical), remove the buffer region and the central test sample, and adjust the amount of poison in both (up or down) as required.

7. Repeat steps 3, 4, 5, and 6 until the multiplication factor for the poisoned test sample (k_∞^P) is 1.0.

8. Knowing the amount of poison required to make $k_\infty^P = 1.0$, calculate k_∞ for the unpoisoned sample and report these values.

Because of the difficulty associated with making ultra-fine adjustments in the poison content of the test material, the amount of poison required to make k_∞^P exactly 1.0 (cf. steps 7 and 8) was ultimately interpolated using results for poisoned test samples having very long positive and negative periods. Details of the calculations required in step 8 are well documented in refs. 23 and 24.

Throughout the experiments, bare and cadmium-covered gold foils were placed at various positions in the buffer and the central test sample so as to verify that (a) the flux was spatially flat across the entire region and that (b) the flux spectrum had indeed reached the equilibrium state (corresponding to an infinite system) in the vicinity of the central test sample.

Because these experiments were performed at room temperature (293°K), and because the Knight-Modified data for ^{238}U was based on these experiments, the 16-group Knight-Modified Hansen-Roach library now found in the SCALE system should (and does) give good results for other critical experiments at room temperatures despite the fact that much of the data for the other resonance nuclides is the original (unbroadened) Hansen-Roach data at 0 K.

M7.B ALPHABETICAL SUBROUTINE INDEX AND CROSS REFERENCE

This section provides a convenient alphabetical index of the subroutines and functions and common blocks used in the Material Information Processor.

Table M7.B.1 provides an alphabetical listing of the subroutines and functions that comprise the Material Information Processor. The first column lists the subroutine name, the second column lists the subroutine that calls it, and the third column contains a list of the subroutines it calls.

Table M7.B.2 provides an alphabetical index of the common blocks used in the Material Information Processor.

Table M7.B.1 Alphabetical index of Material Information Processor routines

Subroutine Name	Calling Subroutine	Called Subroutine
adan	dan	gauss gdan
agauss	dan sphdan	
archk	dan	
array3	mixtab	crite inquir rite
avg1	clapse	
avg2	twodxs	mgcwrd
avgb	bond	
avgy	twodys	mgcwrd stop
axsdrn	c4data	
ball	dandad	(sqrt) sphdan
binfil	ice xsdrn	

Table M7.B.1 (continued)

Subroutine Name	Calling Subroutine	Called Subroutine
binrcf	bonami ice nitawl xsdrn	
binrcx	bonami ice nitawl xsdrn	
bonami	c4data	binrcf binrcx inquir lchkmx rite
bond	clapse	avgb fold io unfold
bonda	resda	(sqrt)
c4data		axsdrn bonami calcms cellmx clapse clear epsig ice knight lrderr mipchk nitawl prelps rmunit shortx smmtba stop verify xsdrn xsmesh

Table M7.B.1 (continued)

Subroutine Name	Calling Subroutine	Called Subroutine
calcms	c4data	lchkmx
cellmx	c4data	lchkmx
cinit	setupb	clear inquir openda rite
clapse	c4data	avg1 bond clear copy dean io io4 stop twodxs twodys
csparm	setupa	aread lcompr smmtba
dan	dandad	adan agauss archk
dancof	resda	dandad e3 shelc stop
dandad	dancof	ball dan sdan
dean	clapse	kaul
epsig	c4data	
fax	stdcmp	fread iread

Table M7.B.1 (continued)

Subroutine Name	Calling Subroutine	Called Subroutine
faxprt	stdcmp	
finner	outer	
fix	stdcmp	
fold	bond	
fox	scdata	
gauss	adan outer	
gdan	adan	ki3
gflux	prelps	
hoggie	twodys	stop
ice	c4data	binfil binrcf binrcx inquir rite volfrc
idents	mtable	iscan nofrac
iscan	idents modify nitawl reordr resda scdata slns	
kaul	dean	
knight	c4data	closda mesage openda reed setupa stop

Table M7.B.1 (continued)

Subroutine Name	Calling Subroutine	Called Subroutine
latcel	setupb	aread fread iread lcompr mixerr scanof scanon
lchkmx	bonami calcms cellmx xsdrn	
logid	shortx	
mipchk	c4data	wot8
mixerr	latcel moredt multrg	
mixtab	setupb	array3 modify mtable reordr stop
modify	mixtab	iscan
moredt	setupb	allowc aread fread iread lread mixerr resetc scanof scanon
mtable	mixtab	idents stop

Table M7.B.1 (continued)

Subroutine Name	Calling Subroutine	Called Subroutine
multrg	setupb	aread fread iread lcompr lread mixerr scanof scanon
nflux	prelps	
nitawl	c4data	binrcf binrcx clear inquir iscan rite
nofrac	idents	wtinv
outer	sphdan	finner gauss
patch	twodxs twodys	
poke	setupb	
prelps	c4data	gflux nflux
reordr	mixtab	iscan
resda	setupb	bonda dancof iscan lcompr
scdata	stdcmp	aread clear fox fread iread iscan reed

Table M7.B.1 (continued)

Subroutine Name	Calling Subroutine	Called Subroutine
sdan	dandad	e3
setupa	knight	aread
		creed
		csparm
		fread
		inquir
		iread
		lcompr
		lread
		opnfil
		reed
		scanon
		setupb
		smmtba
		stop
setupb	setupa	aread
		cinit
		clear
		inquir
		iread
		latcel
		lcompr
		mixtab
		moredt
		multrg
		poke
		resda
		rite
		stdcmp
		stop
shortx	c4data	closda
		copy
		dtaset
		iowrt
		logid
		openda
		opnfil
		reed
		y0trns

Table M7.B.1 (continued)

Subroutine Name	Calling Subroutine	Called Subroutine
slname	stdcmp	
slns	stdcmp	iscan
smmtba	c4data	lcompr
	csparm	
	setupa	
sphdan	ball	agauss
		outer
stdcmp	setupb	aread
		clear
		fax
		faxprt
		fix
		fread
		iread
		lread
		reed
		scanof
		scdata
		slname
		slns
twodxs	clapse	avg2
		clear
		copy
		io
		io4
		patch
twodys	clapse	avgy
		clear
		copy
		hoggie
		io
		io4
		move
		patch
		stop

Table M7.B.1 (continued)

Subroutine Name	Calling Subroutine	Called Subroutine
unfold	bond	
verify	c4data	voljb
volfrc	ice	
voljb	verify	
wtinv	nofrac	
xsdrn	c4data	binfil binrcf binrcx clear inquir lchkmx rite stop
xsmesh	c4data	iread stop

Table M7.B.2 lists the labeled common blocks used in the Material Information Processor and an alphabetical listing of the subroutines that reference them.

Table M7.B.2 Commons used in the Material Information Processor

Common Name	Referencing Subroutine
blklnc	cinit
	moredt
	setupb
	stdcmp
ccdata	c4data
	knight
	setupa
	setupb
cdata	c4data
	knight
	setupa
	setupb
celmix	cellmx
clad	dandad
	gdan
	sdan
compoz	calrho
	knight
	mtable
cunit	archk
	calrho
	csparm
	faxprt
	idents
	knight
	latcel
	mixtab
	moredt
	mtable
	multrg
	nofrac
	poke
	reordr
	scdata
	setupa
	setupb
	shortx
	slname
	slns
	stdcmp

Table M7.B.2 (continued)

Common Name	Referencing Subroutine
deal	c4data
	dancof
	latcel
	multrg
	poke
	resda
	setupb
dimen	c4data
drtacs	array3
	bonami
	cinit
	ice
	nitawl
	setupb
	shortx
	xsdrn
flg	archk
	c4data
	dancof
	fax
	latcel
	moredt
	multrg
	nofrac
	scdata
	setupa
	setupb
	shortx
	slns
	stdcmp
	verify
	xsmesh
gin	adan
	ball
	dan
	dandad
	finner
	gdan
	outer
	sphdan

Table M7.B.2 (continued)

Common Name	Referencing Subroutine
liba	c4data
	epsig
	fix
	fox
	knight
	latcel
	mipchk
	mixtab
	modify
	multrg
	resda
	scdata
	setupa
	setupb
	shortx
	stdcmp
libc	c4data
	epsig
	fix
	fox
	knight
	latcel
	mipchk
	mixtab
	modify
	multrg
	resda
	scdata
	setupa
	setupb
	shortx
	stdcmp
lpnt	c4data
	cinit
	setupb
parm	c4data
	moredt
	setupa
	setupb

Table M7.B.2 (continued)

Common Name	Referencing Subroutine
pass	c4data
	dancof
	knight
	latcel
	mipchk
	mixtab
	modify
	moredt
	multrg
	poke
	resda
	setupa
	setupb
	verify
	xsdrn
pass2	c4data
	knight
	mixtab
	moredt
	setupa
	setupb
	xsdrn
pointa	c4data
	setupa
	setupb
pointb	c4data
	setupa
	setupb
pointc	c4data
	setupa
	setupb

Table M7.B.2 (continued)

Common Name	Referencing Subroutine
unit	array3
	bonami
	cinit
	ice
	nitawl
	resda
	setupb
	shortx
	xsdrn
units	c4data
xsdrnc	ice
	moredt
	nitawl
	setupb
	xsdrn

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STANDARD COMPOSITION LIBRARY

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ABSTRACT

This document provides a listing of the Standard Composition Library currently available within the SCALE system. A separate listing is also provided for available standard solutions that may be specified.

CONTENTS

LIST OF TABLES

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M8.1 INTRODUCTION

The Standard Composition Library has been included within the SCALE system to provide the user with a simple and straightforward method of specifying the material mixtures for a given problem. The library consists of over 600 mixtures and isotopes commonly used within shielding and criticality problems. This library is tabulated in Sect. M8.2 with the various features of each composition. Additionally, a number of standard fissile solutions available for use are tabulated in Sect. M8.3.

As the need arises, the Standard Composition Library will be updated to include an even greater selection of mixtures and solutions. However, if the user has a need to specify a mixture not currently in the library, this step may be achieved using the procedures described in Sect. M7.5.5.2.

M8.2 THE STANDARD COMPOSITION LIBRARY

The Standard Composition Library describes the various isotopes, elements (both symbols and full name), and compounds/alloys that can be used to define the material mixtures for a given problem. Typically, the alphanumeric description of one or more of these materials will be used to define a material mixture, as noted in Sect. M7.4.4.

Full-name elements reference Z*1000 identifier. If this identifier is not available on the cross-section library, the isotope table is then referenced. Elements with symbol names reference the same identifier as full-name elements with a few exceptions. Elements with 100% abundance of one isotope (e.g., gold) reference that isotope. Some light elements reference the principal isotopes. (Examples O - 8016, N - 7014, C - 6012, H - 1001)

When formulating a mixture, it is often necessary to know the density (g/cc) of the various constituent materials. For convenience, the reference values given in the library have been listed in Tables M8.2.1 through M8.2.5 (at end of this section). Note that the given reference values represent the actual theoretical density, except in the case of isotopes and some individual nuclides where a default value of 1.0 g/cc was used. The actual theoretical densities are fixed values at naturally occurring or nominal conditions. These default densities should not be used for materials containing enriched isotopes, especially light elements with strong absorbers such as boron, B_4C, or lithium.

The temperature of a given material can be entered, but is not required (cf. Sect. M7.4.4). However, the temperature should be entered if resonance data or Bondarenko data are available for the material, or if thermal-scattering data are available at more than one temperature. Note that nuclides having resonance data differ from one master cross-section library to another. Section M4 (SCALE Cross-Section Libraries) addresses resonance data and Bondarenko data in more detail. Users may find this information interesting and/or helpful.

Multiple sets of iron, nickel, and chromium nuclides are available in the Standard Composition Library (see Tables M8.2.1 through M8.2.6). These sets correspond to different weighting functions used in generating the multigroup cross sections. The special weighting functions correspond to 1/E σ_t (E), where σ_t (E) is the total cross section of either stainless steel 304 or Inconel for use in mixing such alloys. These weighting functions specifically apply to the 27- and 218-group libraries generated from ENDF/B-IV data. In order for the stainless steel and Inconel standard composition identifiers to be usable with the Hansen Roach library, the 218-group library sets with the special weighting functions were collapsed to 16 groups and added to the Hansen Roach data set. For the 44- and 238-group libraries generated from ENDF/B-V data, there are two special weighting functions. One special weighting function corresponds to 1/E σ_t (E), where σ_t (E) is the total cross section of stainless steel 304. In the other special weighting, σ_t (E) is the cross section for the referenced nuclide. Two standard composition names, SS304S and INCONELS, have been added to reference the standard iron, nickel, and chromium nuclides instead of the specially weighted ones. Entries have been added to the isotopic distribution table so that standard weighted isotopes will be requested if the desired nuclide is not on the specified library.

The nuclide identifying numbers (ID) are listed in column 3 of Tables M8.2.1 through M8.2.5. Typically, the ID number is A +1000*Z, where Z and A are the charge and mass numbers for the nuclide (e.g., 1001 for hydrogen and 8016 for oxygen). Exceptions to this rule include metastable nuclides, nuclides with bound thermal scattering data, and nuclides whose cross sections have a special weighting. Also, elements with isotopic mixtures (typically natural abundance) have ID numbers of Z*1000.

The nuclide's mass, σ_t and σ_s, are shown in Table M8.2.6, the nuclide identification table. The σ_t and σ_s values are used in generating resonance self-shielding parameters and in generating the spatial mesh for XSDRN. If the nuclide occurs in the 238-group ENDF/B-V cross-section library, the values in the table are

the result of integrating the data for that nuclide over the groups between 5 eV and 5 keV using a flat in lethargy over σ_t weight function. Nuclides that do not occur in this library but do occur in a 199-group ENDF/B-VI library are generated from that library in the same fashion. Data for other nuclides are of unknown origin. If a nuclide identifier is listed in this table, it can be accessed and used in an arbitrary material. Arbitrary materials require the user to provide all the information normally found in the Standard Composition Library.

Those materials in the Standard Composition Library containing multiple isotopes of a single element are denoted in columns 4 and 5 of Table M8.2.3. For these materials, the user is free to specify the isotopic distribution using items 6a and 6b of the Standard Composition Specification Card discussed in Sects. M7.4.4 and C4.4.4. Alternatively, the user may elect not to enter this data, thereby telling the code to assume the default values shown in column 3 of Table M8.2.3. In all cases except plutonium, Table M8.2.3 lists the naturally occurring abundance of each isotope. In describing an arbitrary material, a multiple isotope ID of Z * 1000 (where Z is the nuclide charge number) can be used to denote the elements of Table M8.2.3. Then, if an isotope distribution other than the default values of Table M8.2.3 is desired, items 6a and 6b of the Standard Composition Specification Card (see Sect. M7.4.4) must be included.

Atomic masses for the isotopes were taken from ENDF/B-VI[1] where available except for ^{16}O. The atomic masses of remaining nuclides were taken from ENDF/B-V[2] if available there. If not available from the above sources, the atomic masses were taken from the GE Chart of the Nuclides.[3] Potassium-40 was not available in any of these sources and was taken from the Trilinear Chart of the Nuclides.[4] The atom percents of the isotopic distribution table were taken from the GE Chart of the Nuclides. Densities were taken from the CRC Handbook.[5] Gases and explicit isotopes were changed to all have a theoretical density of 1.0 g/cc.

To more fully document the composition of each compound and/or document the assumptions used in producing the associated cross-section data, a brief description of each material in Tables M8.2.4 and M8.2.5 is included here:

Compounds (atoms per molecule)

B4C	Boron carbide: B_4C; natural isotopic distribution obtained by default, 2.52 g/cc
BALSA	Balsa wood: $C_6H_{10}O_5$, 0.125 g/cc
D2O	Heavy Water: D_2O, 1.1054 g/cc
GRAPHITE	Graphite Carbon: 2.3 g/cc
H2O	Water: cross sections developed using 1/E weighting everywhere, 0.9982 g/cc
H2O-X(E)-HR	Water: cross sections developed using fission spectrum weighting at high energies and 1/E at lower energies, 0.9982 g/cc (Hansen-Roach library only)
HFACID	Hydrafluoric acid: HF
HNO3	Nitric acid: HNO_3
NORPAR13	Normal Paraffin 13: $C_{13}H_{28}$ 0.76 g/cc

NORPAR(H2O)	Normal Paraffin 13: $C_{13}H_{28}$ 0.76 g/cc, uses hydrogen in water thermal kernel
OAK	Oak wood: $C_6H_{10}O_5$, 0.700 g/cc
PARA(H2O)	Paraffin: $C_{25}H_{52}$, 0.90 g/cc, uses hydrogen in water thermal kernel
PARAFFIN	Paraffin: $C_{25}H_{52}$, 0.90 g/cc
PLEXIGLAS, PLEXIGLASS	Plexiglas: $C_5H_8O_2$, 1.18 g/cc
POLY(H2O)	Polyethylene: CH_2, 0.923 g/cc uses hydrogen in water thermal kernel
POLYETHYLENE	Polyethylene: CH_2, 0.92 g/cc
POLYVINYLCL	Polyvinyl chloride: C_2H_3Cl, 1.6 g/cc
PU(NO3)4	Plutonium nitrate: $Pu(NO_3)_4$, 2.447 g/cc
PUC	Plutonium carbide: PuC, 13.6 g/cc
PUF4	Plutonium tetrafluoride: PuF_4, 7.0 g/cc
PUN	Plutonium nitride: PuN, 14.25 g/cc
PUO2	Plutonium oxide: PuO_2, 11.46 g/cc
PVC	Polyvinyl chloride: C_2H_3Cl, 1.6 g/cc
PVC(H2O)	Polyvinyl chloride: C_2H_3Cl, 1.6 g/cc uses hydrogen in water thermal kernel
REDWOOD	Redwood: $C_6H_{10}O_5$, 0.387 g/cc
TBP	Tributyl phosphate: $(C_4H_9)_3PO_4$, 0.9724 g/cc
TBP(H2O)	Tributyl phosphate: $(C_4H_9)_3PO_4$, 0.9724 g/cc uses hydrogen in water thermal kernel
U3O8	Uranium oxide (yellowcake): U_3O_8, 8.3 g/cc
UC	Uranium carbide: UC, 13.63 g/cc
UF4	Uranium tetrafluoride: UF_4, 6.70 g/cc
UF6	Uranium hexafluoride: UF_6, 4.68 g/cc
UN	Uranium nitride: UN, 14.31 g/cc

UO2	Uranium dioxide: UO_2, 10.96 g/cc
UO2(NO3)2	Uranyl nitrate: $UO_2(NO_3)_2$, 2.203 g/cc
UO2F2	Uranyl fluoride: UO_2F_2, 6.37 g/cc
UO3	Uranium trioxide: UO_3, 7.29 g/cc
ZIRCALLOY	Zircaloy-2 is approximated by adding a 1/V capture to zirconium. The thermal capture cross section and resonance capture integrals for Zr-2 and Zr-4 are equal within the experimental measurement uncertainties and the variance allowed on the contents of the alloying agents of Zr-2 and Zr-4. ENDF/B-IV 6.56 g/cc
ZRH2	Zirconium hydride: ZrH_2, 5.61 g/cc
ZR5H8	Zirconium hydride as a mixture of ZrH and ZrH_2, with an effective composition of Zr_5H_8; 5.61 g/cc

Compounds (weight percent)

CARBONSTEEL	Carbon steel: 99 wt % iron, 1 wt % carbon, cross sections developed using 1/E weighting, 7.8212 g/cc
INCONEL	Inconel: 73 wt % nickel, 15 wt % chromium, 7 wt % iron, 2.5 wt % titanium, 2.5 wt % silicon, 8.3 g/cc
INCONELS	Inconel: 73 wt % nickel, 15 wt % chromium, 7 wt % iron, 2.5 wt % titanium, 2.5 wt % silicon, (standard nuclides were used instead of special weighted nuclides) 8.3 g/cc
KEROSENE	Average kerosene: 84 wt % carbon, 16 wt % hydrogen, 0.82 g/cc
KERO(H2O)	Average kerosene: 84 wt % carbon, 16 wt % hydrogen, 0.82 g/cc uses hydrogen for water thermal kernel
MGCONCRETE	Magnuson's Concrete: 49.94 wt % oxygen, 22.63 wt % calcium, 10.53 wt % carbon, 0.9445 wt % potassium, 9.420 wt % magnesium, 4.210 wt % silicon, 0.7859 wt % aluminum, 0.5595 wt % iron, 0.3319 wt % hydrogen, 0.2483 wt % sulfur, 0.148 wt % titanium, 0.1411 wt % sodium, 0.523 wt % chlorine, 0.0512 wt % manganese, 2.147 g/cc
ORCONCRETE	Oak Ridge Concrete: 41.02 wt % oxygen, 32.13 wt % calcium, 17.52 wt % carbon, 3.448 wt % silicon, 3.265 wt % magnesium, 1.083 wt % aluminum, 0.7784 wt % iron, 0.6187 wt % hydrogen, 0.1138 wt % potassium, .0271 wt % sodium, 2.2994 g/cc
PYREX	Pyrex: 53.5 wt % oxygen, 37.7 wt % silicon, 4.1 wt % sodium, 3.7 wt % boron, 1.0 wt % aluminum, 2.23 g/cc

REG-CONCRETE	Regular Concrete: 53.2 wt % oxygen, 33.7 wt % silicon, 4.4 wt % calcium, 3.4 wt % aluminum, 2.9 wt % sodium, 1.4 wt % iron, 1.0 wt % hydrogen, 2.3 g/cc
RFCONCRETE	Rocky Flats Concrete: 48.49 wt % oxygen, 23 wt % calcium, 15.5 wt % silicon, 5.52 wt % carbon, 2.17 wt % aluminum, 1.37 wt % potassium, 1.25 wt % magnesium, 1.01 wt % iron, 0.75 wt % hydrogen, 0.63 wt % sodium, 0.19 wt % sulfur, 0.1 wt % itianium, 0.02 wt % nitrogen, 2.231 g/cc
SS304	Stainless steel-304: 68.375 wt % iron, 19 wt % chromium, 9.5 wt % nickel, 2 wt % manganese, 1 wt % silicon, 0.08 wt % carbon, 0.045 wt % phosphorus, 7.94 g/cc
SS304S	Stainless steel-304: 68.375 wt % iron, 19 wt % chromium, 9.5 wt % nickel, 2 wt % manganese, 1 wt % silicon, 0.08 wt % carbon, 0.045 wt % phosphorus (standard nuclides were used instead of special weighted nuclides) 7.94 g/cc
SS316	Stainless steel-316: 65.375 wt % iron, 17 wt % chromium, 12 wt % nickel, 2.5 wt % molybdenum, 2 wt % manganese, 1 wt % silicon, 0.08 wt % carbon, 0.045 wt % phosphorus, 8.03 g/cc
SS316S	Stainless steel-316: 65.42 wt % iron, 17 wt % chromium, 12 wt % nickel, 2.5 wt % molybdenum, 2 wt % manganese, 1 wt % silicon, 0.08 wt % carbon, 0.045 wt % phosphorus (standard nuclides were used instead of special weighted nuclides) 8.03 g/cc
U(.27)METAL	Depleted uranium metal having a fixed isotope distribution: 0.27 wt % ^{235}U, 99.73 wt % ^{238}U 19.05 g/cc (to specify a different distribution, the user should use URANIUM instead of U(.27)METAL) 19.05 g/cc
ZIRC2	Zircaloy-2: 98.250 wt % zirconium, 1.45 wt % tin, 0.100 wt % chromium, 0.135 wt % iron, 0.055 wt % nickel, 0.01 wt % hafnium, 6.56 g/cc
ZIRC4	Zircaloy-4: 98.23 wt % zirconium, 1.45 wt % tin, 0.1 wt % chromium, 0.210 wt % iron, 0.01 wt % hafnium, 6.56 g/cc

Table M8.2.1 The Standard Composition Library - isotopes

Alphanumeric isotope identifier	Default density	Nuclide identifier	Alphanumeric isotope identifier	Default density	Nuclide identifier
AG-107	1.0	47107	BR-79	1.0	35079
AG-109	1.0	47109	BR-81	1.0	35081
AG-111	1.0	47111	C-12	1.0	6012
AM-241	1.0	95241	C-13	1.0	6013
AM-242	1.0	95242	CA-40	1.0	20040
AM-242M	1.0	95601	CA-42	1.0	20042
AM-243	1.0	95243	CA-43	1.0	20043
AR-36	1.0	18036	CA-44	1.0	20044
AR-38	1.0	18038	CA-46	1.0	20046
AR-40	1.0	18040	CA-48	1.0	20048
AS-75	1.0	33075	CD-106	1.0	48106
B-10	1.0	5010	CD-108	1.0	48108
B-11	1.0	5011	CD-110	1.0	48110
BA-130	1.0	56130	CD-111	1.0	48111
BA-132	1.0	56132	CD-112	1.0	48112
BA-134	1.0	56134	CD-113	1.0	48113
BA-135	1.0	56135	CD-114	1.0	48114
BA-136	1.0	56136	CD-115	1.0	48115
BA-137	1.0	56137	CD-115M	1.0	48601
BA-138	1.0	56138	CD-116	1.0	48116
BA-140	1.0	56140	CE-136	1.0	58136
BI-209	1.0	83209	CE-138	1.0	58138
BK-249	1.0	97249	CE-140	1.0	58140

Table M8.2.1 (continued)

Alphanumeric isotope identifier	Default density	Nuclide identifier	Alphanumeric isotope identifier	Default density	Nuclide identifier
CE-141	1.0	58141	CR-54	1.0	24054
CE-142	1.0	58142	CS-133	1.0	55133
CE-143	1.0	58143	CS-134	1.0	55134
CE-144	1.0	58144	CS-135	1.0	55135
CF-249	1.0	98249	CS-136	1.0	55136
CF-250	1.0	98250	CS-137	1.0	55137
CF-251	1.0	98251	CU-63	1.0	29063
CF-252	1.0	98252	CU-65	1.0	29065
CF-253	1.0	98253	DY-156	1.0	66156
CL-35	1.0	17035	DY-158	1.0	66158
CL-37	1.0	17037	DY-160	1.0	66160
CM-241	1.0	96241	DY-161	1.0	66161
CM-242	1.0	96242	DY-162	1.0	66162
CM-243	1.0	96243	DY-163	1.0	66163
CM-244	1.0	96244	DY-164	1.0	66164
CM-245	1.0	96245	ER-162	1.0	68162
CM-246	1.0	96246	ER-164	1.0	68164
CM-247	1.0	96247	ER-166	1.0	68166
CM-248	1.0	96248	ER-167	1.0	68167
CO-59	1.0	27059	ER-168	1.0	68168
CR-50	1.0	24050	ER-170	1.0	68170
CR-52	1.0	24052	ES-253	1.0	99253
CR-53	1.0	24053	EU-151	1.0	63151

Table M8.2.1 (continued)

Alphanumeric isotope identifier	Default density	Nuclide identifier	Alphanumeric isotope identifier	Default density	Nuclide identifier
EU-152	1.0	63152	GE-76	1.0	32076
EU-153	1.0	63153	H-3	1.0	1003
EU-154	1.0	63154	HE-3	1.0	2003
EU-155	1.0	63155	HF-174	1.0	72174
EU-156	1.0	63156	HF-176	1.0	72176
EU-157	1.0	63157	HF-177	1.0	72177
FE-54	1.0	26054	HF-178	1.0	72178
FE-56	1.0	26056	HF-179	1.0	72179
FE-57	1.0	26057	HF-180	1.0	72180
FE-58	1.0	26058	HG-196	1.0	80196
GA-69	1.0	31069	HG-198	1.0	80198
GA-71	1.0	31071	HG-199	1.0	80199
GD-152	1.0	64152	HG-200	1.0	80200
GD-154	1.0	64154	HG-201	1.0	80201
GD-155	1.0	64155	HG-202	1.0	80202
GD-156	1.0	64156	HG-204	1.0	80204
GD-157	1.0	64157	HO-165	1.0	67165
GD-158	1.0	64158	I-127	1.0	53127
GD-160	1.0	64160	I-129	1.0	53129
GE-70	1.0	32070	I-130	1.0	53130
GE-72	1.0	32072	I-131	1.0	53131
GE-73	1.0	32073	I-135	1.0	53135
GE-74	1.0	32074	IN-113	1.0	49113

Table M8.2.1 (continued)

Alphanumeric isotope identifier	Default density	Nuclide identifier	Alphanumeric isotope identifier	Default density	Nuclide identifier
IN-115	1.0	49115	MO-100	1.0	42100
IR-191	1.0	77191	MO-92	1.0	42092
IR-193	1.0	77193	MO-94	1.0	42094
K-39	1.0	19039	MO-95	1.0	42095
K-40	1.0	19040	MO-96	1.0	42096
K-41	1.0	19041	MO-97	1.0	42097
KR-78	1.0	36078	MO-98	1.0	42098
KR-80	1.0	36080	MO-99	1.0	42099
KR-82	1.0	36082	N-14	1.0	7014
KR-83	1.0	36083	N-15	1.0	7015
KR-84	1.0	36084	NB-93	1.0	41093
KR-85	1.0	36085	NB-94	1.0	41094
KR-86	1.0	36086	NB-95	1.0	41095
LA-138	1.0	57138	ND-142	1.0	60142
LA-139	1.0	57139	ND-143	1.0	60143
LA-140	1.0	57140	ND-144	1.0	60144
LI-6	1.0	3006	ND-145	1.0	60145
LI-7	1.0	3007	ND-146	1.0	60146
LU-175	1.0	71175	ND-147	1.0	60147
LU-176	1.0	71176	ND-148	1.0	60148
MG-24	1.0	12024	ND-150	1.0	60150
MG-25	1.0	12025	NE-20	1.0	10020
MG-26	1.0	12026	NE-21	1.0	10021

Table M8.2.1 (continued)

Alphanumeric isotope identifier	Default density	Nuclide identifier	Alphanumeric isotope identifier	Default density	Nuclide identifier
NE-22	1.0	10022	PB-206	1.0	82206
NI-58	1.0	28058	PB-207	1.0	82207
NI-59	1.0	28059	PB-208	1.0	82208
NI-60	1.0	28060	PD-102	1.0	46102
NI-61	1.0	28061	PD-104	1.0	46104
NI-62	1.0	28062	PD-105	1.0	46105
NI-64	1.0	28064	PD-106	1.0	46106
NP-237	1.0	93237	PD-107	1.0	46107
NP-238	1.0	93238	PD-108	1.0	46108
NP-239	1.0	93239	PD-110	1.0	46110
O-16	1.0	8016	PM-147	1.0	61147
O-17	1.0	8017	PM-148	1.0	61148
O-18	1.0	8018	PM-148M	1.0	61601
OS-184	1.0	76184	PM-149	1.0	61149
OS-186	1.0	76186	PM-151	1.0	61151
OS-187	1.0	76187	PR-141	1.0	59141
OS-188	1.0	76188	PR-142	1.0	59142
OS-189	1.0	76189	PR-143	1.0	59143
OS-190	1.0	76190	PT-190	1.0	78190
OS-192	1.0	76192	PT-192	1.0	78192
PA-231	1.0	91231	PT-194	1.0	78194
PA-233	1.0	91233	PT-195	1.0	78195
PB-204	1.0	82204	PT-196	1.0	78196

Table M8.2.1 (continued)

Alphanumeric isotope identifier	Default density	Nuclide identifier	Alphanumeric isotope identifier	Default density	Nuclide identifier
PT-198	1.0	78198	RU-106	1.0	44106
PU-236	1.0	94236	RU-96	1.0	44096
PU-237	1.0	94237	RU-98	1.0	44098
PU-238	1.0	94238	RU-99	1.0	44099
PU-239	1.0	94239	S-32	1.0	16032
PU-240	1.0	94240	S-33	1.0	16033
PU-241	1.0	94241	S-34	1.0	16034
PU-242	1.0	94242	S-36	1.0	16036
PU-243	1.0	94243	SB-121	1.0	51121
PU-244	1.0	94244	SB-123	1.0	51123
RB-85	1.0	37085	SB-124	1.0	51124
RB-86	1.0	37086	SB-125	1.0	51125
RB-87	1.0	37087	SB-126	1.0	51126
RE-185	1.0	75185	SC-45	1.0	21045
RE-187	1.0	75187	SE-74	1.0	34074
RH-103	1.0	45103	SE-76	1.0	34076
RH-105	1.0	45105	SE-77	1.0	34077
RU-100	1.0	44100	SE-78	1.0	34078
RU-101	1.0	44101	SE-80	1.0	34080
RU-102	1.0	44102	SE-82	1.0	34082
RU-103	1.0	44103	SI-28	1.0	14028
RU-104	1.0	44104	SI-29	1.0	14029
RU-105	1.0	44105	SI-30	1.0	14030

Table M8.2.1 (continued)

Alphanumeric isotope identifier	Default density	Nuclide identifier	Alphanumeric isotope identifier	Default density	Nuclide identifier
SM-144	1.0	62144	SR-86	1.0	38086
SM-147	1.0	62147	SR-87	1.0	38087
SM-148	1.0	62148	SR-88	1.0	38088
SM-149	1.0	62149	SR-89	1.0	38089
SM-150	1.0	62150	SR-90	1.0	38090
SM-151	1.0	62151	TA-180	1.0	73180
SM-152	1.0	62152	TA-181	1.0	73181
SM-153	1.0	62153	TA-182	1.0	73182
SM-154	1.0	62154	TB-159	1.0	65159
SN-112	1.0	50112	TB-160	1.0	65160
SN-114	1.0	50114	TC-99	1.0	43099
SN-115	1.0	50115	TE-120	1.0	52120
SN-116	1.0	50116	TE-122	1.0	52122
SN-117	1.0	50117	TE-123	1.0	52123
SN-118	1.0	50118	TE-124	1.0	52124
SN-119	1.0	50119	TE-125	1.0	52125
SN-120	1.0	50120	TE-126	1.0	52126
SN-122	1.0	50122	TE-127	1.0	52127
SN-123	1.0	50123	TE-127M	1.0	52601
SN-124	1.0	50124	TE-128	1.0	52128
SN-125	1.0	50125	TE-129	1.0	52129
SN-126	1.0	50126	TE-129M	1.0	52611
SR-84	1.0	38084	TE-130	1.0	52130

Table M8.2.1 (continued)

Alphanumeric isotope identifier	Default density	Nuclide identifier	Alphanumeric isotope identifier	Default density	Nuclide identifier
TE-132	1.0	52132	TI-47	1.0	22047
TH-230	1.0	90230	TI-48	1.0	22048
TH-232	1.0	90232	TI-49	1.0	22049
TI-46	1.0	22046	TI-50	1.0	22050
TI-47	1.0	22047	TL-203	1.0	81203
TI-48	1.0	22048	TL-205	1.0	81205
TI-50	1.0	22050	TM-169	1.0	69169
TM-169	1.0	69169	U-232	1.0	92232
U-232	1.0	92232	U-233	1.0	92233
U-233	1.0	92233	U-234	1.0	92234
U-234	1.0	92234	U-235	1.0	92235
TE-125	1.0	52125	U-236	1.0	92236
TE-126	1.0	52126	U-237	1.0	92237
TE-127	1.0	52127	U-238	1.0	92238
TE-127M	1.0	52601	V-50	1.0	23050
TE-128	1.0	52128	V-51	1.0	23051
TE-129	1.0	52129	W-180	1.0	74180
TE-129M	1.0	52611	W-182	1.0	74182
TE-130	1.0	52130	W-183	1.0	74183
TE-132	1.0	52132	W-184	1.0	74184
TH-230	1.0	90230	W-186	1.0	74186
TH-232	1.0	90232	XE-124	1.0	54124
TI-46	1.0	22046	XE-126	1.0	54126

Table M8.2.1 (continued)

Alphanumeric isotope identifier	Default density	Nuclide identifier	Alphanumeric isotope identifier	Default density	Nuclide identifier
XE-128	1.0	54128	YB-173	1.0	70173
XE-129	1.0	54129	YB-174	1.0	70174
XE-130	1.0	54130	YB-176	1.0	70176
XE-131	1.0	54131	ZN-64	1.0	30064
XE-132	1.0	54132	ZN-66	1.0	30066
XE-133	1.0	54133	ZN-67	1.0	30067
XE-134	1.0	54134	ZN-68	1.0	30068
XE-135	1.0	54135	ZN-70	1.0	30070
XE-136	1.0	54136	ZR-90	1.0	40090
Y-89	1.0	39089	ZR-91	1.0	40091
Y-90	1.0	39090	ZR-92	1.0	40092
Y-91	1.0	39091	ZR-93	1.0	40093
YB-168	1.0	70168	ZR-94	1.0	40094
YB-170	1.0	70170	ZR-95	1.0	40095
YB-171	1.0	70171	ZR-96	1.0	40096
YB-172	1.0	70172			

Table M8.2.2 The Standard Composition Library – elements and special nuclides by symbols

Alphanumeric element symbols	Density[a]	Nuclide identifier	Alphanumeric element symbols	Density[a]	Nuclide identifier
1/VABSORBER	1.0	999	CRINCONEL	7.20	24404
ACTIVITIES	1.0	900	CRSS	7.20	24304
AC	10.07	89000	CS	1.879	55000
AG	10.5	47000	CU	8.92	29000
AL	2.702	13027	D	1.0	1002
AR	1.0	18000	DFREEGAS	1.0	1802
AS	5.73	33000	DY	8.55	66000
AT	1.0	85000	ER	9.006	68000
AU	18.88	79197	EU	5.243	63000
B	2.370	5000	F	1.0	9019
BA	3.51	56000	FE	7.86	26000
BE	1.85	4009	FE-ESIGT	7.86	26301
BEBOUND	1.85	4309	FEINCONEL	7.86	26404
BI	9.80	83209	FESS	7.86	26304
BR	3.12	35000	FISP-1	1.0	901
C	2.1	6012	FISP-2	1.0	902
C-GRAPHITE	2.3	6312	FR	1.0	87000
CA	1.55	20000	GA	5.904	31000
CD	8.642	48000	GD	7.900	64000
CE	6.657	58000	GE	5.35	32000
CL	1.0	17000	H	1.0	1001
CO	8.9	27059	H-X(E)-HR	1.0	1301
CR	7.20	24000	H-ZRH2	1.0	1701
CR-ESIGT	7.20	24301	HFREEGAS	1.0	1801

Table M8.2.2 (continued)

Alphanumeric element symbols	Density[a]	Nuclide identifier	Alphanumeric element symbols	Density[a]	Nuclide identifier
H-POLY	1.0	1901	NIINCONEL	8.90	28404
HE	1.0	2004	NISS	8.90	28304
HF	13.31	72000	NP	20.45	93000
HG	13.546	80000	O	1.0	8016
HO	8.795	67000	OS	22.48	76000
I	4.93	53000	P	1.82	15031
IN	7.30	49000	PA	15.37	91000
IR	22.421	77000	PB	11.344	82000
K	0.86	19000	PD	12.02	46000
KR	1.0	36000	PM	7.22	61000
LA	6.145	57000	PO	9.4	84000
LI	0.534	3000	PR	6.773	59000
LU	9.840	71000	PT	21.45	78000
MG	1.74	12000	PU	19.84	94000
MN	7.20	25055	RA	5.0	88000
MNSS	7.20	25304	RB	1.532	37000
MO	10.2	42000	RE	20.53	75000
N	1.0	7014	RH	12.4	45000
NA	0.97	11023	RN	1.0	86000
NB	8.57	41093	RU	12.30	44000
ND	6.80	60000	S	2.07	16000
NE	1.0	10000	SB	6.684	51000
NI	8.90	28000	SC	2.989	21000
NI-ESIGT	8.90	28301	SE	4.81	34000

Table M8.2.2 (continued)

Alphanumeric element symbols	Density[a]	Nuclide identifier	Alphanumeric element symbols	Density[a]	Nuclide identifier
SI	2.33	14000	TM	9.321	69000
SM	7.520	62000	U	19.05	92000
SN	7.31	50000	V	5.96	23000
SR	2.6	38000	W	19.35	74000
TA	16.6	73000	XE	1.0	54000
TB	8.229	65000	Y	4.469	39000
TC	11.50	43000	YB	6.965	70000
TE	6.25	52000	ZN	7.14	30000
TH	11.7	90000	ZR	6.49	40000
TI	4.5	22000	ZR-ZRH2	1.0	40701
TL	11.85	81000			

Table M8.2.3 The Standard Composition Library – elements by full name

Alphanumeric element name	Density[a]	Nuclide identifier	Isotopic distribution[b] ID	wt %	Atm. %
ACTINIUM	10.070	89000			
ALUMINUM	2.702	13000	13027	100.000	100.000
AMERICIUM	13.670	95000			
ANTIMONY	6.684	51000	51121	56.998	57.400
			51123	43.002	42.600
ARGON	1.000	18000	18036	0.303	0.337
			18038	0.060	0.063
			18040	99.637	99.600
ARSENIC	5.730	33000	33075	100.000	100.000
ASTATINE	1.000	85000			
BARIUM	3.510	56000	56130	0.100	0.106
			56132	0.097	0.101
			56134	2.360	2.420
			56135	6.477	6.593
			56136	7.769	7.850
			56137	11.196	11.230
			56138	72.001	71.700
BERKELIUM	14.000	97000			
BERYLLIUM	1.850	4000	4009	100.000	100.000
BISMUTH	9.800	83000	83209	100.000	100.000
BORON	2.370	5000	5010	18.431	19.900
			5011	81.569	80.100
BROMINE	3.120	35000	35079	50.065	50.690
			35081	49.935	49.310
CADMIUM	8.642	48000	48106	1.178	1.250
			48108	0.854	0.890
			48110	12.211	12.490
			48111	12.628	12.800
			48112	24.021	24.130
			48113	12.273	12.220
			48114	29.111	28.730
			48116	7.723	7.490
CALCIUM	1.550	20000	20040	96.671	96.941
			20042	0.675	0.647
			20043	0.144	0.135
			20044	2.281	2.086
			20046	0.005	0.004
			20048	0.223	0.187
CARBON	2.100	6000	6012	98.809	98.900
			6013	1.191	1.100
CERIUM	6.657	58000	58136	0.184	0.190
			58138	0.246	0.250
			58140	88.297	88.430
			58142	11.272	11.130
CESIUM	1.879	55000	55133	100.000	100.000

Table M8.2.3 (continued)

Alphanumeric element name	Density[a]	Nuclide identifier	Isotopic distribution[b] ID	wt %	Atm. %
CHLORINE	1.000	17000	17035	74.736	75.770
			17037	25.264	24.230
CHROMIUM	7.200	24000	24050	4.174	4.345
			24052	83.700	83.790
			24053	9.673	9.500
			24054	2.453	2.365
COBALT	8.900	27000	27059	100.000	100.000
COPPER	8.920	29000	29063	68.499	69.170
			29065	31.501	30.830
CURIUM	13.510	96000			
DYSPROSIUM	8.550	66000	66156	0.058	0.060
			66158	0.097	0.100
			66160	2.303	2.340
			66161	18.717	18.900
			66162	25.410	25.500
			66163	24.966	24.900
			66164	28.448	28.200
ERBIUM	9.006	68000	68162	0.136	0.140
			68164	1.578	1.610
			68166	33.334	33.600
			68167	22.906	22.950
			68168	26.908	26.800
			68170	15.139	14.900
EUROPIUM	5.243	63000	63151	47.471	47.800
			63153	52.529	52.200
FLUORINE	1.000	9000	9019	100.000	100.000
FRANCIUM	1.000	87000			
GADOLINIUM	7.900	64000	64152	0.193	0.200
			64154	2.134	2.180
			64155	14.581	14.800
			64156	20.297	20.470
			64157	15.617	15.650
			64158	24.946	24.840
			64160	22.232	21.860
GALLIUM	5.904	31000	31069	59.422	60.110
			31071	40.578	39.890
GERMANIUM	5.350	32000	32070	19.736	20.500
			32072	27.132	27.400
			32073	7.831	7.800
			32074	37.148	36.500
			32076	8.153	7.800
GOLD	18.880	79000	79197	100.000	100.000
HAFNIUM	13.310	72000	72174	0.158	0.162
			72176	5.132	5.206
			72177	18.445	18.606
			72178	27.214	27.297

Table M8.2.3 (continued)

Alphanumeric element name	Density[a]	Nuclide identifier	ID	Isotopic distribution[b] wt %	Atm. %
HAFNIUM (continued)			72179	13.664	13.629
			72180	35.387	35.100
HELIUM	1.000	2000	2003	0.000	0.000
			2004	100.000	100.000
HOLMIUM	8.795	67000	67165	100.000	100.000
HYDROGEN	1.000	1000	1001	99.970	99.985
			1002	0.030	0.015
INDIUM	7.300	49000	49113	4.228	4.300
			49115	95.772	95.700
IODINE	4.930	53000	53127	100.000	100.000
IRIDIUM	22.421	77000	77191	37.056	37.300
			77193	62.944	62.700
IRON	7.860	26000	26054	5.699	5.900
			26056	91.870	91.720
			26057	2.141	2.100
			26058	0.290	0.280
KRYPTON	1.000	36000	36078	0.325	0.350
			36080	2.146	2.250
			36082	11.339	11.600
			36083	11.378	11.500
			36084	57.076	57.000
			36086	17.736	17.300
LANTHANUM	6.145	57000	57138	0.090	0.090
			57139	99.910	99.910
LEAD	11.344	82000	82204	1.378	1.400
			82206	23.955	24.100
			82207	22.075	22.100
			82208	52.592	52.400
LITHIUM	0.534	3000	3006	6.500	7.500
			3007	93.500	92.500
LUTETIUM	9.840	71000	71175	97.396	97.410
			71176	2.604	2.590
MAGNESIUM	1.740	12000	12024	78.098	78.990
			12025	10.211	10.000
			12026	11.691	11.010
MANGANESE	7.200	25000	25055	100.000	100.000
MERCURY	13.546	80000	80196	0.146	0.150
			80198	9.869	10.000
			80199	16.763	16.900
			80200	23.028	23.100
			80201	13.225	13.200
			80202	30.004	29.800
			80204	6.965	6.850
MOLYBDENIUM	10.200	42000	42092	14.230	14.840
			42094	9.053	9.250
			42095	15.748	15.920

Table M8.2.3 (continued)

Alphanumeric element name	Density[a]	Nuclide identifier	Isotopic distribution[b] ID	wt %	Atm. %
MOLYBDENIUM (continued)			42096	16.673	16.680
			42097	9.646	9.550
			42098	24.623	24.130
			42100	10.028	9.630
NEODYMIUM	6.800	60000	60142	26.691	27.130
			60143	12.068	12.180
			60144	23.745	23.800
			60145	8.339	8.300
			60146	17.389	17.190
			60148	5.907	5.760
			60150	5.862	5.640
NEON	1.000	10000	10020	89.639	90.480
			10021	0.281	0.270
			10022	10.080	9.250
NEPTUNIUM	20.450	93000			
NICKEL	8.900	28000	28058	67.395	68.270
			28060	26.653	26.100
			28061	1.173	1.130
			28062	3.788	3.590
			28064	0.991	0.910
NIOBIUM	8.570	41000	41093	100.000	100.000
NITROGEN	1.000	7000	7014	99.604	99.630
			7015	0.396	0.370
OSMIUM	22.480	76000	76184	0.019	0.020
			76186	1.544	1.580
			76187	1.572	1.600
			76188	13.140	13.300
			76189	15.992	16.100
			76190	26.361	26.400
			76192	41.371	41.000
OXYGEN	1.000	8000	8016	99.732	99.760
			8017	0.043	0.040
			8018	0.225	0.200
PALLADIUM	12.020	46000	46102	0.977	1.020
			46104	10.877	11.140
			46105	22.013	22.330
			46106	27.199	27.330
			46108	26.830	26.460
			46110	12.104	11.720
PHOSPHORUS	1.820	15000	15031	100.000	100.000
PLATINUM	21.450	78000	78190	0.010	0.010
			78192	0.777	0.790
			78194	32.712	32.900
			78195	33.780	33.800
			78196	25.415	25.300
			78198	7.307	7.200

Table M8.2.3 (continued)

Alphanumeric element name	Density[a]	Nuclide identifier	Isotopic distribution[b] ID	wt %	Atm. %
PLUTONIUMALP	19.840	94000			
PLUTONIUMDLT	15.920	94000	94239	100.000	100.000
POLONIUM	9.400	84000			
POTASSIUM	0.860	19000	19039	92.937	93.258
			19040	0.012	0.012
			19041	7.051	6.730
PRASEODYMIUM	6.773	59000	59141	100.000	100.000
PROMETHIUM	7.220	61000			
PROTACTINIUM	15.370	91000			
RADIUM	5.000	88000			
RADON	1.000	86000			
RHENIUM	20.530	75000	75185	37.148	37.400
			75187	62.852	62.600
RHODIUM	12.400	45000	45103	100.000	100.000
RUBIDIUM	1.532	37000	37085	71.691	72.160
			37087	28.309	27.840
RUTHENIUM	12.300	44000	44096	5.257	5.540
			44098	1.802	1.860
			44099	12.428	12.700
			44100	12.455	12.600
			44101	17.073	17.100
			44102	31.862	31.600
			44104	19.122	18.600
SAMARIUM	7.520	62000	62144	2.967	3.100
			62147	14.656	15.000
			62148	11.116	11.300
			62149	13.668	13.800
			62150	7.378	7.400
			62152	26.977	26.700
			62154	23.238	22.700
SCANDIUM	2.989	21000	21045	100.000	100.000
SELENIUM	4.810	34000	34074	0.842	0.900
			34076	8.748	9.100
			34077	7.402	7.600
			34078	23.283	23.600
			34080	50.493	49.900
			34082	9.231	8.900
SILICON	2.330	14000	14028	91.873	92.230
			14029	4.818	4.670
			14030	3.308	3.100
SILVER	10.500	47000	47107	51.377	51.840
			47109	48.623	48.160
SODIUM	0.970	11000	11023	100.000	100.000

Table M8.2.3 (continued)

Alphanumeric element name	Density[a]	Nuclide identifier	Isotopic distribution[b] ID	wt %	Atm. %
STRONTIUM	2.600	38000	38084	0.536	0.560
			38086	9.668	9.860
			38087	6.943	7.000
			38088	82.852	82.580
SULFUR	2.070	16000	16032	94.746	95.020
			16033	0.771	0.750
			16034	4.460	4.210
			16036	0.022	0.020
TANTALUM	16.600	73000	73180	0.012	0.012
			73181	99.988	99.988
TECHNETIUM	11.500	43000			
TELLURIUM	6.250	52000	52120	0.089	0.095
			52122	2.475	2.590
			52123	0.872	0.905
			52124	4.652	4.790
			52125	6.970	7.120
			52126	18.680	18.930
			52128	31.778	31.700
			52130	34.485	33.870
TERBIUM	8.229	65000	65159	100.000	100.000
THALLIUM	11.850	81000	81203	29.316	29.520
			81205	70.684	70.480
THORIUM	11.700	90000	90232	100.000	100.000
THULIUM	9.321	69000	69169	100.000	100.000
TIN	7.310	50000	50112	0.914	0.970
			50114	0.624	0.650
			50115	0.348	0.360
			50116	14.186	14.530
			50117	7.563	7.680
			50118	24.055	24.220
			50119	8.594	8.580
			50120	32.917	32.590
			50122	4.755	4.630
			50124	6.043	5.790
TITANIUM	4.500	22000	22046	7.678	8.000
			22047	7.158	7.300
			22048	73.903	73.800
			22049	5.622	5.500
			22050	5.639	5.400
TUNGSTEN	19.350	74000	74180	0.117	0.120
			74182	26.028	26.300
			74183	14.210	14.280
			74184	30.716	30.700
			74186	28.928	28.600

Table M8.2.3 (continued)

Alphanumeric element name	Density[a]	Nuclide identifier	Isotopic distribution[b] ID	wt %	Atm. %
URANIUM	19.050	92000	92234	0.005	0.005
			92235	0.711	0.720
			92238	99.284	99.275
VANADIUM	5.960	23000	23050	0.245	0.250
			23051	99.755	99.750
XENON	1.000	54000	54124	0.094	0.100
			54126	0.086	0.090
			54128	1.861	1.910
			54129	25.920	26.400
			54130	4.057	4.100
			54131	21.137	21.200
			54132	27.025	26.900
			54134	10.607	10.400
			54136	9.213	8.900
YTTERBIUM	6.965	70000	70168	0.126	0.130
			70170	2.995	3.050
			70171	14.127	14.300
			70172	21.761	21.900
			70173	16.111	16.120
			70174	31.966	31.800
			70176	12.914	12.700
YTTRIUM	4.469	39000	39089	100.000	100.000
ZINC	7.140	30000	30064	47.510	48.600
			30066	28.126	27.900
			30067	4.196	4.100
			30068	19.527	18.800
			30070	0.642	0.600
ZIRCONIUM	6.490	40000	40090	50.707	51.450
			40091	11.181	11.220
			40092	17.278	17.150
			40094	17.891	17.380
			40096	2.944	2.800

Table M8.2.4 The Standard Composition Library – compounds/alloys
(atoms per molecule)

Alphanumeric compound/alloy identifier	Density[a]	Nuclide	Number of atoms per molecule
B4C	2.52	5000	4
		6012	1
BALSA	0.125	6012	6
		1001	10
		8016	5
D2O	1.1054	1002	2
		8016	1
GRAPHITE	2.3	6312	1
H2O	0.9982	1001	2
		8016	1
H2O-X(E)-HR	0.9982	1301	2
		8016	1
HFACID	1.0	1001	1
		9019	1
HNO3	1.0	1001	1
		7014	1
		8016	3
NORPAR13	0.76	1901	28
		6012	13
NORPAR(H2O)	0.76	1001	28
		6012	13
OAK	0.700	6012	6
		1001	10
		8016	5
PARA(H2O)	0.90	1001	52
		6012	25
PARAFFIN	0.90	1901	52
		6012	25
PLEXIGLAS	1.18	1001	8
		6012	5
		8016	2

Table M8.2.4 (continued)

Alphanumeric compound/alloy identifier	Density	Nuclide	Number of atoms per molecule
PLEXIGLASS	1.18	1001	8
		6012	5
		8016	2
POLY(H2O)	0.923	1001	2
		6012	1
POLYETHYLENE	0.92	1901	2
		6012	1
POLYVINYLCL	1.6	1901	3
		6012	2
		17000	1
PU(NO3)4	2.447	94000	1
		7014	4
		8016	12
PUC	13.6	94000	1
		6012	1
PUF4	7.0	94000	1
		9019	4
PUN	14.25	94000	1
		7014	1
PUO2	11.46	94000	1
		8016	2
PVC	1.6	1901	3
		6012	2
		17000	1
PVC(H2O)	1.6	1001	3
		6012	2
		17000	1
REDWOOD	0.387	6012	6
		1001	10
		8016	5
TBP	0.9724	1901	27
		6012	12
		8016	4
		15031	1

Table M8.2.4 (continued)

Alphanumeric compound/alloy identifier	Density	Nuclide	Number of atoms per molecule
TBP(H2O)	0.9724	1001	27
		6012	12
		8016	4
		15031	1
U3O8	8.30	92000	3
		8016	8
UC	13.63	92000	1
		6012	1
UF4	6.70	92000	1
		9019	4
UF6	4.68	92000	1
		9019	6
UN	14.31	92000	1
		7014	1
UO2	10.96	92000	1
		8016	2
UO2(NO3)2	2.203	92000	1
		7014	2
		8016	8
UO2F2	6.37	92000	1
		8016	2
		9019	2
UO3	7.29	92000	1
		8016	3
ZIRCALLOY	6.56[b]	40302	1
ZRH2	5.61[c]	40701	1
		1701	2
ZR5H8	5.61[c]	40701	5
		1701	8

[a]See ref. 5.
[b]See ref. 6.
[c]See ref. 7.

Table M8.2.5 The Standard Composition Library – compounds/alloy
(weight percent)

Alphanumeric compound/alloy name	Density[a]	Nuclide	Weight %
CARBONSTEEL	7.8212	26000	99.0
		6012	1.0
INCONEL	8.3	14000	2.5
		22000	2.5
		24404	15.0
		26404	7.0
		28404	73.0
INCONELS	8.3	14000	2.5
		22000	2.5
		24000	15.0
		26000	7.0
		28000	73.0
KEROSENE	0.82	1901	16
		6012	84
KERO(H2O)	0.82	1001	16
		6012	84
MGCONCRETE	2.147	26000	0.5595
		1001	0.3319
		6012	10.5321
		8016	49.9430
		11023	0.1411
		12000	9.4200
		13027	0.7859
		14000	4.2101
		16000	0.2483
		17000	0.0523
		19000	0.9445
		20000	22.6318
		22000	0.1488
		25055	0.0512
ORCONCRETE	2.2994	26000	0.7784
		1001	0.6187
		6012	17.52
		8016	41.02
		11023	0.02706
		12000	3.265
		13027	1.083

Table M8.2.5 (continued)

Alphanumeric compound/alloy name	Density	Nuclide	Weight %
ORCONCRETE (continued)	14000	3.448	
		19000	0.1138
		20000	32.13
PYREX 2.23	5000	3.7	
		13027	1.0
		8016	53.5
		14000	37.7
		11023	4.1
REG-CONCRETE	2.3	26000	1.4
		1001	1.0
		13027	3.4
		20000	4.4
		8016	53.2
		14000	33.7
		11023	2.9
RFCONCRETE	2.321	26000	1.01
		1001	0.75
		6012	5.52
		7014	0.02
		8016	48.49
		11023	0.63
		12000	1.25
		13027	2.17
		14000	15.5
		16000	0.19
		19000	1.37
		20000	23.0
		22000	0.1
SS304	7.94	6012	0.08
		14000	1.0
		15031	0.045
		24304	19.0
		25055	2.0
		26304	68.375
		28304	9.5

Table M8.2.5 (continued)

Alphanumeric compound/alloy name	Density	Nuclide	Weight %
SS304S	7.94	6012	0.08
		14000	1.0
		15031	0.045
		24000	19.0
		25055	2.0
		26000	68.375
		28000	9.5
SS316	8.03	6012	0.08
		14000	1.0
		15031	0.045
		24304	17.0
		25055	2.0
		26304	65.375
		28304	12.0
		42000	2.5
SS316S	8.03	6012	0.08
		14000	1.0
		15031	0.045
		24000	17.0
		25055	2.0
		26000	65.375
		28000	12.0
		42000	2.5
U(.27)METAL	19.05	92235	0.27
		92238	99.73
ZIRC2	6.56[b]	40000	98.25
		50000	1.45
		26000	0.135
		24000	0.100
		28000	0.055
		72000	0.10
ZIRC4	6.56[b]	40000	98.23
		50000	1.45
		26000	0.21
		24000	0.10
		72000	0.01

[a]See ref. 5.
[b]See ref. 6.

Table M8.2.6 The Standard Composition Library – nuclide identification

Nuclide identifier	Mass[a]	σ_s (resonance energy scattering cross section)	σ_t (resonance energy total cross section)
900	0.6022	0.000	0.000
901	0.6022	0.000	0.000
902	0.6022	0.000	0.000
999	0.6022	0.000	0.064
1000	1.0079	20.450	20.450
1001	1.0078	20.38087	20.38782
1002	2.0141	3.39486	3.39487
1003	3.0161	1.30000	1.30000
1301	1.0078	20.450	20.450
1701	1.0078	20.450	20.450
1801	1.0078	20.38072	20.38767
1802	2.0141	3.39486	3.39487
1901	1.0078	20.38087	20.38782
2000	4.0026	0.759	0.759
2003	3.0149	1.00000	48.43520
2004	4.0026	0.75914	0.75914
3000	6.9410	1.025	4.556
3006	6.0151	0.70640	9.49837
3007	7.0160	1.05000	1.05077
4000	9.0122	6.000	6.000
4009	9.0122	6.00000	6.00023
4309	9.0122	6.00000	6.00023
5000	10.8126	4.430	41.800
5010	10.0129	2.02361	36.99886
5011	11.0093	5.03432	5.03443
6000	12.0011	4.740	4.740
6012	12.0000	4.73651	4.73658
6013	13.0034	4.400	4.400
6312	12.0000	4.73651	4.73658
7000	14.0067	9.830	10.000
7014	14.0031	9.37454	9.41251
7015	14.9999	4.26969	4.26969
8000	15.9994	3.750	3.750
8016	15.9906	3.88696	3.88696
8017	16.9991	3.74000	3.74501
8018	17.9992	3.790	3.790
9000	18.9984	3.640	3.640
9019	18.9982	3.64311	3.64331
10000	20.1800	3.520	3.520
10020	19.9924	3.540	3.540
10021	20.9938	3.400	3.400
10022	21.9914	3.260	3.260

Table M8.2.6 (continued)

Nuclide identifier	Mass[a]	σ_s (resonance energy scattering cross section)	σ_t (resonance energy total cross section)
11000	22.9895	3.130	3.130
11023	22.9895	3.68074	3.69501
12000	24.3051	3.56188	3.56322
12024	24.1928	3.60	3.63
12025	24.9858	3.60	3.63
12026	25.9826	3.60	3.63
13000	26.9815	1.347	1.350
13027	26.9818	1.34652	1.35195
14000	28.0853	2.07886	2.08242
14028	27.9769	2.086	2.090
14029	28.9765	2.290	2.290
14030	29.9738	2.160	2.160
15000	30.9738	4.100	4.110
15031	30.9741	4.10000	4.10940
16000	32.0636	0.96801	0.98647
16032	31.9717	1.07917	1.16292
16033	32.9715	1.770	1.770
16034	33.9679	1.650	1.650
16036	35.9671	1.460	1.460
17000	35.4526	3.87615	4.09662
17035	34.9688	14.600	16.100
17037	36.9659	14.600	16.100
18000	39.9480	0.500	0.510
18036	35.9675	1.460	1.460
18038	37.9627	1.310	1.310
18040	39.9624	0.500	0.510
19000	39.1019	1.57649	1.61912
19039	38.9637	1.748	1.795
19040	39.9766	1.280	1.280
19041	40.9618	3.190	3.190
20000	40.0803	2.93420	2.94575
20040	40.0803	2.990	3.000
20042	41.9586	1.320	1.320
20043	42.9588	1.420	1.420
20044	43.9555	1.530	1.530
20046	45.9537	1.860	1.860
20048	47.9525	2.310	2.310
21000	44.9559	24.000	24.000
21045	44.9541	24.000	24.000
22000	47.8789	4.76379	4.84643
22046	45.9526	4.470	4.500

Table M8.2.6 (continued)

Nuclide identifier	Mass[a]	σ_s (resonance energy scattering cross section)	σ_t (resonance energy total cross section)
22047	46.9513	4.470	4.500
22048	47.9479	4.470	4.500
22049	48.9479	2.560	2.560
22050	49.9995	3.570	3.570
23000	50.9416	6.08597	6.22050
23050	49.9448	3.080	3.080
23051	50.9416	5.000	5.250
24000	51.9957	4.80606	4.88958
24050	49.9461	3.65041	4.06749
24052	51.9402	2.93131	2.95963
24053	52.9408	11.36418	11.85856
24054	53.9394	2.59604	2.60402
24301	51.9957	4.80332	4.88691
24304	51.9957	4.80524	4.87986
24404	51.9957	4.340	4.560
25055	54.9381	4.11673	4.66220
25304	54.9380	1.620	2.510
26000	55.8447	10.14041	10.21196
26054	53.9394	0.54078	0.56419
26056	55.9345	10.34167	10.41600
26057	56.9351	2.18651	2.24484
26058	57.9337	2.93278	3.02954
26301	55.8447	10.13435	10.18683
26304	55.8447	10.13958	10.20438
26404	55.8447	11.330	11.500
27059	58.9332	4.01701	4.56253
28000	58.6868	17.40151	17.49917
28058	57.9357	22.89210	22.98659
28059	59.1179	6.160	6.160
28060	59.9308	0.60130	0.64445
28061	60.9314	7.03812	7.08748
28062	61.9280	13.83746	14.13414
28064	63.9282	0.03621	0.06739
28301	58.6871	17.39816	17.49579
28304	58.6871	17.39386	17.49143
28404	58.6871	17.850	18.170
29000	63.5456	7.67365	7.87143
29063	62.9296	4.96604	5.15628
29065	64.9278	11.04072	11.17869
30000	65.3900	3.970	4.045
30064	63.9291	3.970	4.045

Table M8.2.6 (continued)

Nuclide identifier	Mass[a]	σ_s (resonance energy scattering cross section)	σ_t (resonance energy total cross section)
30066	65.9260	5.930	5.930
30067	66.9271	5.990	5.990
30068	67.9248	6.050	6.050
30070	69.9253	6.170	6.170
31000	69.7200	7.24099	7.85971
31069	68.9256	6.110	6.110
31071	70.9247	6.200	6.200
32000	72.6100	6.240	6.240
32070	69.9242	6.170	6.170
32072	71.9221	2.75260	2.79731
32073	72.9235	1.77701	2.66178
32074	73.9212	2.21790	2.23275
32076	75.9214	3.14968	3.21560
33000	74.9216	6.300	6.300
33075	74.9216	2.40061	3.05509
34000	78.9600	6.330	6.330
34074	73.9220	2.40836	3.86328
34076	75.9192	2.18392	3.89666
34077	76.9199	3.23300	4.87295
34078	77.9174	2.57555	2.70517
34080	79.9165	0.74908	0.78460
34082	81.9167	2.83395	2.83491
35000	79.9040	6.330	6.330
35079	78.9184	3.84062	5.73140
35081	80.9163	4.39900	5.12874
36000	83.8000	6.240	6.240
36078	77.9204	9.67690	10.32532
36080	79.9163	9.99815	10.87241
36082	81.9135	11.00954	12.39253
36083	82.9141	7.60811	8.90037
36084	83.9114	7.37167	7.61555
36085	84.9125	4.35119	4.42300
36086	85.9106	5.37942	5.38389
37000	85.4678	6.200	6.200
37085	84.9118	6.78018	7.12265
37086	85.9112	4.82311	6.23901
37087	86.9090	4.57199	4.67865
38000	87.6200	6.150	6.150
38084	83.9139	4.47559	4.69884
38086	85.9093	2.16458	2.27995
38087	86.9089	3.84809	4.21824

Table M8.2.6 (continued)

Nuclide identifier	Mass[a]	σ_s (resonance energy scattering cross section)	σ_t (resonance energy total cross section)
38088	87.9057	3.61505	3.61518
38089	88.9075	4.20130	4.21933
38090	89.9078	3.67100	3.68981
39089	88.9058	3.48300	3.52674
39090	89.9072	5.18952	5.42417
39091	90.9074	4.66901	4.75126
40000	91.2196	6.40229	6.44668
40090	89.9043	5.63609	5.63665
40091	90.9029	9.63672	9.88639
40092	91.9015	4.60604	4.62334
40093	92.9064	5.25481	6.23552
40094	93.9027	6.39770	6.40101
40095	94.9080	4.66893	5.01030
40096	95.9049	6.63752	6.69435
40302	91.2196	6.57039	6.64760
40701	91.2196	6.40229	6.44668
41000	92.9064	5.990	5.990
41093	92.9032	6.24149	6.91965
41094	93.9073	6.37552	9.18253
41095	94.9068	5.00376	6.09320
42000	95.9402	6.66278	7.55771
42092	92.0003	4.69744	4.75108
42094	93.9051	3.60965	3.64971
42095	94.9059	3.88602	5.22943
42096	95.9047	3.12306	3.29786
42097	96.9061	4.15422	4.86886
42098	97.9055	4.05373	4.33084
42099	98.9078	4.96830	7.33397
42100	99.9075	4.12708	4.26029
43099	99.0005	8.48843	11.89032
44000	101.0700	5.650	5.650
44096	95.9079	8.15755	8.91747
44098	97.9051	8.25404	8.87823
44099	98.9060	4.85653	8.10904
44100	99.9042	4.82418	5.23917
44101	100.9058	4.16608	6.78565
44102	101.9044	4.03206	4.27401
44103	102.9060	5.35181	8.38870
44104	103.9056	4.36130	4.64186
44105	104.9082	4.79934	5.28506
44106	105.9078	4.29521	4.41311
45000	102.9055	5.560	5.560

Table M8.2.6 (continued)

Nuclide identifier	Mass[a]	σ_s (resonance energy scattering cross section)	σ_t (resonance energy total cross section)
45103	102.9050	6.73505	8.47520
45105	104.9062	5.82661	12.45579
46000	106.4200	5.370	5.370
46102	101.9054	7.52110	8.21081
46104	103.9036	4.65932	5.18701
46105	104.9052	3.84954	7.39375
46106	105.9038	4.34964	4.59382
46107	106.9054	3.96261	9.22079
46108	107.9040	3.78627	5.25835
46110	109.9051	4.60048	5.24374
47000	107.8682	5.290	5.290
47107	106.9054	6.53019	8.73731
47109	108.9046	7.03860	10.78046
47111	110.9057	4.73012	8.66196
48000	112.4258	5.96439	7.35874
48106	105.9098	6.98897	7.76262
48108	107.9040	4.77742	5.02427
48110	109.9031	3.78265	4.44252
48111	110.9047	4.62964	6.82803
48112	111.9033	4.41276	4.88232
48113	112.8999	5.82412	7.65733
48114	113.9035	4.06873	4.52448
48115	114.9061	4.400	8.450
48116	115.9047	4.47517	4.62149
48601	114.9060	5.08049	12.14392
49000	113.8340	6.54499	11.55700
49113	112.9039	4.73201	8.29204
49115	114.9041	4.95874	7.68116
50000	118.6900	5.08197	5.19374
50112	111.9013	5.83299	6.40444
50114	113.8985	5.90196	6.09166
50115	114.9031	5.03967	6.20347
50116	115.9017	4.31898	4.50526
50117	116.9033	4.83833	5.54342
50118	117.9018	4.74617	4.97918
50119	118.9035	5.07381	5.41780
50120	119.9020	4.44965	4.56804
50122	121.9032	4.26749	4.31517
50123	122.9058	5.14967	5.30259
50124	123.9054	4.51436	4.61335
50125	124.9080	5.14050	5.89974

Table M8.2.6 (continued)

Nuclide identifier	Mass[a]	σ_s (resonance energy scattering cross section)	σ_t (resonance energy total cross section)
50126	125.9076	4.59500	4.60129
51000	121.7500	4.220	4.220
51121	120.9036	5.01859	7.95345
51123	122.9038	4.74831	6.06791
51124	123.9064	5.15754	7.73459
51125	124.9050	6.09719	7.18684
51126	125.9076	6.31921	8.93292
52000	127.6000	3.650	3.650
52120	119.9000	6.62139	7.64407
52122	121.9032	3.97031	4.63531
52123	122.9048	6.29093	9.41775
52124	123.9034	4.36331	4.82319
52125	124.9040	5.07637	6.15076
52126	125.9036	4.27202	4.40841
52127	126.9052	5.020	6.270
52128	127.9048	4.78246	4.95040
52129	128.9074	4.670	4.740
52130	129.9060	4.62586	4.64628
52132	131.9082	4.74000	4.74004
52601	126.9050	6.96475	9.34985
52611	128.9070	6.31616	6.62837
53000	126.9045	3.720	3.720
53127	126.9042	4.73310	7.40698
53129	128.9054	6.33669	8.31838
53130	129.9070	7.57110	13.76491
53131	130.9066	6.35574	6.73260
53135	134.9100	4.81200	4.81242
54000	131.2900	3.330	3.330
54124	123.9064	11.50989	14.44249
54126	125.9046	5.72483	6.14354
54128	127.9038	4.63051	4.91435
54129	128.9044	5.89874	8.14997
54130	129.9039	4.44554	4.60329
54131	130.9056	11.95602	15.37690
54132	131.9041	4.37973	4.39941
54133	132.9057	11.32614	24.91361
54134	133.9053	4.73044	4.77503
54135	134.9069	11.88843	12.58943
54136	135.9075	5.21155	5.21643
55000	132.9054	3.210	3.210
55133	132.9057	8.36492	12.39438

Table M8.2.6 (continued)

Nuclide identifier	Mass[a]	σ_s (resonance energy scattering cross section)	σ_t (resonance energy total cross section)
55134	133.9073	14.07658	27.01808
55135	134.9059	8.53004	13.49562
55136	135.9075	5.86240	6.55006
55137	136.9071	5.38316	5.40325
56000	137.3270	3.040	3.040
56130	129.9063	3.430	3.430
56132	131.9050	3.290	3.290
56134	133.9043	4.83515	5.12520
56135	134.9059	5.16108	6.38253
56136	135.9045	5.01188	5.15380
56137	136.9051	5.63901	5.89302
56138	137.8996	7.00000	7.02446
56140	139.9109	5.07550	5.77947
57000	138.9055	3.090	3.090
57138	138.9071	3.090	3.090
57139	138.9063	6.72696	6.94693
57140	139.9099	9.42548	10.92764
58000	140.1150	3.180	3.180
58136	135.9071	3.060	3.060
58138	137.9060	3.030	3.030
58140	139.9059	5.15576	5.16960
58141	140.9085	11.89578	13.20776
58142	141.9091	5.97662	6.00512
58143	142.9127	9.02059	10.05762
58144	143.9133	5.78863	5.95060
59141	140.9075	4.05503	4.55001
59142	141.9101	16.60534	21.30440
59143	142.9107	20.29262	27.55482
60000	144.2400	4.220	4.220
60142	141.9081	4.60720	5.01585
60143	142.9097	4.49254	5.39538
60144	143.9103	1.76757	1.92650
60145	144.9129	4.74528	7.34156
60146	145.9135	1.76913	1.91672
60147	146.9161	44.77876	75.87045
60148	147.9167	0.78075	0.93393
60150	149.9209	4.55604	4.78174
61147	146.9151	29.41382	40.44508
61148	147.9177	12.63462	55.47230
61149	148.9183	19.91237	69.02393
61151	150.9215	10.23679	16.89389

Table M8.2.6 (continued)

Nuclide identifier	Mass[a]	σ_s (resonance energy scattering cross section)	σ_t (resonance energy total cross section)
61548	147.9177	14.120	501.560
61601	147.9160	12.50349	84.52424
62000	150.3600	8.410	8.410
62144	143.9163	8.70659	9.12992
62147	146.9151	8.55485	14.41743
62148	147.9147	10.98818	11.54683
62149	148.9173	10.67280	26.70062
62150	149.9169	5.60014	7.41767
62151	150.9195	27.74949	91.09621
62152	151.9201	12.20033	14.96736
62153	152.9217	33.18710	61.24710
62154	153.9223	3.93533	4.45460
63000	151.9624	19.79401	77.43832
63151	150.9195	19.49246	82.69254
63152	151.9251	20.01232	97.97688
63153	152.9217	16.26340	51.92801
63154	153.9223	14.41121	52.45164
63155	154.9229	7.48674	26.34428
63156	155.9245	9.93960	16.11951
63157	156.9251	9.67766	14.05592
64000	157.2500	2.900	30.900
64152	151.9201	5.80773	9.31788
64154	153.9213	7.12720	11.55622
64155	154.9229	11.33346	42.56798
64156	155.9225	7.51759	9.00551
64157	156.9241	4.56730	10.01622
64158	157.9237	4.37880	5.12278
64160	159.9269	4.61818	4.85875
65000	158.9253	7.530	7.530
65159	158.9253	13.31429	24.24897
65160	159.9273	16.15331	28.68471
66000	162.5000	7.340	7.340
66156	155.9243	7.770	7.770
66158	157.9244	7.610	7.610
66160	159.9249	26.55838	53.53649
66161	160.9274	21.09521	50.16882
66162	161.9270	7.78376	10.77485
66163	162.9287	7.41391	12.14881
66164	163.9282	16.92097	18.10130
67000	164.9303	7.240	7.240
67165	164.9298	13.87232	26.66914

Table M8.2.6 (continued)

Nuclide identifier	Mass[a]	σ_s (resonance energy scattering cross section)	σ_t (resonance energy total cross section)
68000	167.2600	7.200	7.200
68162	161.9288	7.370	7.370
68164	163.9292	7.280	7.280
68166	165.9304	5.71682	8.14902
68167	166.9320	19.20864	36.77205
68168	167.9324	7.190	7.190
68170	169.9355	7.160	7.160
69000	168.9342	7.180	7.180
69169	168.9342	12.000	115.000
70000	173.0400	7.220	7.220
70168	167.9339	7.190	7.190
70170	169.9348	7.160	7.160
70171	170.9363	7.180	7.180
70172	171.9364	7.200	7.200
70173	172.9382	7.220	7.220
70174	173.9389	7.240	7.240
70176	175.9426	7.330	7.330
71000	174.9670	7.260	7.260
71175	174.9408	13.09388	26.00653
71176	175.9414	13.10944	30.47302
72000	178.4873	21.82691	35.23405
72174	173.9402	15.81409	30.24438
72176	175.9414	8.00761	11.52188
72177	176.9430	19.51120	39.34697
72178	177.9436	11.39213	13.77346
72179	178.9462	14.03141	23.58469
72180	179.9468	12.50468	13.34719
73000	180.9479	7.820	7.820
73180	180.9479	7.820	7.820
73181	180.9545	10.59555	18.60863
73182	181.9500	21.39445	37.89878
74000	183.8564	18.06516	21.95447
74180	179.9467	7.640	7.640
74182	181.9531	11.50250	13.36487
74183	182.9517	7.92861	11.86607
74184	183.9502	5.95709	6.30797
74186	185.9575	14.14692	17.10276
75000	186.2070	8.950	8.950
75185	184.9528	21.76644	36.67757
75187	186.9561	14.34111	22.17058
76000	190.2000	10.230	10.230

Table M8.2.6 (continued)

Nuclide identifier	Mass[a]	σ_s (resonance energy scattering cross section)	σ_t (resonance energy total cross section)
76184	183.9525	8.370	8.370
76186	185.9538	8.870	8.870
76187	186.9557	9.190	9.190
76188	187.9558	9.510	9.510
76189	188.9581	9.830	9.830
76190	189.9584	10.160	10.160
76192	191.9615	10.690	10.690
77000	192.2200	10.760	10.760
77191	190.9606	82.050	82.050
77193	192.9629	25.628	25.628
78000	195.0800	11.520	11.520
78190	189.9599	10.170	10.170
78192	191.9610	10.690	10.690
78194	193.9627	11.230	11.230
78195	194.9648	11.500	11.500
78196	195.9649	11.590	11.590
78198	197.9679	11.750	11.750
79000	196.9665	11.670	11.670
79197	196.9660	14.47990	19.48166
80000	200.5900	11.690	11.690
80196	195.9658	11.590	11.590
80198	197.9667	11.750	11.750
80199	198.9683	11.730	11.730
80200	199.9683	11.700	11.700
80201	200.9703	11.690	11.690
80202	201.9706	11.670	11.670
80204	203.9735	11.640	11.640
81000	204.3833	11.640	11.640
81203	202.9723	11.660	11.660
81205	204.9744	11.630	11.630
82000	207.2100	11.22196	11.22639
82204	203.9730	11.640	11.640
82206	205.9694	10.82533	10.83220
82207	206.9780	10.72854	10.74918
82208	207.9766	11.35993	11.35994
83209	208.9803	10.04156	10.05296
90000	232.0381	11.190	11.190
90230	230.0361	12.18722	14.73401
90232	232.0333	14.46822	16.76003
91231	231.0347	9.87229	39.59202
91233	233.0399	10.87494	28.26477

Table M8.2.6 (continued)

Nuclide identifier	Mass[a]	σ_s (resonance energy scattering cross section)	σ_t (resonance energy total cross section)
92000	238.0289	11.480	11.480
92232	232.0333	10.87214	32.30190
92233	233.0450	12.46693	37.62292
92234	234.0405	12.18716	16.09542
92235	235.0441	11.90249	35.22383
92236	236.0458	12.27302	14.93351
92237	237.0484	14.24581	24.68619
92238	238.0510	12.32636	14.62708
93237	237.0484	12.17113	32.69289
93238	238.0510	10.85823	36.53173
93239	239.0526	12.35728	42.01463
94000	239.0526	8.950	29.040
94236	236.0458	12.87549	21.65514
94237	237.0484	11.68929	45.26585
94238	238.0500	15.70542	20.02287
94239	239.0526	11.51819	28.47182
94240	240.0542	11.11239	14.06522
94241	241.0487	12.45935	40.20634
94242	242.0584	13.03224	15.35400
94243	243.0620	12.90616	28.13765
94244	244.0647	12.60434	15.21899
95241	241.0568	13.15588	36.54988
95242	242.0594	10.69250	33.91222
95243	243.0610	11.93284	32.23324
95601	242.0600	11.69557	67.76985
96241	241.0578	11.64334	42.63003
96242	242.0584	11.78203	15.48221
96243	243.0610	12.95100	47.19994
96244	244.0626	12.98077	17.89164
96245	245.0653	10.60726	38.13534
96246	246.0669	12.09723	13.54742
96247	247.0725	10.36968	16.68160
96248	248.0721	8.59636	10.26753
97249	249.0797	27.18501	70.44259
98249	249.0797	10.98123	36.83376
98250	250.0763	13.01097	17.80937
98251	251.0799	13.62784	26.60932
98252	252.0815	11.08669	15.01721
98253	253.0841	12.37956	45.71291
99253	253.0414	19.02553	28.06653

M8.3 TABLE OF AVAILABLE SOLUTIONS

The Standard Composition Library (Tables M8.2.1 through M8.2.6) describes the various compounds, alloys, elements, and isotopes one may use in defining the material mixtures for a given problem. In addition to the various materials listed there, one is also free to use any of the fissile solutions listed in Table M8.3.1. Indeed, the user is encouraged to treat the solutions listed in Table M8.3.1 as he would any other standard composition. Using empirical fits to experimental data, the code will then automatically calculate the volume fraction corresponding to the heavy metal, acid, and water components of the solution.

Table M8.3.1 Table of available solutions

Alphanumeric description of the solution	List of nuclides in this fissile solution (first nuclide listed is a variable isotope nuclide)
SOLNUO2F2	92000 1001 8016 9019
SOLNUO2(NO3)2	92000 1001 7014 8016
SOLNPU(NO3)4	94000 1001 7014 8016

M8.4 REFERENCES

1. *ENDF-201 - ENDF/B-VI Summary Documentation*, Compiled and edited by P. F. Rose, BNL-NCS-17541 [ENDF-201], Brookhaven National Laboratory, National Nuclear Data Center, October 1991.

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3. "Chart of the Nuclides," *Nuclides and Isotopes, Fourteenth Edition*, General Electric Company, Revised 1989.

4. William H. Sullivan, *Trilinear Chart of Nuclides*, U.S. Atomic Energy Commission, January 1957.

5. *CRC Handbook of Chemistry and Physics*, 64th Edition, CRC Press, Boca Raton, Florida, 1983-1984.

6. *International Methods Handbook*, Vol. III, 10th Ed., American Society for Metals, 1990.

7. Atlantic Equipment Engineers, Division of Micron Metals, http://www.micronmetals.com/zirconium_hydride.htm.

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Computational Physics and Engineering Division

MARS: A MULTIPLE-ARRAY SYSTEM USING COMBINATORIAL GEOMETRY

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ABSTRACT

MARS is a combinatorial geometry method for modeling a Multiple-ARray System. It allows the user the ability to model many unique rectangular arrays with unlimited array nesting. In this system, arrays may contain arbitrary vacancies and may be arbitrarily positioned in space. Geometry may be modeled around an array and optionally repeated with the array. Array repetition and array nesting does not require additional computer memory; hence, MARS can model very complicated geometry systems with a minimum of computer memory requirements.

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ACKNOWLEDGMENTS

The direction and guidance of L. M. Petrie in developing the MARS system were invaluable. His patience and consultation aided in overcoming programming obstacles and spawning several fresh approaches to lattice modeling. This development is an offshoot of the array lattice modeling system originally developed by G. E. Whitesides in his KENO Monte Carlo program. The efforts of R. M. Westfall and R. H. Odegaarden, formerly of the U.S.Nuclear Regulatory Commission, are appreciated for their support and encouragement in funding this work.

M9.1 INTRODUCTION

Rectangular lattice modeling demands as demonstrated by shipping casks, spent fuel pools, and reactor cores require a geometry system with a multiple-array capability and array manipulation techniques. The MARS geometry system has been developed to allow the nuclear analyst the ability to model complex lattice geometries efficiently and quickly with a minimum of geometric approximation and a minimum of computer memory requirements. The MARS system is a versatile system, meeting the most rigid modeling requirements in a flexible and general manner. The features the MARS system offers are as follows:

1. Many arrays may be modeled - each being unique.

2. Arrays may contain other arrays embedded in their lattice positions. The user may nest arrays inside arrays with no program limitation.

3. Arrays may be repeated by simple reference.

4. Arrays may have vacant lattice positions to model irregular array shapes. A particle may enter or exit an array from any cell in an array.

5. Geometry may be optionally modeled around an array and repeated with the array.

6. Arrays may be arbitrarily oriented. An array may be rotated as well as translated when it is repeated.

7. User geometry is modeled in simple coordinate systems called "universes," which are separate and independent from other parts of a geometry model.

8. Array input is verified for logical consistency and fit during input.

9. Basic geometry modeling uses combinatorial geometry for ease of input and flexibility. No restrictions are placed on the shape or complexity of individual cell content provided the outer shape of the cell is rectangular.

10. Efficient geometry data management minimizes the computer space requirements and has no external disk requirements. All geometry data reside in computer memory. Repeating a universe, repeating an array, and nesting arrays inside arrays do not require additional memory. Computer memory requirements are primarily a function of the number of unique arrays modeled and the size of each array. This feature allows complex models to be run on small computers.

11. MARS runs within MORSE-SGC. MORSE-SGC supergroups both the material cross sections and the particle tracking to minimize the computer memory requirements. Extensive effort has been placed on verifying and benchmarking this version of MORSE with the MARS geometry system. This version of MORSE is in the SCALE system and may run either in a

stand-alone mode or in a SCALE control sequence. Further description of MORSE-SGC may be found in Sect. F9 of the SCALE manual.

This document is intended to give a detailed description of the MARS geometry concepts and to illustrate some applications of the MARS modeling capability. Section M9.2 describes the rudiments of combinatorial geometry by introducing the concepts of material zone construction using basic combinatorial bodies. Section M9.3.1 discusses the MARS approach to lattice modeling and introduces the "universe concept," which is the link between combinatorial particle tracking and MARS lattice construction. In addition, Sect. M9.3.2 examines array nesting and the advantages nesting offers in lattice modeling. Section M9.3.3 recommends some broad procedures for the novice MARS user in model construction and development. Section M9.4 discusses the array analysis portion of MARS. The analysis part of MARS is a collision flux estimator with an edit feature that allows the user to obtain very specific and detailed reaction rate information from complicated models. Section M9.5 is a summary of the concepts introduced in Sects. M9.2 through M9.4. Section M9.6 discusses some subtle aspects of MARS tracking logic, including its weaknesses and some recommended corrective techniques for preventive modeling.

Appendices M9.A through M9.F give the mechanics for applying the MARS geometry system. Appendix M9.A gives the input requirements for both the combinatorial and array portions of MARS. Appendix M9.B gives three examples of problems modeled with MARS. Many of the MARS concepts are best understood in these applications. Appendix M9.C describes the combinatorial geometry zone transfer table printed at the completion of MARS tracking. Appendix M9.D describes how the MARS collection of subroutines may be interfaced into other Monte Carlo codes. Appendix M9.E discusses the MARS tracking logic and program flow. Appendix M9.F is presented as complementary information to the combinatorial ray tracing discussed in Sect. M9.2.4. A detailed numerical illustration of combinatorial tracking is given in Appendix M9.F. This appendix is a reprint of material presented in past MORSE workshops.

This document should orient the new MARS user to both combinatorial geometry modeling concepts and multiple nested-array concepts unique to the MARS system. The user should attempt to understand the geometry concepts developed in this document before generating MARS input. Users familiar with combinatorial geometry may wish to omit Sect. M9.2 and Appendix M9.C and concentrate on Sects. M9.3 and M9.6.

M9.2 COMBINATORIAL GEOMETRY THEORY AND TRACKING LOGIC

The combinatorial geometry package in the MARS system was obtained from earlier versions of the MORSE Monte Carlo code. Combinatorial geometry allows the description of physical structures by the combination of certain basic geometric shapes (bodies) such as rectangular parallelepipeds, right circular cylinders, etc. These basic shapes are combined using three logical operators—the AND operator using the "+" notation, the NOT operator using the "–" notation, and the OR operator using the "OR" notation. This section will introduce the concepts of simple geometric bodies, the operators to combine bodies into zones, and two types of zones—the input zone and its subset, the code zone.

M9.2.1 BODY DESCRIPTIONS

Combinatorial geometry (CG or COMJOM) describes general three-dimensional (3-D) material configurations by considering unions, differences, and intersections of simple bodies such as spheres, boxes, cylinders, etc. The description of material zones is accomplished by describing simple bodies and their relationships. This method allows space to be subdivided into unique zones of arbitrary shape. Each zone is the result of combining one or more of the following geometric bodies:

1. Rectangular Parallelepiped (RPP)
2. Box (an RPP arbitrarily rotated in space)
3. Sphere (SPH)
4. Right Circular Cylinder (RCC)
5. Right Elliptical Cylinder (REC)
6. Truncated Right-Angle Cone (TRC)
7. Arbitrary Convex Polyhedron of 4, 5, or 6 sides
8. Ellipsoid of Revolution (ELL)
9. Right-Angle Wedge (WED)

Body types 2–9 may be arbitrarily oriented with respect to the x, y, and z coordinate axes. Body 1, the RPP, must have its sides all parallel to coordinate planes. Alternative input descriptions for the BOX and the WED are described later in this section.

The information required to specify each type of body is as follows:

1. Rectangular Parallelepiped (RPP) - Specify the minimum and maximum values of the x, y and z coordinates that bound the parallelepiped.

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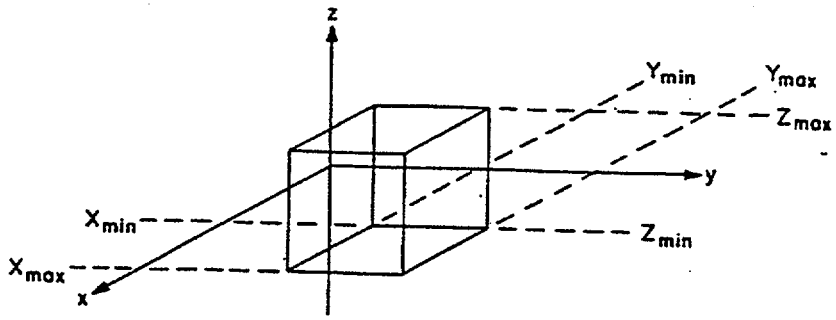

2. Sphere (SPH) - Specify the vertex, V, at the center and the scalar, R, denoting the radius.

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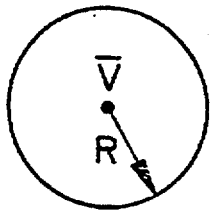

3. Right Circular Cylinder (RCC) - Specify the vertex, V, at the center of one base; a height vector, H, expressed in terms of its x, y, and z components; and a scalar, R, denoting the radius.

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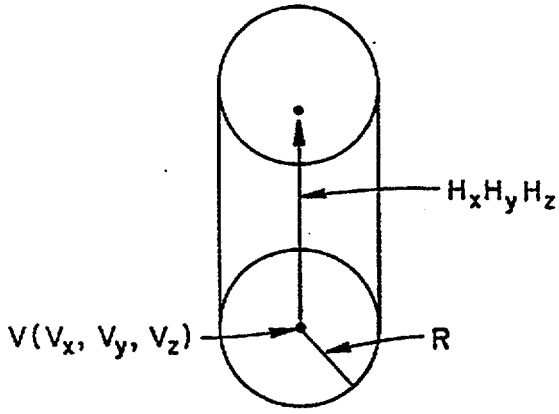

4. Right Elliptical Cylinder (REC) - Specify coordinates of the center of the base ellipse, a height vector, and two vectors in the plane of the base defining the major and minor axes.

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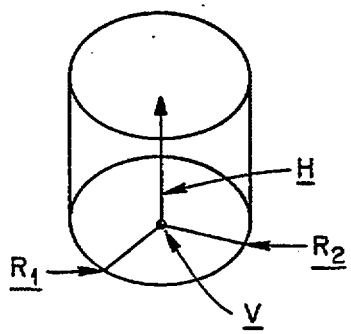

5. Truncated Right-Angle Cone (TRC) - Specify a vertex, V, at the center of the lower base; the height vector, H, expressed in terms of its x, y, and z components; and two scalars, R_1 and R_2, denoting the radii of the lower and upper bases.

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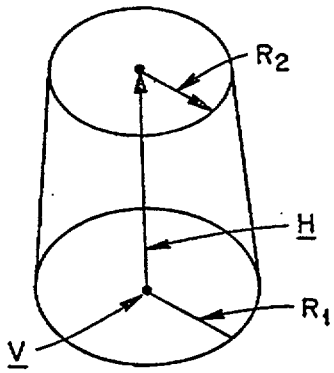

6. Ellipsoid (ELL) - Specify two vertices, V_1 and V_2, denoting the coordinates of the foci and a scalar, R, denoting the length of the major axis.

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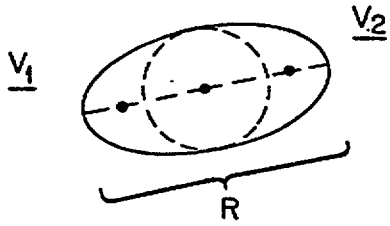

7. Right-Angle Wedge (WED) or (RAW) - Specify the vertex, V, at one of the corners by giving its (x, y, z) coordinates. Specify a set of three mutually perpendicular vectors, a_i, with a_1 and a_2 describing the two legs of the right triangle of the wedge, that is, the x, y, and z components of the height, width, and length vectors are given.

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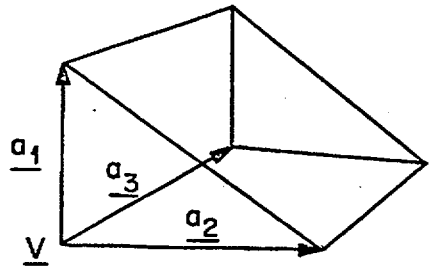

8. Box (BOX) - Specify the vertex, V, at one of the corners by giving its (x, y, z) coordinates. Specify a set of three mutually perpendicular vectors, a_i, representing the height, width, and length of the box, respectively. That is, the x, y, and z components of the height, width, and length vectors are given.

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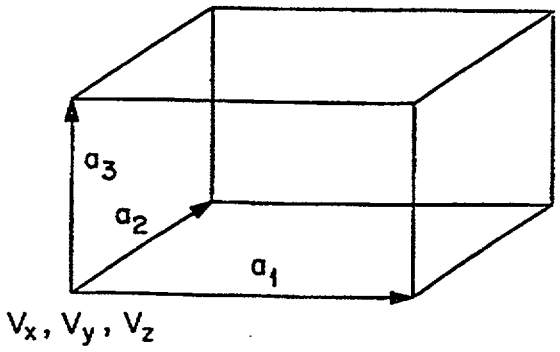

9. Arbitrary Polyhedron (ARB) - Assign an index (1 to 8) to each vertex. For each vertex, give the x, y, and z coordinates. Each of the six faces is then described by a four-digit number giving the indices of the four vertex points in that face. For each face, these indices must be entered in either clockwise or counterclockwise order.

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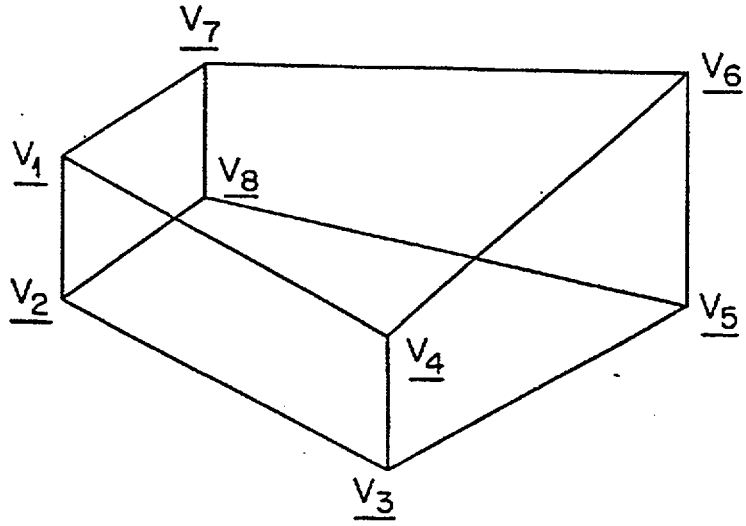


Alternative body descriptions for the BOX and the wedge (WED) are provided in the MARS version of combinatorial geometry. Presently the body data for the BOX and the WED (wedge) require the user to input a vertex and three displacement vectors for the axes of the body. An alternative method is available for entering these bodies. Very often the angle of rotation and the size of the body are known. The alternative body input is BPP for the BOX and WPP for the wedge. The "PP" refers to the parallelepiped input description used for the RPP. The BPP and WPP require the user to describe a rectangular parallelepiped, similar to the RPP, and then to enter three rotation angles. These angles are not simple Euclidean angles, but rather rotational angles. The first angle is an X-Y rotation about the Z axis and is positive in the CLOCKWISE direction. This angle defines the first rotation of the RPP. The second angle is an Y-Z rotation about the X axis and is positive in the CLOCKWISE direction. The second angle defines a rotation on the first rotation. The third angle input is an X-Z rotation about the Y axis and is positive in the COUNTERCLOCKWISE direction. The third angle is a rotation on the second rotation. These three angles are input in degrees and may be either positive or negative. It is essential to remember that each angle defines a rotation that operates on the previous rotation. Figure M9.2.1 illustrates these rotations. The input for the BPP and the WPP is then translated into the BOX and WED input description for use by combinatorial geometry. The use of the BPP and WPP is optional, and the user should use the body description that is best understood.

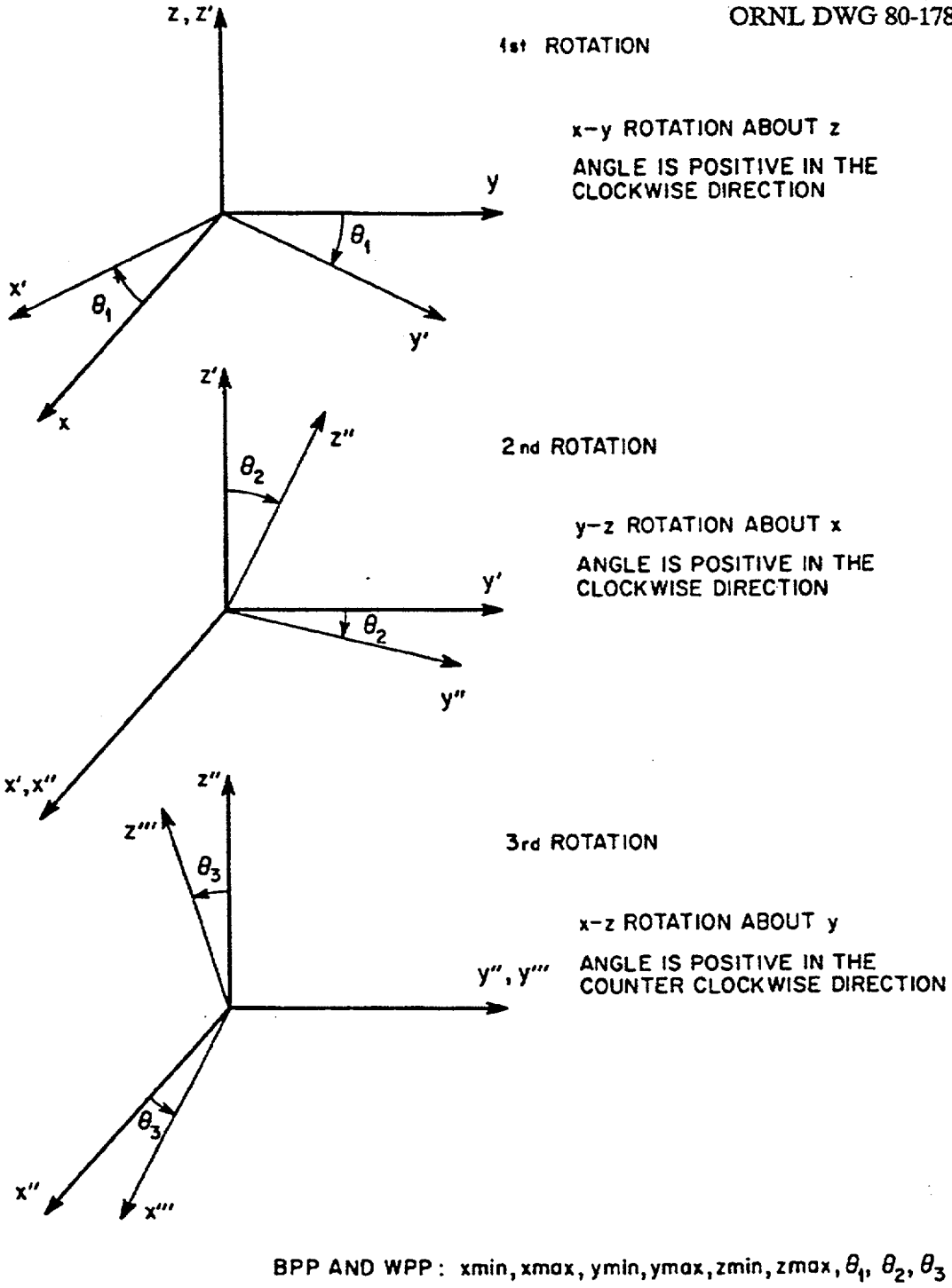


Figure M9.2.1 Rotations defining alternative bodies BPP and WPP

M9.2.2 COMBINATORIAL OPERATORS

The basic technique for the description of the geometry consists of defining the location and shape of the various zones in terms of the intersections and unions of the geometric bodies. A special operator notation involving the symbols (+), (–), and (OR) is used to describe the intersections and unions. These symbols are used by the program to construct information relating material descriptions to the body definitions.

If a body appears in a zone description with a (+) operator, it means that the zone being described is wholly contained in the body. If a body appears in a zone description with a (–) operator, it means that the zone being described is wholly outside the body. If the body appears with an (OR) operator, it means that the input zone being described includes all points in the code zone following the "OR." OR may be considered as a union operator. In some instances, an input zone may be described in terms of subzones, called code zones, lumped together by (OR) statements. Body numbers after an "OR" describe a code zone. Code zones may be thought of as subsets of an input zone.

Techniques for describing a particular geometry are best illustrated by examples. Consider an object composed of a sphere and a cylinder as shown in Fig. M9.2.2. To describe the object, one takes a spherical body (2) penetrated by a cylindrical body (3) (see Fig. M9.2.2); if the materials in the sphere and cylinder are the same, then they can be considered as one zone, say Zone I (Fig. M9.2.2, Item c). The description of Zone I would be

$$I = OR +2 \; OR +3 \; .$$

This equation means that a point is in Zone I if it is either inside Body 2 or inside Body 3.

If different materials are used in the sphere and cylinder, then the sphere with a cylindrical hole in it would be given a different zone number (e.g., J) from that of the cylinder (K).

The description of Zone J would be (Fig. M9.2.2, Item d):

$$J = +2 - 3 \; .$$

This equation means that points in Zone J are all those points inside Body 2 which are not inside Body 3.

The description of Zone K is simply (Fig. M9.2.2, Item e):

$$K = +3 \; .$$

In other words, all points in Zone K lie inside Body 3.

Combinations of more than two bodies and similar zone descriptions could contain a long string of (+), (–), and (OR) operators. It is important, however, to remember that every spatial point in the geometry must be located in one and only one zone.

As a more complicated example of the use of the (OR) operator, consider the system shown in Fig. M9.2.3 consisting of the shaded zone, A, and the unshaded zone, B. These zones can be described by the two BOXes, Bodies 1 and 3, and the RCC, Body 2. The zone description would be

$$A = +1 \; +2$$

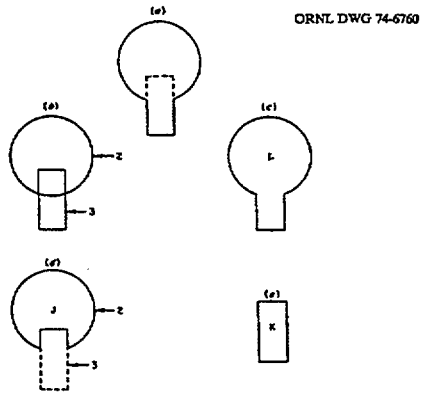


Figure M9.2.2 Examples of combinatorial geometry method

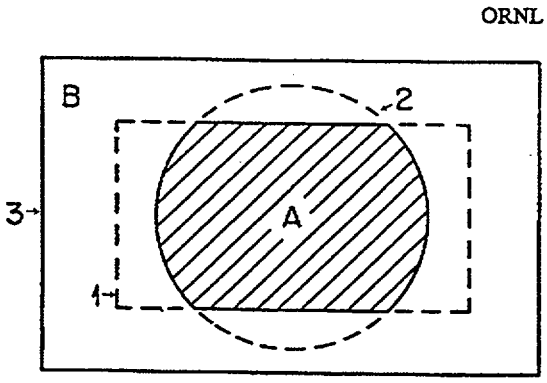
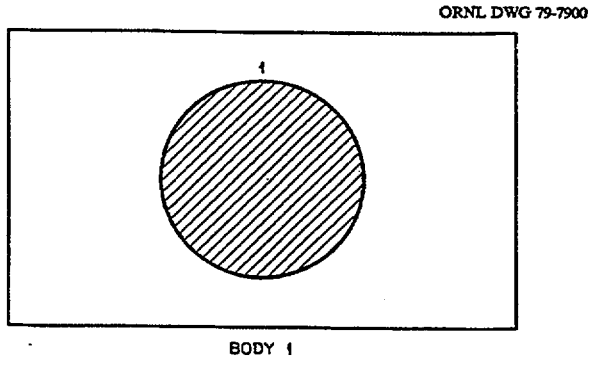


Figure M9.2.3 Use of OR operators

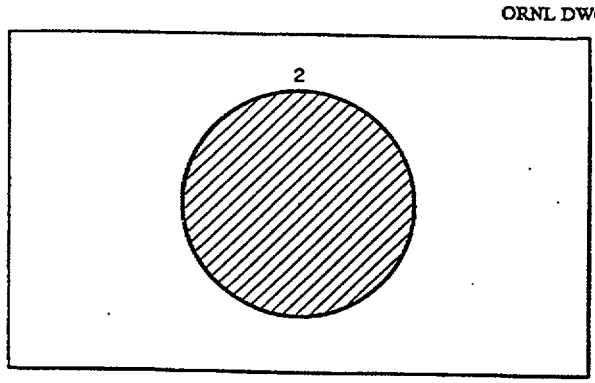
Notice that the OR operator refers to all following body numbers until the next OR operator is reached. For example, let Body 1 be a sphere with vertex (-0.75, 0.0, 0.0) and radius 1.0.



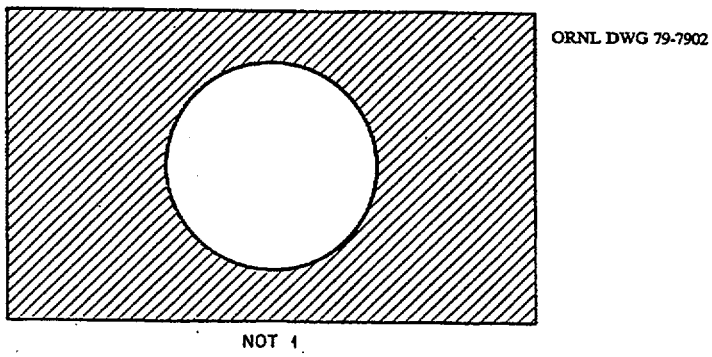
and

$$B = OR +3 -1 OR +3 -2 .$$

And let Body 2 be a sphere with vertex (0.75, 0.0, 0.0) and radius 1.0.



Then, "NOT 1" consists of all points that are not in Body 1.



"1 OR 2" consists of all points that are in Body 1 or in Body 2 (or in both, the OR operation is not an exclusive or).

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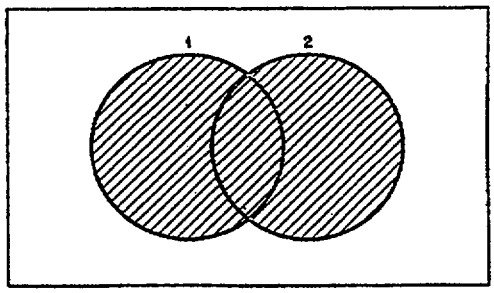

1 OR 2

"1 AND 2" consists of all points that are in Body 1 and are also in Body 2.

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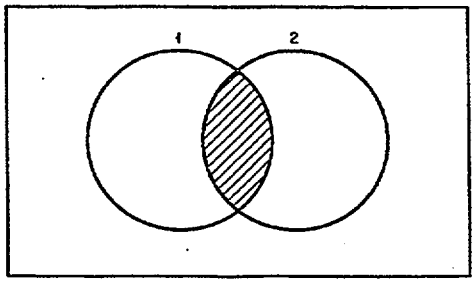

1 AND 2

M9.2.3 COMBINATORIAL ZONE CONSTRUCTION

In combinatorial geometry the most elementary zone description is called a "code zone." The code zone description uses only the "+" and "–" operators to describe a material zone. Code zones may be combined with the "OR" operator to define an "input zone" containing more than one code zone. An input zone may be composed of only one code zone. An input zone is a material zone of only one media, containing one or more code zones. An input zone may describe volumes of space that are not continuous. Figure M9.2.4 illustrates the difference between input zones and code zones.

Figure M9.2.4-A shows the shaded zone, Input Zone 1, as all points in Body 1 "OR" all points in Body 2. Input Zone 1 in Fig. M9.2.4-A contains two code zones. The first code zone is +1, and the second code zone is +2. Alternatively, this material zone could have been described as two input zones, each with only one code zone, as illustrated by Zones 2 and 3 of Fig. M9.2.4-A. In both methods, the set of points shared by Bodies 1 and 2 have been doubly defined; this is valid since both zones contain the same media. If Bodies 1 and 2 contained different material media, then the two bodies could not be combined into a single input zone; and the overlap between the two bodies would be erroneous. Figure M9.2.4-B's shaded zone represents all

points in Body 1; and the clear zone represents all points in Body 2 which are "not" in Body 1. The shaded zone, Zone 1, is described as +1. The clear zone, Zone 2, is described as +2 –1. Figure M9.2.4-C's shaded area is all points in Body 2 and is the opposite description of Fig. M9.2.4-B. Figure M9.2.4-D's shaded zone is all points in Body 1, which are also in Body 2; that is, points which are common to both bodies. This zone is described as +1 +2. Figure M9.2.4 demonstrates the use of the "OR," the "+," and "–" operator. Note that the user is not required to use the "OR" operator (see Fig. M9.2.4-A). The "OR" operator gives the user a shorthand input notation to lump "code zones" logically together into a single "input zone." All combinatorial geometry tracking is done with "code zones." Tracking across code zones is transparent to the user. Program action occurs only when a particle track crosses an input zone boundary. Input zones are a user convenience for consolidating code zones in a more logical, understandable manner.

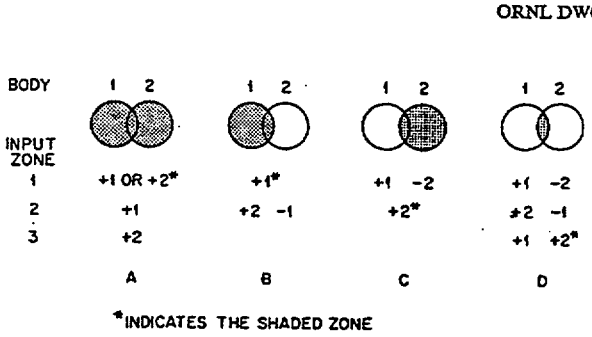

Figure M9.2.4 Illustrative input zone descriptions

M9.2.4 COMBINATORIAL TRACKING LOGIC

Tracking in combinatorial geometry depends on the following criteria:

1. Knowing the particle location in the geometry.

2. Knowing the particle trajectory in the current coordinate system.

3. Knowing the distance a particle can travel before having a collision.

4. Knowing the distance to enter and the distance to exit each body of the zone in which the particle is traversing.

These four criteria determine whether the particle will undergo a collision or cross a zone boundary. If the distance to the next collision is less than the distance to exit the current input zone, then the particle will suffer a collision. If the distance to the next collision is greater than the distance to exit the current input zone, then the particle will encounter a boundary crossing and enter a new input zone. Only crossing an input zone boundary may constitute a possible change in material media. Changing code zones within the same input zone cannot constitute a media change. When combinatorial tracking determines that a boundary crossing has occurred, it then tries to determine the next zone of entry in its current universe. A universe is a collection of

input zones sharing a unique coordinate system. It is necessary for MARS to compute the entrance and exit distances for bodies used in describing other input zones in the current universe. These entrance and exit distances used with the input zone descriptions determine the next zone the particle will enter. This procedure is demonstrated in Fig. M9.2.5.

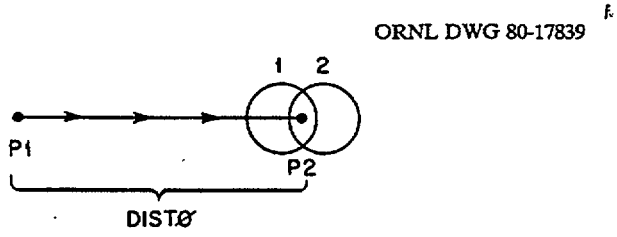

Figure M9.2.5 Particle trajectory moving from P1 to P2

In Fig. M9.2.5 a particle is emitted from point P1 and is traveling in the trajectory defined by direction cosines, U, V, and W. The distance to the next collision for the particle is known to be DIST0. From previous computation, the location of point P1 is known. The problem is to determine the input zone containing the particle collision site. From analytical geometry relations, the entrance and exit distances for the trajectory is computed for Body 1 and Body 2. The distance to enter Body i will be RINi, and the distance to exit Body i will be ROUTi. If RINi < DIST0 < ROUTi, then the particle trajectory will terminate inside Body i. The relation of the RINis and ROUTis to DIST0 may be used to construct a "truth table" to determine which bodies contain the collision site. Knowing the bodies containing the collision site, and the code zone descriptions, the code zone containing the collision is known. Assuming the zone description for Fig. M9.2.5 is given in Fig. M9.2.4-D, the following relations will exist:

BODY	[Relation of RINi to ROUTi]	Collision in Body
1	RIN1 < DIST0 < ROUT1	YES
2	RIN2 < DIST0 < ROUT2	YES

Knowing the bodies containing the collision site, the zone containing the collision site can be determined.

ZONE	Description	Collision in Zone?	Reason
1	+1 –2	NO	Collision is inside Body 2
2	+2 –1	NO	Collision is inside Body 1
3	+1 +2	YES	Collision is inside Body 1 and Body 2

MARS can quickly determine the input zone containing a coordinate after all bodies containing the coordinate have been determined and a comparison with the zone description table has been performed. This method is efficient and effective provided (a) all space has been uniquely defined, and (b) all points in all bodies are satisfied by a given zone description with the correct relationship of bodies to each point.

M9.3 MARS GEOMETRY THEORY

M9.3.1 THE UNIVERSE BUILDING BLOCK

A universe is a separate independent dimension in space defined by a collection of input zones bounded by a special boundary media. Every input zone resides in a universe. Every input zone description must include a universe number containing the zone. A particle can be in one and only one universe at a time. A particle may not change universes at a boundary crossing between input zones without first exiting the current universe. Each universe defines a unique coordinate system. Particle coordinates used while tracking through a universe are relative to the universe. This eliminates absolute coordinate space defined in a universe from conflicting with the same absolute coordinate space defined in other universes. Each universe is a microcosm with a separate unique geometry model. The most global universe in a model is Universe 0, the absolute universe. Universe 0 must contain an array in order to enter other universes in a model. All universes with the exception of the absolute universe must be surrounded by a special boundary media, Media –1000. This special –1000 media acts as a boundary flag to signify particle translation out of the current universe. The inner body of the zone containing the –1000 media then becomes the real outer boundary of the universe. This body is referred to as the universe reference body. The universe reference body may be either an RPP or a BOX. The reference body determines the absolute coordinate system inside the universe. The ability to differentiate universes makes the actual modeling construction of universes much simpler since they do not interact, interfere, or share space with any other zones not in the universe. After universes have been modeled, they may be combined arbitrarily into geometric arrays. The contents of a universe are arbitrary, and a universe may contain an array in one or more of its input zones. These concepts are illustrated in Appendix M9.B by several examples. Studying Appendix M9.B will make the universe concepts, array construction, and array nesting more comprehensible.

There are two types of universes: the combinatorial universe and the simple universe. The simple universe is composed of input zones analogous to KENO zones, where every zone completely encompasses the previous zone. Simple universe zone descriptions are composed of two or less bodies and do not reference any negative media numbers. A simple universe input zone may contain only one code zone. Universes erroneously declared simple containing input zones with more than one code zone, or a code zone with more than two bodies, or an input zone with a negative media number will be correctly recognized by MARS as combinatorial universes, and the user will receive warning messages of the alteration. Tracking through simple universes is approximately 30% faster than tracking through combinatorial universes. The MARS user is encouraged to use simple universes in his model description wherever possible.

M9.3.2 MARS "ARRAY OF ARRAYS" CAPABILITY

MARS allows the user the ability to describe rectangular cells of arbitrary content and to combine these cells to form unique arrays. These arrays may subsequently be referenced for inclusion in a geometry model. The arrays could be referenced in an input zone in a universe, or they could be referenced in lattice cell positions in a larger array. Thus, there is a nested-array capability in the MARS system.

Arrays are assigned a numeric name as each array description is entered. Hence, the first array entered into the MARS input becomes Array 1; the second array entered becomes Array 2, etc.

It is necessary in constructing a MARS model to distinguish array names from universe names. This is accomplished by referencing universe names as positive integers and array names as negative integers.

Therefore, Array 1 would be referenced as –1 and Universe 1 would be referenced as +1. Universes are referenced ONLY in array descriptions. Arrays may be referenced by TWO methods: (1) in the zone media input or (2) as the lattice cell content of other array descriptions.

One of the most important portions of the MARS input is the description of arrays (i.e., their dimensions and their content). The array input description in MARS combines the universes and other arrays into a complete model. Initially in the array input portion of MARS, the size of each array is entered. Array numbers (names) are assigned sequentially as each array size is entered. The size of an array is described by the number of lattice cells along each coordinate dimension, that is, the number of cells along the X-axis, the number along the Y-axis, and the number of cells along the Z-axis. Next, the content of each lattice cell position in each array must be defined. MARS allows the user three different techniques for entering this information. The technique used is strictly based on individual user preference. These array description input techniques are described in detail in Appendix M9.A. Regardless of the method chosen by the user to describe the contents of each array, the contents of each lattice cell position of each array will be defined at the completion of the array description portion of the MARS input. A lattice cell position in an array may contain either a universe, entered with a positive integer; an array, entered with a negative integer; or a vacancy, entered with a zero. A zero in an array description defines a vacant lattice cell position and should not be confused with the absolute universe zero. Vacant lattice positions give the user flexibility in determining the shape of an array. Vacant lattice cell positions may be located either internally or on the periphery of an array.

Since the contents of a universe are arbitrary, a universe may contain an array. This arrangement allows geometry to be built around an array and then to be automatically repeated with the universe. An array is placed in a universe by describing a zone that snugly fits the nonvacant lattice cell positions of an array. The media for the input zone is given as a negative array number. This inserts by reference the array into the input zone. The array must fit snugly in the input zone; otherwise, a gap of undefined space may exist.

The simplest method to repeat an array is to directly reference a smaller array in a lattice cell position of a larger array. This method does not require any additional input to be specified, but wherever it is referenced, this method does require the smaller array to completely fill the lattice position of the larger array. Whenever a smaller array is referenced in a lattice cell position of a larger array, the smaller array may not contain vacant lattice positions.

Two methods for nesting an array have been described: (1) an array may be referenced in any input zone of any universe, and the universe may be referenced in any array description, and (2) an array may completely fill a lattice cell position of a larger array. A third technique is made possible through the use of arbitrarily located vacancies in a larger array. This technique is illustrated in Fig. M9.3.1.

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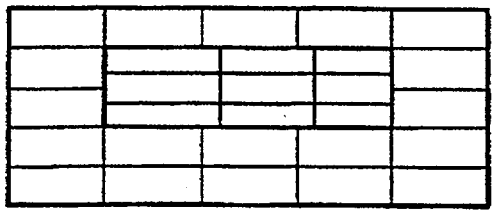

Figure M9.3.1 A nested-array lattice

The larger array shown in Fig. M9.3.1 is a 5 × 5 × 1 array with a 3 × 3 × 1 array embedded in its vacant lattice locations. The lattice cell description for the larger array could be

```
1 2 1 2 1

2 0 0 0 2

2 0 0 0 2

2 1 2 1 2
1 2 1 2 1
```

Note the 1's and 2's are positive integers referencing Universes 1 and 2. The 0's are array vacancies.

The actual input zone containing the two arrays would be

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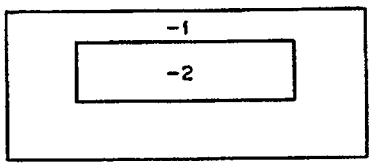


Every MARS model must contain one or more input zones in Universe 0. The absolute universe in MARS contains the entire MARS model. Universe 0 may be bounded by a vacuum boundary, a reflected boundary, or an albedo boundary. These special boundaries are described in Sect. M9.5.1, Media Notation. Each input zone exists in a universe. Universe 0 is the beginning or top of the geometry hierarchy in the MARS system. Transfer into an array from the absolute universe is accomplished by entering an input zone defined in the absolute universe containing a negative media.

The term "level of geometry" represents the geometry hierarchy in MARS. The level concept is necessary to understand MARS model construction and MARS tracking logic. (See Sect. M9.6.1.)

The absolute universe is in the zero*th* (0*th*) level of the geometry hierarchy. Any array referenced in an input zone defined in the absolute universe exists in the first level of the geometry hierarchy. The level of an array establishes the level of all universes referenced in the array. The universe level is the same as the array level, and all universes in an array exist at the same level. Any subarray referenced either directly in an array or in an input zone in a universe in an array is in the next level of the geometry nesting. There is no program limit to the extent of geometry nesting in the MARS system. Furthermore, array nesting in MARS is independent of computer memory requirements. The concept of a "geometry level" allows MARS to construct a nesting table which uniquely defines each point in a multilevel geometry model. Therefore, even though particle tracking utilizes a local universe coordinate system, the nesting table constructed during tracking allows MARS to uniquely define a particle location relative to any higher geometry level. The universe coordinate system utilized during particle tracking is always in the largest geometry level number (the most local) necessary to define the particle in an input zone containing a positive media number.

M9.3.3 ARRAY ROTATION

The Combinatorial MARS System has the ability to rotate an array arbitrarily in space. An array may be referenced either by a negative media notation for an input zone or by a negative entry in an array lattice description. When an array is referenced in an input zone, the first body of the input zone description becomes the reference body for the array. The reference body determines the coordinate translation and rotation for particles entering and exiting the array. The reference body for an array may be either an "RPP" or a "BOX" body type. If the reference body for an array is an "RPP" body type, then no rotation occurs and the boundaries of the array are parallel to coordinate planes. If the reference body for an array is a "BOX" body type, then the array will be oriented according to the definition of the BOX. Section M9.2.1 describes the combinatorial body types. The "BOX" is described as the eighth body type. In the figure accompanying this description, three displacement vectors, A1, A2, and A3, are shown. For an array with a BOX reference body, vector A1 defines the X axis for the array, vector A2 defines the Y axis for the array, and vector A3 defines the Z axis for the array.

Arrays repeated with a BOX reference body may have arbitrary vacancies, just as an array referenced with an RPP reference body. The space external to the array inside the reference body must be defined by another input zone. The input zone containing the array must have the shape of the boundaries of the array.

All universes and/or arrays referenced in a rotated array are automatically rotated in space. Particle trajectories in a rotated array are in a rotated coordinate system. This requires particles entering a rotated array to have their coordinates translated and rotated and their direction cosines to be rotated. Particles exiting a rotated array must have their coordinates translated and undergo a reverse rotation and must have their direction cosines undergo the same reverse rotation. Each BOX body that is an array reference body has an orthogonal rotational matrix associated with it. The inverse rotation for an orthogonal matrix is the transpose of the original rotational matrix.

M9.3.4 MODEL CONSTRUCTION WITH MARS

Lattice array nesting is a different modeling technique from many of the conventional modeling schemes. Therefore, the following suggestions are presented to aid the novice MARS user in preparing his model.

1. *Examine your geometry for unique repeatable rectangular cells.* These cells will be your universes. Decide how many unique cells exist in your model and identify each.

2. *Define combinatorial bodies for each unique type of universe in your system.* Bodies are numbered by the order in which they are entered in the combinatorial input. Make marginal notations in your notes of each body type and number. These notations will be convenient for future reference when describing input zones.

3. *Identify a reference body for each universe.* This determines the origin of each universe. All bodies used to model input zones in a given universe will have the same coordinate system as the universe reference body surrounding the universe. This body may be either an RPP or a BOX body. Always use the RPP as your reference body unless geometry rotation is required.

4. *Determine the number of unique, simple arrays in your system.* These arrays are composed entirely of universes. Assign universe numbers for these "building blocks" to be used in forming arrays. List your simple arrays noting the array description and array number.

5. *Examine your system for the possibility of forming larger arrays that contain either the simple arrays and/or universes.* This step may involve surrounding a simple array with its peripheral geometry features (such as a sheath surrounding a fuel assembly as in the typical PWR) to define a new universe. Then, the entire new universe can be referenced in the larger arrays as often as required. Remember to reference arrays with negative integers. Arrays may be inserted in combinatorial input zones with negative zone media designation. Arrays may be referenced in larger arrays with a negative array number for the content of a given cell in the larger array. Remember, universes are referenced with positive integers in array lattice descriptions.

6. *In specifying the elements of the input, it is likely that further simplifications through array nesting as described in (5) will be recognized.* It is difficult to adjust to the concept of examining a geometry model for the possibility of nesting arrays inside of larger arrays. In some models it may be apparent, but in most models nesting arrays is a subtle thought acquired after careful reflection. Thus, some iteration in the input zone and array content description may be desirable. For convenience, marginal notation of the actual description of the universe will be useful records for later reference.

7. Use PICTURE to check the geometry model before attempting to perform a Monte Carlo calculation.

M9.4 ARRAY ANALYSIS — COLLISION EDITS

In tracking through a complicated array, it is often necessary to obtain specific reaction rates dependent on location and/or media criteria. MARS has a generalized method of allowing the user to obtain this information without impacting on computer time requirements. MARS allows the user to specify both location criteria and media criteria to selectively sample specific collisions. The desired reaction rate is generated by multiplying the user-selected, collided flux times an arbitrary, user-defined response set. The combination of location criteria, media criteria, and response criteria allows the user to "edit" his collisions into special reaction rate bins. The criteria are general enough to cover many different lattice reaction rates of interest.

The order of the array analysis input is as follows:

1. The number of "edits" required is input in the first data block of the MORSE input.

2. For each "edit," the location criteria are entered.

3. For each "edit," the media criteria and the response criteria required are entered.

The location, media, and response criteria will be described in this section, along with some illustrative examples. It is important to remember that both the specified location and media criteria for each edit must be met before the collided flux is multiplied by the specified user response and banked in the appropriate edit bin.

M9.4.1 ANALYSIS CRITERIA

M9.4.1.1 Location Criteria

The location criteria are input in three parts, but only the first part is required. For each edit the location criteria input will be less than or equal to five entries. The three parts of the location criteria available for each edit are described below:

1. (1 REQUIRED ENTRY) The user may edit either an array or a universe. If the user is editing an array, the array name is entered as a negative entry. If the user is editing a universe, then the universe number is entered as a positive entry. If Universe "0," the absolute universe, is specified, then no additional location criteria input for the edit is required.

2. (1 OPTIONAL ENTRY) A larger array in which the subarray or universe resides in may be entered. If zero is entered, then collisions for this edit will be tallied at all locations where the subarray or universe occurs. If a positive array number is entered, then collisions only in the specified subarray or universe occurring in the larger array will be tallied. The subarray or universe may occur in any sublevel of the larger array. The subarray or universe does not have to be directly referenced in the larger array.

3. (3 OPTIONAL ENTRIES) A specific location in the larger array specified in Part 2 may be entered. If zero is entered, then the edit is not location-dependent in the larger array specified in Part 2. The location given is entered as the NX, NY, NZ coordinate of the lattice position in the larger array.

A zero input for any of the above entries terminates the location criteria for the edit being entered.

After the location criteria have been entered for all edits, then the media and response criteria will be input as a pair of entries for each edit.

M9.4.1.2 Media Criteria

The media criteria are specified by entering a media number to selectively bank collisions by material composition. All collisions meeting the location criteria occurring in the specified media for an edit will be banked. If zero is entered, then only the location criteria will be observed and the edit will not have any media dependence.

M9.4.1.3 Response Criteria

When a collision site has met both the location and media criteria for a given edit, the collided flux is calculated and multiplied times an arbitrary response set specified in the response input for the edit. MORSE allows the user to input arbitrary response functions (NRESP). These response functions are referenced in the response input to the array analysis. The MARS array analysis system computes only one reaction rate for each edit required by the user.

For each edit, the user inputs the media criteria and response criteria. At the end of the MORSE calculation each edit is output with the reaction rate and the fractional standard deviation. If the user edit is for a universe, then only one result and deviation is output. If the user edit is for an array, then results will be given for all lattice positions in the array. The contents of the lattice positions are arbitrary and independent of the array analysis performed. Therefore, the user may obtain array-averaged reactions by editing a larger array containing the arrays to be averaged.

M9.4.2 ILLUSTRATIVE EXAMPLES

The following free form input is given for six edits:

–2 0, –2 3 0, –2 3 12 10 8, 30 0, 30 2 0, 30 2 1 1 1,

0 1, 2 3, 1 3, 2 4, 3 5, 1 2

The Location Criteria for each of the six edits were given first, followed by the Media and Response Criteria for each edit. Each edit is discussed below:

Edit 1
Location Criteria: –2 0
Media/Response Criteria: 0 1
Bank all collisions in Array 2 wherever Array 2 occurs. No media dependence. Use Response Set 1 for this edit.

Edit 2
Location Criteria: –2 3 0
Media/Response Criteria: 2 3
Bank collisions in Array 2 whenever Array 2 occurs inside Array 3. Bank collisions in Media 2 only; use Response Set 3 for this edit.

Edit 3
Location Criteria: –2 3 12 10 8
Media/Response Criteria: 1 3
Bank collisions in Array 2, whenever Array 2 occurs in the 12 10 8 position of Array 3. Array 2 may occur in any sublevel of Array 3. For example, Array 3 may reference Array 4 which references Array 2. Bank collisions only in Media 1; use Response Set 3 for this edit.

Edit 4
Location Criteria: 30 0
Media/Response Criteria: 2 4
Bank collisions occurring in Universe 30 wherever Universe 30 occurs. Bank collisions only in Media 2; use Response Set 4 for this edit.

Edit 5
Location Criteria: 30 2 0
Media/Response Criteria: 3 5
Bank collisions in Universe 30 whenever it occurs in Array 2. Bank collisions only in Media 3 and use Response Set 5 for this edit.

Edit 6
Location Criteria: 30 2 1 1 1
Media/Response Criteria: 1 2
Bank collisions in Universe 30 whenever it occurs in the 1 1 1 position of Array 2. Bank collisions only in Media 1; use Response Set 2 for this edit.

M9.5 COMBINATORIAL MARS OVERVIEW

Sections M9.2 and M9.3 introduced the user to combinatorial geometry concepts and MARS array logic. This section is a summary of some of the important concepts developed in previous sections. The use of media input is introduced in this section with some discussion on special combinatorial MARS media notation.

M9.5.1 MEDIA NOTATION

The input to combinatorial MARS requires the user to input a media number for each input zone. This entry may have the following definition:

1. If positive, it refers to a valid cross-section mixture provided it is not equal to 1000 or to MEDALB.

2. If negative, it refers to an array residing in the input zone, provided it is not –1000.

The absolute value of the entry is the array number. The following several special media are used in combinatorial geometry in the MARS system:

Media	Description
0	External void - all particles entering Media 0 leak out of the system; their history is terminated.
1000	Internal void - all particles traversing Media 1000 have no interactions; they simply pass through the input zone without any change in direction or energy.
–1000	Universe boundary flag - signals the exit of a particle from a universe. Translation and/or rotation occurs; no tracking is performed in Media –1000; this media is seen only on exiting a zone but never on entering a zone.
MEDALB	Reflection Media - can occur in any level of geometry model; specular reflection occurs; reflecting surface for MARS must be on an RPP or BOX. The body number of the RPP or BOX must be referenced both in the zone exiting and the zone entering.

M9.5.2 TERMS AND DEFINITIONS

1. Bodies - Nine basic geometric shapes with fully enclosed volumes. (Polyhedrals) RPP, BOX, BPP, WED, WPP, ARB, (Revolved Surfaces) SPH, ELL, RCC, TRC, REC. BPP is an alternate specification for BOX; WPP is an alternative for WED.

2. Operators - + Include – Exclude OR Combine.

3. Code Zones - One or more bodies used to describe a portion of problem space having a single media number.

4. Input Zones - One or more code zones used to describe a portion of problem space having a single media number. Code zones may be combined with the OR operator in forming input zones. The complete description for an input zone includes a media number, a region number, and a universe number.

5. Media Number - Explicitly specified in the media number list. In addition to designating a cross-section mixture number, the media number can be used for five other purposes.

Purpose	Numerical value	Use
A	0 < Media Number < 1000 Media Number ≠ MEDALB	Cross-section mixture number
B	Media Number = 0	External void
C	Media Number = 1000	Internal void
D	Media Number = MEDALB	Reflection media number
E	Media Number = –1000	Universe boundary for enclosed space
F	–1000 < Media Number < 0	IABS(MEDIA) = ARRAY number

6. Region Number - Explicitly specified in the region number list. Used to designate a set of weights (Russian roulette, splitting, pathlength stretching) for each input zone.

7. Universe Number - Explicitly specified in the universe number list. Used to designate a set of two or more input zones (in a single coordinate system) bounded by an outer input zone with the media number equal to –1000. The simple Universe (analogue to KENO BOX-TYPE) is the basic "building block" for specifying an array; however, more complicated lattice geometry may be modeled in a universe. The contents of a universe is completely arbitrary. The outer shape of a universe must conform to an RPP or BOX.

8. Array Number - Implicitly determined from the order of arrays specified in the array size list. Explicitly referenced as a negative media number (see Purpose F under Definition 5) OR as a negative entry in the array content list. Thus, an array can contain another array. Positive entries in the array list are universe numbers. A ZERO entry in the array content list designates a vacancy described by other geometry specifications external to the array.

9. MEDALB - Single variable specified in MORSE-SGC (SAS3) to designate a reflective boundary on an RPP surface or combination of RPP surfaces (see Purpose D under Definition 5).

10. Internal Void - Specified as Media 1000 (see Purpose C under Definition 5 listed above). All particles traversing Media 1000 have no interactions.

11. External Void - Specified as Media Number 0 (see Purpose B under Definition 5 listed above). All particles entering Media 0 leak out of the system. Their histories are terminated.

12. Levels - Depth of geometry nesting starting with the absolute or zero universe being Level 0. Higher levels are defined by embedded arrays. The entire system is in Level 0. Large portions of the system are in Level 1. Smaller portions are in Level 2, and so on. All universes within an array are at the same level as the array itself. Each array is at a lower level number than the level number of any arrays embedded in it. Hence, the lower the level number, the more global the level.

M9.5.3 RULES FOR ARRAY REPETITION

1. All arrays must fit snugly in the zone in which they are referenced.

2. The first body referenced in a zone containing an array is used as the array reference body. All translations for particles entering or exiting an array is performed relative to the reference body.

3. An array directly referenced in a lattice cell position of a larger array may not contain any vacant lattice cell positions.

4. A universe containing an array may not have the same reference body as the array it contains.

M9.6 MARS TRACKING LOGIC, SHORTFALLS, AND CORRECTIONS

M9.6.1 PARTICLE NESTING TABLE FOR TRACKING

During tracking in the MARS geometry system, a particle frequently changes universes and arrays. With the ability to repeat and nest arrays in MARS, it is necessary to have a method of determining the particle location relative to the complete geometry model. As each particle tracks through the geometry, a "nesting table" is continually updated on the particle's present location. This nesting table gives detailed information on where the particle is relative to each level of the geometry model. The size of the table is 6*NLEV+4, where NLEV is the total number of geometry levels in a given model. Six entries in the table are given for each geometry level:

FIRST LEVEL:	NBU	LM	NXY(1)	NXY(2)	NXY(3)	NLU
SECOND LEVEL:	"	"	"	"	"	"
	.	.	.	.	.	.
	.	.	.	.	.	.
NLEV LEVEL:	.	.	.	.	.	.

where

NBU is the reference body for the current array if the array was entered by a combinatorial input zone in a universe.

LM is the content of the lattice position of the current array. This value is positive for a universe and negative for an array. This value cannot be zero.

NXY is the current lattice position in Array NLU that is the X, Y, Z position of the lattice.

NLU is the current array number.

For example:

FIRST LEVEL:	12	-5	1	2	1	3
SECOND LEVEL:	0	6	3	1	1	5
THIRD LEVEL:	21	1	5	7	1	1

This is the nesting table for a pin in the center assembly of the typical shipping cask.

The particle location described in the above example is in the 5 7 1 position of the fuel assembly described as Array 1. Array 1 is in Universe 6 referenced at the 3 1 1 location of Array 5. Array 5 is referenced explicitly in the array description of Array 3 in the 1 2 1 position. Array 3 was entered in Input Zone 28. The reference body for Array 3 is Body 12. Input Zone 28 occurs in the absolute universe.

NBU is zero if the array for the current level was explicitly referenced in an array description for the next lowest level of the geometry. NBU cannot be zero for the first level description of the nesting array table. LM may either be positive or negative but not zero. It is positive if a universe is referenced at the NXY location of Array NLU, and it is negative if an array was referenced at the NXY location of Array NLU.

The last four locations in the nesting table after the level data are:

NL ...current level of the particle in the geometry.

NLO ...last effective level change. It is +1 if the particle increased in level number; it is –1 if the particle decreased in level number; it is 0 if the particle changed array location without a change in level. For example, if the particle went from Level 2 to Level 3, NLO would be +1. If a particle went from Level 3 to Level 2, NLO would be –1.

NLUOLD ...The last array the particle was inside before entering the current universe.

NLU ...The current array the particle is inside. This number will be the same as the 6*NL location in the nesting table.

M9.6.2 MARS ARRAY PITFALLS

By now the user is familiar with the concepts of MARS and combinatorial geometry. The relation between MARS and combinatorial geometry is important. MARS determines the universe and the universe location in a geometry model. After the universe is known, then combinatorial geometry determines the code zone and input zone in the universe in which the particle or particle trajectory resides. MARS handles the array bookkeeping and particle translation, as described in the previous section on the MARS-generated nesting table. Combinatorial geometry knows the correct universe number from MARS, and then performs the particle tracking in the universe. MARS logic involves arrays and does not involve zone descriptions. This relationship between MARS and combinatorial geometry is essential to user understanding of the tracking process and should be understood before he ventures forward into constructing a model. Input preparation is one element of building a complex geometry model; but by far, the most difficult part is model debugging. Even the most careful users will find themselves sooner or later examining a geometry dump. Geometry tracking errors are almost inevitable. The purpose of this section is to make the user aware of the pitfalls of MARS array modeling so as to minimize the number of geometry dumps. The success or failure of the MARS combinatorial geometry will depend on the ability of its users to master its many features with reasonable effort.

Before beginning a discussion of geometry model debugging it is imperative that the user have a basic understanding of the combinatorial geometry and MARS array tracking logic. The concepts of MARS universes, arrays, and geometry levels will be essential to understanding this section. The discussion of the nesting table concept introduced in the preceding section is important to interpreting the particle location in a geometry dump. This section will further discuss how MARS enters and exits an array during tracking. This is necessary in order to understand the failures that may occur during entering or exiting arrays.

Arrays are inserted into combinatorial input zones with negative media numbers. This insertion is more of a superpositioning of one geometry model, an array model, onto (not into) a combinatorial geometry input zone. Many warnings were given that the nonvacant lattice positions of an array must fit snugly in the combinatorial input zones where the array is referenced. More exactly, the array must completely fill and preferably slightly overflow the input zone boundary. This is necessary because of the method of entering and exiting arrays. The method of entering an array is described as follows:

1. A particle trajectory in combinatorial geometry encounters an input zone with a negative media number. The negative media number is not –1000; therefore, the particle is entering an array.

2. The particle coordinates must be translated into the array reference system in order to determine the lattice position in the array the particle is entering. The first body in the zone description is the array reference body. The coordinates of the origin of the reference body are subtracted from the particle coordinates, yielding the particle coordinates relative to the origin of the array.

3. Knowing the array being entered determines the lattice cell boundaries. The particle coordinates relative to the array origin must be within a valid nonvacant lattice cell position, or the particle cannot enter the array properly.

4. Next are translated the particle coordinates relative to the lattice cell being entered. The vertex, or the origin, of the lattice cell, XMIN, YMIN, ZMIN, is subtracted from the particle coordinates. This gives the coordinates of the particle relative to the lattice cell position.

5. If the lattice cell contains a universe, the particle coordinates are added to the reference body origin of the universe to give the absolute coordinates of the particle in the universe. Tracking then continues in combinatorial geometry.

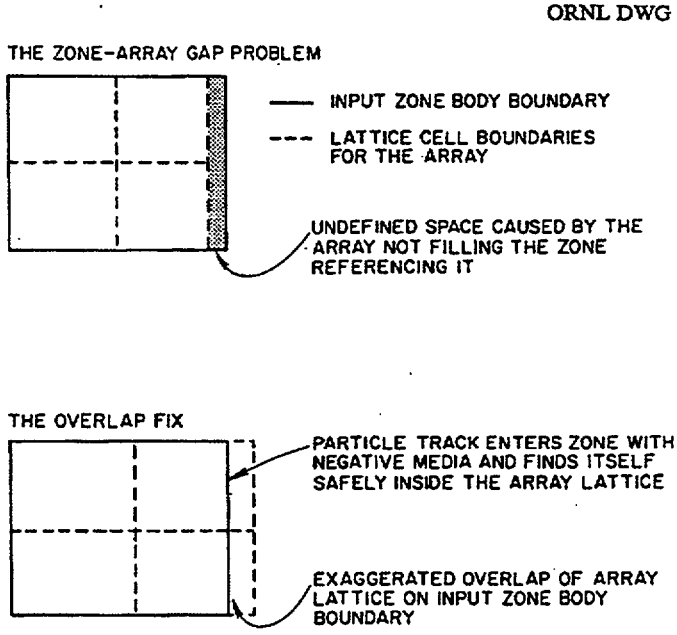
6. If the lattice cell contains a subarray, the result of Step 4 is analogous to Step 2 for entering an array. Therefore, Steps 3, 4, and 5 are repeated for the subarray. When entering subarrays explicitly referenced in a larger array, no absolute coordinate relative to a universe is calculated. This is efficient but may lead to roundoff problems. Tracking into or out of universes helps to reduce roundoff error by translating relative to the universe reference body. This translation gives the particle a fresh update on its coordinates and tends to stabilize the tracking.

Frequently when a particle has made an incorrect entry into an array, the error is due to computer roundoff, or by an insignificant gap between the array lattice and the code zone referencing it. The size of each array and ALL lattice cell boundaries in each array are computed at input time. The size of an array and its lattice cell boundaries are calculated from the reference body of each universe composing each lattice position. The simple arrays, containing no subarrays, in the highest geometry level are computed first, then the larger arrays in the next lower level are computed until all arrays and their respective lattice positions have been calculated. A rigid test is performed to verify the proper fitting of universe reference bodies in lattice positions and the proper fitting of arrays in their reference bodies. If the "FIT Test" fails, then the job is terminated. The figure shown on the next page illustrates an unintentional gap between an array lattice position and a combinatorial input zone.

The gap illustrated may be small, less than 1.0E-09 cm, but it would be sufficient to cause a particle track to be lost. The correction is illustrated as the "overlap fix." If the overlap is greater than 1.0E-09 cm, then Subroutine FINEFI will fatally warn the user, "THE ARRAY ... IN BODY ... REFERENCED IN CODE ZONE ... DOES NOT FIT." Therefore, the overlap applied should be small or it may itself be a fatal error. This is a rigid requirement. The overlap fix is beneficial in exiting the array correctly as well as entering the array correctly.

M9.6.3 COMBINATORIAL MODELING PITFALLS

Now that the user has some appreciation for the pitfalls in array tracking, it is necessary to discuss pitfalls in combinatorial geometry tracking. Whenever two floating-point numbers resulting from separate calculations are compared on a computer of finite precision, it is bad practice to test and depend on direct



equality. In combinatorial tracking it is not always possible to avoid this problem. User input description is the best place to avoid ambiguity on zone boundaries. When two bodies share a common surface, the user should never assume the computer is capable of recognizing the two surfaces are actually a single surface. Furthermore, try to avoid having two bodies sharing a common surface occur on an input zone boundary, especially if the two bodies are referenced in both the adjacent input zone descriptions. In your geometry model, when constructing code zones, always attempt to describe your geometry with combinatorial logic, the union or intersection of bodies, without falling into the dangerous trap of defining bodies with common surfaces. When this is not possible, a less dangerous alternative exists. A small overlap between two body surfaces is preferable to a single surface. Combinatorial geometry will unwittingly let the user double-define space. Combinatorial tracking is always happy with the first definition for a portion of space it finds. It does not check to see if any other definitions exist. The danger comes in trying to leave the doubly defined space and in depending on which definition of the space is used.

M9.6.4 COMPUTER TRACKING AND MODELING

This section deals with the combinatorial MARS tracking logic and considerations involved in geometry model development. It is essential at this point that the user understand the following concepts and definitions before continuing:

A. how combinatorial logic determines in which code zone a particle is located,

B. the meaning of the following combinatorial variables: RIN, ROUT, DIST, DIST0 (see Table M9.E.6 for labelled common /PAREM/),

C. the different roles of combinatorial geometry tracking and MARS array tracking (see Sect. M9.6.3). The complex modeling capabilities of combinatorial MARS are accompanied with a complex debugging output dump requiring user understanding of the tracking methods.

The most important questions combinatorial geometry and MARS must answer during tracking are the following:

MARS Tracking Questions:

A. In which universe is the particle located?

B. Will the particle exit the current universe? If so, then what will be the universe entered and in what array?

Combinatorial Tracking Questions:

A. In which input zone in the current universe is the particle located?

B. Will the particle exit the current input zone? If so, then what will be the next input zone the particle will enter?

These questions for MARS and combinatorial geometry are related in the following way. The first question in each system is asking the basic question:

Where is the particle located?

Each system, MARS and combinatorial, is answering the question from its own perspective. The second question in each system is asking the basic question:

Where is the particle going?

This question cannot be answered without knowing the answer to the first question in both the combinatorial and MARS systems. In changing lattice locations in an array, the dialogue between combinatorial tracking and MARS tracking may go:

Combinatorial: The particle is entering Media –1000; therefore, the particle is exiting the current universe.

MARS: The lattice cell being entered is in the same array as the current lattice cell location; therefore, the new universe being entered is NLU. The new coordinates are computed as X, Y, Z for the new universe.

Combinatorial: The particle is in input zone IR in the current universe. The particle will be entering input zone IRPRIM in the new universe.

MARS: The lattice cell being entered is in the same array as the current lattice cell location; therefore, the new universe being entered is NLU. The new coordinates are computed as X, Y, Z for the new universe.

Combinatorial: The particle is in input zone IRPRIM in the new universe. The particle will be entering input zone IR in the new universe.

Computer tracking in the MARS/combinatorial geometry system is very often a combination of both questions in both systems. A very definite flow exists between the MARS and combinatorial tracking systems which is essential to a nested multiple-array geometry logic. This flow is best understood in the purpose of some of the more important subroutines in both systems. The MARS subroutines discussed will be CALI and PILOT. The combinatorial subroutines discussed will be LOOKZ, G1, and GG. Question A in MARS logic is answered by Subroutine CALI. It calls Subroutine LOOKZ to answer question A in combinatorial logic. Question B in MARS logic is answered by subroutine PILOT. It calls subroutine G1 in combinatorial logic to answer question B for the combinatorial system. MARS subroutines CALI and PILOT call combinatorial subroutines LOOKZ and G1. Combinatorial subroutines do not call MARS subroutines. Both MARS routines CALI and PILOT call LOOKZ, but only PILOT calls combinatorial routine G1. PILOT must call LOOKZ when a particle has entered a new universe to determine the particle input zone location.

Both combinatorial subroutines G1 and LOOKZ call subroutine GG to compute RIN, the distance to enter a body, and ROUT, the distance to exit a body. This information is stored in a floating point array called FPD for the body. This array contains the body definition data as well as the RIN and ROUT for each body. The address in the FPD array for each body information set is stored in the MA array. During a calculation RIN and ROUT are continually updated. The particle position and direction will be referred to as the particle trajectory. Many times during a particle track, the trajectory will change as a result of collisions and entering new universes. The RIN and ROUT computed in one universe are not valid in other universes. To know the current trajectory, a trajectory index is maintained called KLOOP. This index gives each trajectory a unique identifier. Each time RIN and ROUT are calculated for a body, a body trajectory variable called LOOP is updated. LOOP is set to KLOOP when RIN and ROUT are reset in the FPD array. LOOP is stored in the MA array. The detailed description of the FPD and MA array is given in Tables M9.E.3 and M9.E.4 of Appendix E. These arrays will be dumped out whenever a particle gets lost. The combinatorial MARS user should thoroughly understand the contents of the MA and FPD arrays. Unfortunately, by the time a particle is lost in tracking, many important variables in the MA and FPD array have been destroyed by subsequent calculations. The MA and FPD array should be examined in a broad sense in a dump, for detailed information may not exist at the time of the dump.

The MARS subroutines determine the universe a particle is inside and the particle coordinates relative to that universe. The level nesting table in MARS gives the universe location relative to all lower levels of the

MARS geometry. The nesting table is dumped when a particle is lost in tracking through array geometry. The combinatorial geometry routines are called from the MARS routines for tracking inside of a universe.

Most geometry errors fall into two broad categories:

A. undefined space, making it impossible to determine a particle location or impossible to determine the next zone of entry (a particle trajectory is trying to enter undefined space)

B. roundoff gap problems between arrays and lattice cells or between common surfaces of two or more bodies. The gap problem may create an undefined gap in a model.

Errors of type A are discovered in FINEFI (during array input), CALI, or LOOKZ. Errors of type B are discovered by PILOT or G1 during tracking. Whenever an error is discovered, eventually subroutine PR is called. PR dumps the MA and FPD arrays, a few label commons, and calls DIPR. Subroutine DIPR calls DUPR which dumps all relevant array storage information. The nesting table and the local particle coordinates are the last few lines DUPR dumps.

Most of the error messages indicate the subroutine calling for the error dump. It will be helpful to examine the subroutine listing to determine the initiating event causing the error dump. If the message is from PILOT, it probably relates to an array description error or reference. If the message is from G1, the error is probably due to a confusing or contradictory code zone description. The particle coordinates printed out in a geometry dump are either the coordinate of the last collision site or the coordinates where the particle entered the current universe. The value DIST is the trajectory distance from the coordinate site in the direction WB, where WB(1), WB(2), and WB(3) are the particle direction cosines. Examine KLOOP and all the bodies where LOOP is the same as KLOOP. These bodies were the last bodies where RIN and ROUT were computed. The only bodies combinatorial geometry considers the particle trajectory to be located in are those bodies in which RIN is negative and ROUT is positive. Combinatorial geometry considers the particle trajectory is external to all other bodies in which this combination of RIN and ROUT does not exist.

There are normally many combinations of bodies for describing a geometric material zone. Combinatorial logic makes body possibilities very flexible. Frequently, the quickest and most efficient attempt at correction may simply be to try another zone description. It is important to understand geometry errors, but frequently it is more important to obtain results from a geometry model. After examining RIN and ROUT for the current KLOOP, determine if a code zone exists fitting the combination of included and excluded bodies. If the body combination can exist, then an undefined volume of space may exist. If the body combination cannot exist, then G1 will have a roundoff problem in tracking. The user may correct this problem by describing a code zone with the nonexistent combination of bodies. Be careful not to doubly define the geometry model with a second contradictory zone description.

No danger exists in describing an input zone with a nonexistent body description that may not exist. If such a description is necessary to avoid a tracking error, it will not be encountered at any other time during the tracking process.

M9.A FREE-FORM COMBINATORIAL MARS INPUT INSTRUCTIONS

M9.A.1 TITLE* CARD

FORMAT (15A4)

M9.A.2 OPTIONS CARD (four entries required)

IVOPT – Volume option not implemented - enter 0.

IDBG – Debug print option if positive; otherwise, enter 0.

IBOD – Body numbers are assigned by the user if IBOD is greater than zero; otherwise, enter 0.

NAZ – Number of zones to be added to the data storage for next zone of entry memory table. Enter any large number if extra storage is required. Default value allows for five zones to be entered from any single code zone. This option is normally not required; enter 0.

M9.A.3 BODY DEFINITION CARDS

Each new body must start on a new card. The allowable body types are given in Table M9.A.1 along with the required input variables to describe each body. An END card must be used to signify the end of the body definition cards. For each body, the following input is required:

ITYPE – Specifies the alphanumeric body type or END to terminate reading of body data (for example, BOX, RPP, ARB, RCC, etc.)

IALP – Body number assigned by the user if IBOD is greater than zero; otherwise, it is not entered.

FPD(I) – Real data required for the given body as shown in Table M9.A.1. These data must be in cm.

M9.A.4 INPUT ZONE DESCRIPTION CARDS

Each new zone must start on a new card. A three-character title should be given for each new input zone (not necessarily unique) which must start with an alpha-type character. An END card must be used to signify the end of the input zone description cards. For each input zone, the data needed are the title and zone data. Input zone numbers are assigned sequentially.

IALP – The three-character title for the zone where the first character is a letter.

Table M9.A.1 Input required for each body type[a]

Body type	ITYPE	IALP	Real data defining particular body					
Box	BOX	IALP is assigned by the user or by the code if left blank.	Vx	Vy	Vz	H1x	H1y	H1z
			H2x	H2y	H2z	H3x	H3y	H3z
Right parallelepiped	RPP		Xmin	Xmax	Ymin	Ymax	Zmin	Zmax
Sphere	SPH		Vx	Vy	Vz	R	--	--
Right circular cylinder	RCC		Vx	Vy	Vz	Hx	Hy	Hz
			R	--	--	--	--	--
Right elliptical cylinder	REC		Vx	Vy	Vz	Hz	Hy	Hz
			R1x	R1y	R1z	R2x	R2y	R2z
Ellipsoid	ELL		V1x	V1y	V1z	V2x	V2y	V2z
			R	--	--	--	--	--
Truncated right cone	TRC		Vx	Vy	Vz	Hx	Hy	Hz
			R1	R2	--	--	--	--
Right angle wedge	WED or RAW		Vx	Vy	Vz	H1x	H1y	H1z
			H2x	H2y	H2z	H3x	H3y	H3z
Arbitrary polyhedron	ARB		V1x	V1y	V1z	V2x	V2y	V2z
			V3x	V3y	V3z	V4x	V4y	V4z
			V5x	V5y	V5z	V6x	V6y	V6z
			V7x	V7y	V7z	V8x	V8y	V8z
			Face descriptions (see note below)					
Alternative body	BPP		Xmin	Xmax	Ymin	Ymax	Zmin	Zmax
			θ_1	θ_2	θ_3			
Descriptions	WPP		Xmin	Xmax	Ymin	Ymax	Zmin	Zmax
			θ_1	θ_2	θ_3			
Termination of body input data	END							

[a]NOTE: The arbitrary polyhedron input contains a four-digit number for each of the six faces of an ARB body.

IIBIAS(I) – Specify the "OR" operator if required for the JTY(I) body.

JTY(I) - Body number with the (+) or (–) sign as required for the zone description.

Example:

```
PEL +1
CLD +2 –1
H2O +3 –2
END
```

M9.A.5 REGION CARD

One entry is required for each input zone. This entry specifies the importance region each input zone is inside. This step determines which set of weights for splitting, Russian roulette, and pathlength stretching to use in each zone during tracking.

M9.A.6 UNIVERSE CARD

This array specifies which universe each input zone is inside. One entry is required for each input zone. The entry must be either a zero or a positive integer. A negative entry is not valid. Each universe, with the exception of the absolute universe, must contain one and only one zone with a –1000 media. The absolute universe cannot contain any –1000 media zone.

M9.A.7 MEDIA CARD

This array specifies the media contained in each input zone. One entry is required for each input zone. If the entry is positive, it references a valid cross-section mixture or a reflected boundary, MEDALB. If the entry is negative, it references a valid array number as the absolute value of the entry. If the entry is –1000, it references a universe external boundary media. If the entry is 1000, it references an internal void. If the entry is 0, it references an external void.

M9.A.8 ARRAY SIZE SPECIFICATIONS INPUT

An array is a regular rectangular lattice composed of rectangular cells of arbitrary content. The size of each array should be entered as NXMAX, NYMAX, by NZMAX. Arrays are sequentially named as they are entered, starting with 1. The array size entered should include any vacant cells in the array, if any are present. After the size of the last array has been entered, a zero should be entered to terminate the entries. Zero is an illegal entry for an array size. After the zero terminator has been entered, a single integer parameter is entered to determine the means of entering the array specification list. If no array is to be described, only the zero terminator is required.

$NXMAX^i$ – the number of cells along the x-axis of array i

NYMAX^{i} – the number of cells along the y-axis of array i

NZMAX^{i} – the number of cells along the z-axis of array i followed by a "0 terminator"

IOP – array specification input option (required)
= 0 Free-Form Input, FFREAD, type specification
= 1 Standard KENO Mixed Cell (BOX) Orientation Cards
= 2 Standard FIDO Integer Array Input Specification

Example: 15 15 1 6 5 2 7 7 1 0 0

This example describes three arrays. Array 1 will be a 15 × 15 × 1 array. Array 2 will be a 6 × 5 × 2 array. Array 3 will be a 7 × 7 × 1 array. Zero terminates the array size entries. The last zero entered selects the free-form input specification method of describing the array contents.

--End of Geometry Input if no Arrays are Modeled--

M9.A.9 ARRAY CONTENT DESCRIPTION

The contents of each cell of each array must be defined. All contents of Array 1 are defined, then Array 2, etc. The method of entering these data is determined by IOP in Sect. M9.A.8 input. There are three possibilities for each cell entry. These numbers are distinguished by either a positive, zero, or negative entry. A positive entry is a universe number. The universe must fit snugly in the lattice cell position it is referenced inside. The contents of a universe are completely arbitrary. A negative entry is an array entry. The absolute value of the entry is the array being referenced. It must completely fill the lattice position in which it is referenced. It cannot contain any vacancies in its lattice cell positions. Repeating a subarray in a larger array in this manner does not require any additional input. The array must, however, fit snugly in the lattice cell position. The means of entering these data is selected by the user to give flexibility in describing his arrays. The options are the following:

1. IOP = 0 - Free-Form Input Option

   Free-form input is entered using the FFREAD notation. This allows an "*" repeat feature. Data are entered as:

   DO 10 M = 1, NAR (NAR is the number of arrays entered)

   DO 10 K = 1, NZMAX

   DO 10 J = 1, NYMAX

   DO 10 I = 1, NXMAX

   . . .enter the contents of the i^{th}, j^{th}, and z^{th} cell location for array m. . .

10 CONTINUE

All entries must be separated by a blank, and data may be entered in all columns 1 through 80. Entries of the form "L*N" means enter the value N into the input L times. This could also be done with the "R" option by entering "LRN." In either case, blanks within an entry are not allowed.

Example: 2 1 2 2 1 2 2 1 2

This could be the description of a 3 × 3 array of the form,

2 1 2
2 1 2
2 1 2

2. IOP = 1 - Mixed-Cell Orientation Cards

The first field contains the entry followed by three sets of three fields that are treated like FORTRAN DO loops, followed by a field that indicates whether another set of data is to be read. The arrangement of lattice cells may be considered as consisting of a 3-D matrix of numbers, with the cell position increasing in the positive X, Y, and Z directions, respectively. Each set of orientation data consists of the following parameters, separated by one or more blanks.

LTYPE The cell entry. LTYPE may be negative (array #), zero (empty cell), or positive (universe #).

IX1 The starting point in the X direction. IX1 must be at least 1 and less than or equal to NXMAX.

IX2 The ending point in the X direction. IX2 must be at least 1 and less than or equal to NXMAX.

INCX The number of cells by which increments are made in the positive X direction. INCX must be greater than zero and less than or equal to NXMAX.

IY1 The starting point in the Y direction. IY1 must be at least 1 and less than or equal to NYMAX.

IY2 The ending point in the Y direction. IY2 must be at least 1 and less than or equal to NYMAX.

INCY The number of cells by which increments are made in the positive Y direction. INCY must be greater than zero and less than or equal to NYMAX.

IZ1 The starting point in the Z direction. IZ1 must be at least 1 and less than or equal to NZMAX.

IZ2 The starting point in the Z direction. IZ2 must be at least 1 and less than or equal to NZMAX.

INCZ The number of cells by which increments are made in the positive Z direction. INCZ must be greater than zero and less than or equal to NZMAX.

ISTP = 0, read another set of data,
≠ 0, do not read any more mixed-cell orientation data.

An important feature of this type of data description is that, if any portion of an array is defined in a conflicting manner, the last card to define that portion will be the one that determines the array's cell type configuration. To utilize this feature, one can fill an entire array with the most prevalent cell type and then superimpose the other cell types in their proper places to accurately describe the array. The last set of mixed-cell orientation data must have a nonzero entry in the last field.

3. IOP = 2 - Standard FIDO Array Input

The array being entered is integer; therefore, it is a "$" or "$$" array. The array may be entered in the standard free-form FIDO format. The description for each lattice array is entered as a single array block with FIDO. The FIDO integer array number entered is the array number being described plus 100. The data are entered, and each array description is terminated with a "T." All standard FIDO repeat options are available for entering the data. Array 1 would be entered as the "101$$" FIDAS array terminated with a "T." The process would continue until all array descriptions have been entered. The format for the data entry is the same as the description for free-form input. All x entries for the first y row and first z level are entered, then all x entries for the second y row and first z level are entered. This process continues until the entire first z level has been described. Then the second z level is described until the entire array has been described. Then the geometry array description or a given array is terminated with a "T."

M9.A.10 UNIVERSE TYPE

One entry is required for each universe modeled in the combinatorial geometry, starting with Universe 1. The entries should be either a zero or a 1: a zero if the universe is "combinatorial" and a 1 if the universe is "simple." A "simple" universe is a universe composed of concentric zones, where every zone completely surrounds the zone inside of it. Furthermore, input zones in a simple universe may be only one code zone and may be described by only one or two bodies. Tracking through "simple" universes is about 30% or more faster than through regular combinatorial geometry tracking, although the modeling capability is limited. Simple universes may be combined with regular combinatorial universes in arrays without any problems.

--- End of Geometry Input ---

M9.B ILLUSTRATIVE EXAMPLES OF MARS GEOMETRY

M9.B.1 AN UNCOMMON ARRAY SHAPE

Figure M9.B.1 illustrates the geometry being described. The input and some of the output edit are given in Fig. M9.B.2. The MARS input is Cards 2 through 27 in the input list. The remaining input is solely for the JUNEBUG graphics program, which is no longer distributed with the SCALE system. The following correspondence exists between the MARS input instructions and the card image list:

Card number	Input requirement
2	A.1, Title Card
3	A.2, Options Card
4–14	A.3, Body Definition Cards
15–21	A.4, Input Zone Description Cards
22	A.5, Region Card
23	A.6, Universe Card
24	A.7, Media Card
25	A.8, Array Size Specification Input
26	A.9, Array Content Description
27	A.10, Universe Type

The model consists of:

10 Bodies using
3 Body Types (RPP, RCC, and SPH)
6 Input Zones described by
12 Code Zones
1 Universe
1 Array of size 3 × 3 × 1
1 Level of Geometry Nesting

Special attention should be given to:

1. Body 6 is the Reference Body 1 for Universe 1.

2. Input Zone 4 is the Universe 1 boundary zone with the –1000 media.

3. Body 1 is the reference body for Array 1.

4. Input Zone 3 references Array 1 in the media list by a –1 media.

5. Input Zone 3 is described with two code zones, Code Zones 8 and 9.

6. Body 1 is the first body given in the zone description list for Code Zones 8 and 9.

7. Array 1 is a 3 × 3 × 1 array with vacant cell positions on each corner.

8. Array 1 is described with FIDAS input because IOP is 2 on Card 25.

M9.B.1.1 Explanations and Discussions

Universe 1 consists of Input Zones 4, 5, and 6. Input Zone 4 is the universe boundary since it references Media –1000. Zone 6 is described as "+8 –6." The reference body for a universe is the first excluded body in the universe boundary zone description. No tracking occurs in a –1000 media. This acts only as a flag to signify exiting the universe. It is encountered only on exiting a universe. Body 6 not only is the reference body used to translate into and out of Universe 1, but it also defines the size of Universe 1. A universe cannot be referenced in array cells that do not correspond in length, width, and height to the universe's reference body.

Array 1 is referenced in Input Zone 3 which is made up of Code Zones 8 and 9. The reference body for an array is always the first positive body mentioned in the code zone description where the array is referenced.

It must be a positive body reference. An array referenced in an input zone composed of more than one code zone can have only one reference body. Body 1 is the reference body for Array 1. Notice it is the first body mentioned in the descriptions for Code Zones 8 and 9 of Input Zone 3. The reference body for an array must have the same delta x width, delta y depth, and delta z height as the full array. The reference body should be the size of the full array, even though vacancies may exist in the description of the array. The input zone where an array is referenced must fit snugly with the nonvacant lattice positions of the array. It is not necessary to combine Code Zones 8 and 9 into a single input zone as long as they both correctly reference the same reference body.

Notice that, since IOP is 2 on Card 25 of the A.8 input, the array content requirement, A.9, is accomplished with the FIDO input specifications on Card 26.

The nonmaterial media used in this model are the following:

Media number	Description
1000	Internal Void
–1000	Universe Boundary Media
–1	Reference to array 1

The absolute universe, Universe 0, in this model is described with Input Zones 1, 2, and 3. Code Zones 1 through 5 were lumped together into Input Zone 1 since they all contained the same media. This zone definition was done with the "OR" operator. This step is not a requirement. It was done only for logical consistency in the input description. The best way to model any problem is in a manner that the user best understands.

Array 1 contents are

FOR Z = 1

X	1	2	3	
Y				
3	0	1	0	Array 1 is a 3 × 3 × 1 array
2	1	1	1	"0" is a vacant cell position
1	0	1	0	"1" refers to Universe 1

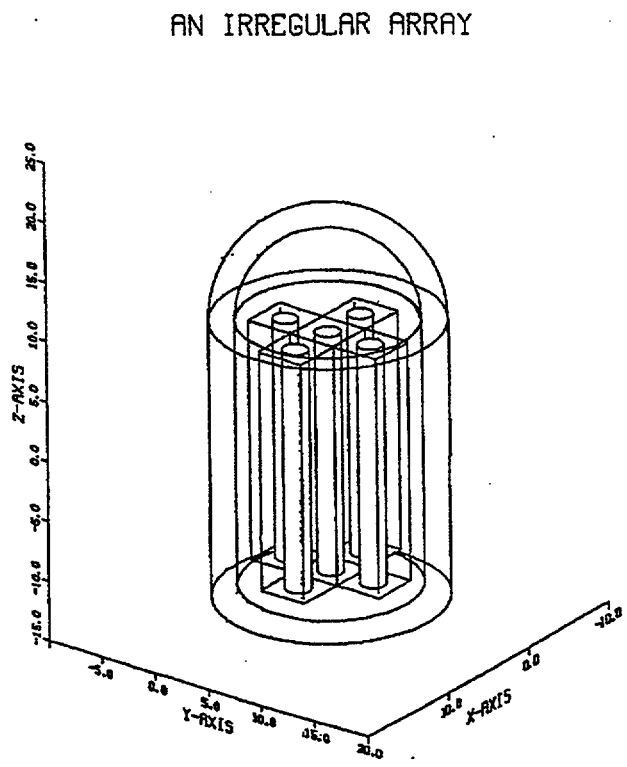


Figure M9.B.1 Computer drawing of Sample Problem 1

```
            the following is a list of card image input

card no.                    data

 1      10 100 10 100 2 1 0 0 0 1.0 .40
 2      an uncommon array shape
 3      3*0 100
 4      rpp  0.0 12.0 0.0 12.0 -10.0 10.0
 5      rcc  6.0 6.0 -11.0 0.0 0.0 22.0 7.0
 6      rcc  6.0 6.0 -12.0 0.0 0.0 23.0 9.0
 7      rpp  4.0  8.0  0.0 12.0  -10.0 10.0
 8      rpp  0.0 12.0 4.0 8.0 -10.0 10.0
 9      rpp  -2.0 2.0 -2.0 2.0 0.0 20.0
10      rcc 0.0 0.0 1.0  0.0 0.0 18.0 1.0
11      rpp  -1.e+08 1.0e+08 -1.0e+08 1.0e+08 -1.0e+08 1.0e+08
12      sph  6.0 6.0 11.0  7.0
13      sph  6.0  6.0 11.0 9.0
14        end
15      spc  +8 -3 -10 or +9 -2  or +2 -4 -5 or +4 -1 or +5 -1
16      cyl  +3 -2 or +10 -9 -3
17      arl  +1  +4  or  +1  +5
18      bdy  +8  -6
19      rod  +7
20      fil  +6 -7
21        end
22       6*1
23      3*0  3*1
24      1000 1 -1 -1000 2 3
25      3 3 1  0  2
26      101$$ 0 1 0 3r1 0 1 0 t
27        1
28        -1
29        1
30      an irregular array$
31        10.0 7.5
32        -10.0 20.0 -10.0 20.0 -15.0 25.0
33        8.5e+03 6.5e+03 5.0e+03
34          0 1 0
35        0 1


            end of card input list
```

Figure M9.B.2 Computer input and output listing of Sample Problem 1

```
an uncommon array shape

                ivopt = 0          idbg = 0


                                                                    body data
 rpp    1  0.0000000E+00  0.1200000E+02  0.0000000E+00  0.1200000E+02 -0.1000000E+02  0.1000000E+02

 rcc    2  0.6000000E+01  0.6000000E+01 -0.1100000E+02  0.0000000E+00  0.0000000E+00  0.2200000E+02
           0.7000000E+01
 rcc    3  0.6000000E+01  0.6000000E+01 -0.1200000E+02  0.0000000E+00  0.0000000E+00  0.2300000E+02
           0.9000000E+01
 rpp    4  0.4000000E+01  0.8000000E+01  0.0000000E+00  0.1200000E+02 -0.1000000E+02  0.1000000E+02

 rpp    5  0.0000000E+00  0.1200000E+02  0.4000000E+01  0.8000000E+01 -0.1000000E+02  0.1000000E+02

 rpp    6 -0.2000000E+01  0.2000000E+01 -0.2000000E+01  0.2000000E+01  0.0000000E+00  0.2000000E+02

 rcc    7  0.0000000E+00  0.0000000E+00  0.1000000E+01  0.0000000E+00  0.0000000E+00  0.1800000E+02
           0.1000000E+01
 rpp    8 -0.1000000E+09  0.1000000E+09 -0.1000000E+09  0.1000000E+09 -0.1000000E+09  0.1000000E+09

 sph    9  0.6000000E+01  0.6000000E+01  0.1100000E+02  0.7000000E+01
 sph   10  0.6000000E+01  0.6000000E+01  0.1100000E+02  0.9000000E+01
number of bodies      10
length of fpd-array   79
```

```
                                                    input zone data
      input zone    code zone          body numbers
 spc          1          1              8     -3    -10
                         2      or      9     -2
                         3      or      2     -4     -5
                         4      or      4     -1
                         5      or      5     -1
 cyl          2          6              3     -2
                         7      or     10     -9     -3
 arl          3          8              1      4
                         9      or      1      5
 bdy          4         10              8     -6
 rod          5         11              7
 fil          6         12              6     -7
number of input zones       6
number of  code zones      12
length of integer array   602
```

code zone	input zone	zone data loc.	no. of bodies	region no.	media no.	box input zone	box code zone
1	1	71	3	1	1000	0	0
2	1	87	2	1	1000	0	0
3	1	98	3	1	1000	0	0
4	1	114	2	1	1000	0	0
5	1	125	2	1	1000	0	0
6	2	136	2	1	1	0	0
7	2	147	3	1	1	0	0
8	3	163	2	1	-1	0	0
9	3	174	2	1	-1	0	0
10	4	185	2	1	-1000	1	1
11	5	196	1	1	2	1	1
12	6	202	2	1	3	1	1

i	kr1(i)	kr2(i)
1	1	5
2	6	7
3	8	9
4	10	10
5	11	11
6	12	12

Figure M9.B.2 (continued)

```
          morse region in input zone(i) array  (mriz(i),i=1,  6)

              1     1     1     1     1     1

          morse media in input zone(i) array (mmiz(i),i=1,  6)

           1000     1    -1-1000     2     3

          morse universe in input zone(i) array (nbiz(i),i=1,  6)

              0     0     0     1     1     1
 option 0 was used in calculating volumes, for  1 regions
0-set volumes = 1, 1-concentric spheres, 2-slabs, 3-inputvolumes.


           volumes ( cc ) used in collisions density and track length estimators.
   reg        1
volume  1.000E+00
  101$ array      9 entries read
     t
                array no.     1      array size is     3 by     3 by     1
```

Figure M9.B.2 (continued)

M9.B.2 OVERLAPPING PINS IN A 2 × 2 ARRAY

Figure M9.B.3 illustrates the geometry described. The input and some of the output edit are given in Fig. M9.B.4. The MARS input is Cards 2 through 55 in the input list. The remaining input is solely for the JUNEBUG graphics program which is no longer distributed with the SCALE system. The following correspondence exists between the MARS input instructions and the card image list:

Card number	Input requirements
2	A.1, Title Card
3	A.2, Options Card
4–18	A.3, Body Definition Card
19–45	A.4, Input Zone Description Cards
46	A.5, Region Card
47	A.6, Universe Card
48–52	A.7, Media Card
53	A.8, Array Size Specification Input
54	A.9, Array Content Description
55	A.10, Universe Type

The model consists of:

14	Bodies using
2	Body Types (RCC and RPP)
26	Input Zones described by
26	Code Zones
4	Universes
1	Array of size 2 × 2 × 1
1	Level of Geometry Nesting

Special attention should be given to:

1. Body 11 is the reference body for Universe 1.
2. Body 12 is the reference body for Universe 2.
3. Body 10 is the reference body for Universe 3.
4. Body 9 is the reference body for Universe 4.
5. Input Zone 6 is the universe boundary zone for Universe 1.
6. Input Zone 12 is the universe boundary zone for Universe 2.
7. Input Zone 18 is the universe boundary zone for Universe 3.
8. Input Zone 24 is the universe boundary zone for Universe 4.

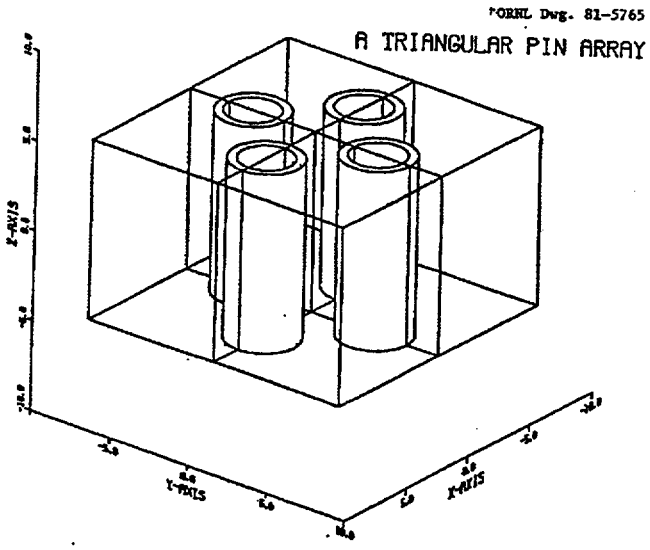


Figure M9.B.3 Computer drawing of Sample Problem 2

```
             the following is a list of card image input

card no.                    data

 1       10 30 10 30 5*0 0.3 0.3
 2       overlapping pins in a 2 by 2 array, jim west ornl
 3       3*0 100
 4      rcc 8.0 12.0 0.0   0.0 0.0 10.0  1.5
 5      rcc 8.0 12.0 0.0   0.0 0.0 10.0   2.0
 6      rcc  12.0 8.0 0.0   0.0 0.0 10.0 1.5
 7      rcc  12.0 8.0 0.0   0.0 0.0 10.0 2.0
 8      rcc  8.0 4.0 0.0 0.0 0.0 10.0 1.5
 9      rcc  8.0 4.0 0.0 0.0 0.0 10.0 2.0
10      rcc  4.0 8.0 0.0 0.0 0.0 10.0 1.5
11      rcc  4.0 8.0 0.0 0.0 0.0 10.0 2.0
12      rpp  0.0 8.0 0.0  8.0 0.0 10.0
13      rpp  8.0 16.0 0.0  8.0 0.0 10.0
14      rpp  0.0 8.0 8.0 16.0 0.0 10.0
15      rpp  8.0 16.0 8.0 16.0 0.0 10.0
16      rpp -8.0 8.0 -8.0 8.0 -5.0 5.0
17      rpp  -1.0e+07 1.0e+07 -1.0e+07 1.0e+07 -1.0e+07 1.0e+07
18       end
19      pi1  +1 +11
20      pc1  +2 -1 +11
21      pi4  +7 +11
22      pc4  +8 -7 +11
23      fi1 +11 -2 -8
24      fb1  +14 -11
25      pi1 +1 +12
26      pc1 +2 -1 +12
27      pi2  +3  +12
28      fc2  +4 -3 +12
29      fi2  +12 -2 -4
30      fb2  +14  -12
31      pi2  +3 +10
32      pc2  +4 -3 +10
33      pi3  +5 +10
34      pc3  +6 -5 +10
35      fi3  +10 -4 -6
36      fb3  +14 -10
37      fi3  +5  +9
38      fc3  +6 -5 +9
39      fi4  +7  +9
40      fc4  +8 -7 +9
41      fi4  +9  -6  -8
42      fb4  +14 -9
43      ar1  +13
44      air  +14 -13
45       end
46       6*1 6*2 6*3 6*4 2*5
47       6*1 6*2 6*3 6*4 2*0
48       1 2 1 2 3 -1000
49       1 2 1 2 3 -1000
50       1 2 1 2 3 -1000
51       1 2 1 2 3 -1000
52       -1 1000
53        2  2  1     0  0
54        4 3 1 2
55        4*1
56        -1
57         1
58       a weird 2 by 2 array$
59        10.0 7.5
60        -10.0 10.0 -10.0 10.0 -10.0  10.0
61      8.5e+03 6.5e+03 5.0e+03
62       0 1 0 1 0 0
63       0 1 0 1 0 0
64       0 1 0 1 0 0
65       0 1 0 1 0 0
66       0 0
67       0 1
          end of card input list
```

Figure M9.B.4 Computer input and output listing of Sample Problem 2

```
      overlapping pins in a 2 by 2 array, jim west ornl

                    ivopt = 0          idbg = 0

                                                                  body data
 rcc     1  0.8000000E+01  0.1200000E+02  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.1000000E+02
            0.1500000E+01
 rcc     2  0.8000000E+01  0.1200000E+02  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.1000000E+02
            0.2000000E+01
 rcc     3  0.1200000E+02  0.8000000E+01  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.1000000E+02
            0.1500000E+01
 rcc     4  0.1200000E+02  0.8000000E+01  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.1000000E+02
            0.2000000E+01
 rcc     5  0.8000000E+01  0.4000000E+01  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.1000000E+02
            0.1500000E+01
 rcc     6  0.8000000E+01  0.4000000E+01  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.1000000E+02
            0.2000000E+01
 rcc     7  0.4000000E+01  0.8000000E+01  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.1000000E+02
            0.1500000E+01
 rcc     8  0.4000000E+01  0.8000000E+01  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.1000000E+02
            0.2000000E+01
 rpp     9  0.0000000E+00  0.8000000E+01  0.0000000E+00  0.8000000E+01  0.0000000E+00  0.1000000E+02

 rpp    10  0.8000000E+01  0.1600000E+02  0.0000000E+00  0.8000000E+01  0.0000000E+00  0.1000000E+02

 rpp    11  0.0000000E+00  0.8000000E+01  0.8000000E+01  0.1600000E+02  0.0000000E+00  0.1000000E+02

 rpp    12  0.8000000E+01  0.1600000E+02  0.8000000E+01  0.1600000E+02  0.0000000E+00  0.1000000E+02

 rpp    13 -0.8000000E+01  0.8000000E+01 -0.8000000E+01  0.8000000E+01 -0.5000000E+01  0.5000000E+01

 rpp    14 -0.1000000E+08  0.1000000E+08 -0.1000000E+08  0.1000000E+08 -0.1000000E+08  0.1000000E+08

number of bodies      14
length of fpd-array  120
```

Figure M9.B.4 (continued)

```
                                                    input zone data
      input zone    code zone          body numbers
 pi1          1          1          1     11
 pc1          2          2          2     -1      11
 pi4          3          3          7     11
 pc4          4          4          8     -7      11
 fi1          5          5         11     -2      -8
 fb1          6          6         14    -11
 pi1          7          7          1     12
 pc1          8          8          2     -1      12
 pi2          9          9          3     12
 fc2         10         10          4     -3      12
 fi2         11         11         12     -2      -4
 fb2         12         12         14    -12
 pi2         13         13          3     10
 pc2         14         14          4     -3      10
 pi3         15         15          5     10
 pc3         16         16          6     -5      10
 fi3         17         17         10     -4      -6
 fb3         18         18         14    -10
 fi3         19         19          5      9
 fc3         20         20          6     -5       9
 fi4         21         21          7      9
 fc4         22         22          8     -7       9
 fi4         23         23          9     -6      -8
 fb4         24         24         14     -9
 arl         25         25         13
 air         26         26         14    -13
number of input zones     26
number of  code zones     26
length of integer array 1129
```

Figure M9.B.4 (continued)

code zone	input zone	zone data loc.	no. of bodies	region no.	media no.	box input zone	box code zone
1	1	99	2	1	1	1	1
2	2	110	3	1	2	1	1
3	3	126	2	1	1	1	1
4	4	137	3	1	2	1	1
5	5	153	3	1	3	1	1
6	6	169	2	1	-1000	1	1
7	7	180	2	2	1	2	2
8	8	191	3	2	2	2	2
9	9	207	2	2	1	2	2
10	10	218	3	2	2	2	2
11	11	234	3	2	3	2	2
12	12	250	2	2	-1000	2	2
13	13	261	2	3	1	3	3
14	14	272	3	3	2	3	3
15	15	288	2	3	1	3	3
16	16	299	3	3	2	3	3
17	17	315	3	3	3	3	3
18	18	331	2	3	-1000	3	3
19	19	342	2	4	1	4	4
20	20	353	3	4	2	4	4
21	21	369	2	4	1	4	4
22	22	380	3	4	2	4	4
23	23	396	3	4	3	4	4
24	24	412	2	4	-1000	4	4
25	25	423	1	5	-1	0	0
26	26	429	2	5	1000	0	0

```
morse region in input zone(i) array  (mriz(i),i=1, 26)

    1   1   1   1   1   1   2   2   2   2   2   2   3   3   3   3   3   3   4   4   4   4

    4   4   5   5

morse media in input zone(i) array (mmiz(i),i=1, 26)

    1   2   1   2   3-1000   1   2   1   2   3-1000   1   2   1   2   3-1000   1   2   1   2

    3-1000   -1 1000

morse universe in input zone(i) array (nbiz(i),i=1, 26)

    1   1   1   1   1   1   2   2   2   2   2   2   3   3   3   3   3   3   4   4   4   4

    4   4   0   0
```

Figure M9.B.4 (continued)

```
 option 0 was used in calculating volumes, for  5 regions
0-set volumes = 1, 1-concentric spheres, 2-slabs, 3-inputvolumes.

          volumes ( cc ) used in collisions density and track length estimators.
   reg        1           2           3           4           5
volume  1.000E+00   1.000E+00   1.000E+00   1.000E+00   1.000E+00
              array no.    1     array size is    2 by    2 by    1


               level     1 of array no.     1

     x =   1  2
   y

   2       1  2

   1       4  3


                    universe specifications

               universe          1-simple/0-comjom


         code zone   2 in universe   1 cannot be a simple universe


                  1                    0

         code zone   8 in universe   2 cannot be a simple universe


                  2                    0

         code zone  14 in universe   3 cannot be a simple universe


                  3                    0

         code zone  20 in universe   4 cannot be a simple universe


                  4                    0
```

Figure M9.B.4 (continued)

9. This model has one code zone for each input zone.

10. The same bodies may be used in more than one universe description, thereby reducing the number of bodies needed to model a given geometry. Notice the cylinders overlap the universe boundaries and each cylinder is referenced in two universes.

11. This model has one array of size 2 × 2 × 1.

12. The reference body for Array 1 is Body 13.

13. The array content description on Card 54 used the free-form specification option with IOP set to 0 on Card 53.

The reference body for a universe is the excluded body in the universe boundary zone description. Everything inside the universe reference body comprises the universe model. This model demonstrates the importance of positioning the universes correctly in an array. If the array content input was reversed, what would the picture look like? Actually, for this model there was not a real need to use the array feature of MARS. This could have been modeled completely in the absolute universe. Notice in the output listing that the universes in this problem are combinatorial and not simple. The input declared the universes as simple, but MARS changed the input to combinatorial and issued warning messages accordingly.

M9.B.3 PLEXIGLAS PIPE CROSS EXPERIMENT

Figure M9.B.5 illustrates the geometry being described. The input and some of the output edit is given in Fig. M9.B.6. The MARS input is Cards 2 through 38 in the input list. The remaining input is solely for the JUNEBUG graphics program which is no longer distributed with the SCALE system. The following correspondence exists between the MARS input instructions and the card image list:

Card number	Input requirements
2	A.1, Title Card
3	A.2, Options Card
4–19	A.3, Body Definition Cards
20–34	A.4, Input Zone Description Cards
35	A.5, Region Card
36	A.6, Universe Card
37	A.7, Media Card
38	A.8, Array Size Specification Input
	Note: Since no arrays were specified, Input A.9 was not entered.

The model consists of:

15	Bodies using
3	Body Types (RPP, RCC, & BOX)
14	Input Zones described by
15	Code Zones
0	Universes
0	Arrays
0	Level of Geometry Nesting

ORNL Dwg. 81-5766

PIPE CROSS EXP.

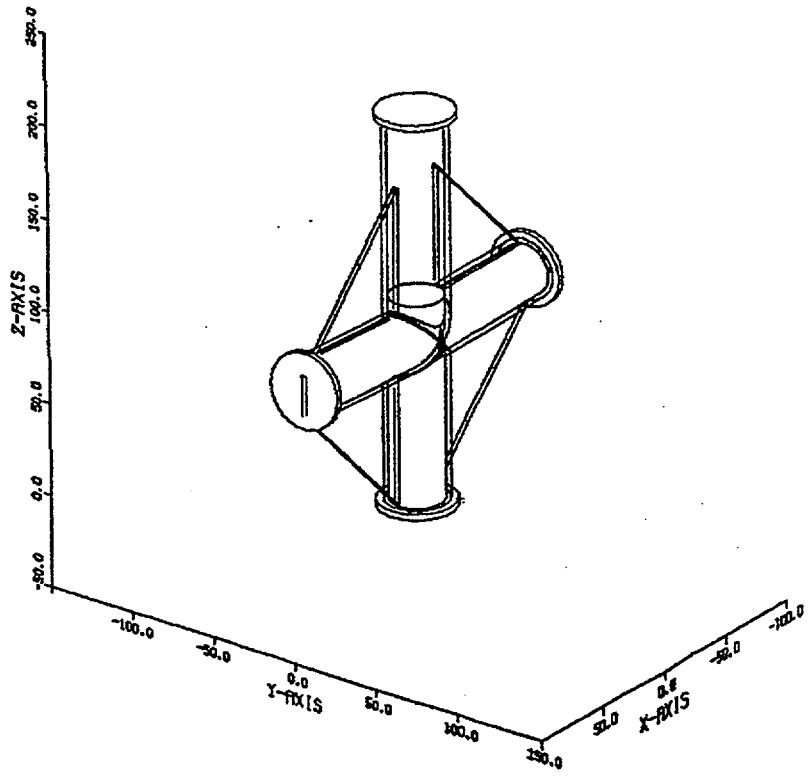


Figure M9.B.5 Computer drawing of Sample Problem 3

```
             the following is a list of card image input

card no.                    data

 1      10 100 10 100 1 4*0   0.5 0.5
 2      plexiglas pipe cross critical experiment
 3      3*0 10
 4      rcc 0.0 0.0 3.175 0.0 0.0 207.01 13.97
 5      rcc 0.0 0.0 3.175 0.0 0.0 207.01 16.51
 6      rcc 0.0 0.0 91.44 88.160559 0.0 3.076759 13.97
 7      rcc 0.0 0.0 91.44 88.160559 0.0 3.076759 16.51
 8      rcc 0.0 0.0 91.44 -88.160559 0.0 3.076759 13.97
 9      rcc 0.0 0.0 91.44 -88.160559 0.0 3.076759 16.51
10      rcc 0.0 0.0 0.0 0.0 0.0 3.175 20.32
11      rcc 0.0 0.0 210.185 0.0 0.0 3.175 20.32
12      rcc 88.150000 0.0 94.518635 3.173066 0.0 0.110806 20.32
13      rcc -88.160559 0.0 94.518635 -3.173066 0.0 0.1108-6 20.32
14      box 0.0 -1.27 -10.80 102.24 0.0 102.24 0.0 2.54 0.0 -102.24 0.0 102.24
15      rpp -300.0 300.0 -300.0 300.0 -300.0 113.175
16      rpp -350.0 350.0 -350.0 350.0 -350.0 350.0
17      rpp  -1.0e+05 1.0e+05 -1.0e+05  1.0e+05  -1.0e+05 1.0e+05
18      rpp -90. 90. -10.0.10.0 0.0 213.36
19       end
20      pg1 +2 -1 -4 -6 -7 -8
21      pg2 +6 -5 -10 -1
22      pg3 +4 -3 -9 -1
23      pg4 +7
24      pg5 +8
25      pg6 +9
26      pg7 +10
27      pg8 +11 -2 -4 -6 -7 -8 -9 -10 +15
28      uf1 +12 +1
29      uf2 +12 +5 -1
30      uf3 +12 +3 -1
31      vod +1 -12
32      fil +13 -2 -4 -6 -7 -8 -9 -10 -11 or +13 +11 -15 -9
33      rfl +14 -13
34       end
35      14*1
36      14*0
37       8*2 3*1 1000 3 0
38        0
39        -1
40        1
41       pipe cross exp.$
42        10.0 7.5
43       -100.0 100.0 -130.0 130.0 -10.0 220.0
44       8.5e+03 6.5e+03 5.0e+03
45       3*0 4*1 0 3*1 4*0
46        0


        end of card input list
```

Figure M9.B.6 Computer input and output listing of Sample Problem 3

```
        plexiglas pipe cross critical experiment

                  ivopt = 0          idbg = 0


                                                                  body data
 rcc     1  0.0000000E+00  0.0000000E+00  0.3175000E+01  0.0000000E+00  0.0000000E+00  0.2070100E+03
            0.1397000E+02
 rcc     2  0.0000000E+00  0.0000000E+00  0.3175000E+01  0.0000000E+00  0.0000000E+00  0.2070100E+03
            0.1651000E+02
 rcc     3  0.0000000E+00  0.0000000E+00  0.9144000E+02  0.8816056E+02  0.0000000E+00  0.3076759E+01
            0.1397000E+02
 rcc     4  0.0000000E+00  0.0000000E+00  0.9144000E+02  0.8816056E+02  0.0000000E+00  0.3076759E+01
            0.1651000E+02
 rcc     5  0.0000000E+00  0.0000000E+00  0.9144000E+02 -0.8816056E+02  0.0000000E+00  0.3076759E+01
            0.1397000E+02
 rcc     6  0.0000000E+00  0.0000000E+00  0.9144000E+02 -0.8816056E+02  0.0000000E+00  0.3076759E+01
            0.1651000E+02
 rcc     7  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.3175000E+01
            0.2032000E+02
 rcc     8  0.0000000E+00  0.0000000E+00  0.2101850E+03  0.0000000E+00  0.0000000E+00  0.3175000E+01
            0.2032000E+02
 rcc     9  0.8815000E+02  0.0000000E+00  0.9451864E+02  0.3173066E+01  0.0000000E+00  0.1108060E+00
            0.2032000E+02
 rcc    10 -0.8816056E+02  0.0000000E+00  0.9451864E+02 -0.3173066E+01  0.0000000E+00  0.1108000E-06
            0.2032000E+02
 box    11  0.0000000E+00 -0.1270000E+01 -0.1080000E+02  0.1022400E+03  0.0000000E+00  0.1022400E+03
            0.0000000E+00  0.2540000E+01  0.0000000E+00 -0.1022400E+03  0.0000000E+00  0.1022400E+03
 rpp    12 -0.3000000E+03  0.3000000E+03 -0.3000000E+03  0.3000000E+03 -0.3000000E+03  0.1131750E+03

 rpp    13 -0.3500000E+03  0.3500000E+03 -0.3500000E+03  0.3500000E+03 -0.3500000E+03  0.3500000E+03

 rpp    14 -0.1000000E+06  0.1000000E+06 -0.1000000E+06  0.1000000E+06 -0.1000000E+06  0.1000000E+06

 rpp    15 -0.9000000E+02  0.9000000E+02 -0.1001000E+02  0.0000000E+00  0.2133600E+03  0.0000000E+00

number of bodies      15
length of fpd-array  136
```

```
                                                                                  input zone data
      input zone   code zone        body numbers
 pg1         1          1              2     -1     -4     -6     -7     -8
 pg2         2          2              6     -5    -10     -1
 pg3         3          3              4     -3     -9     -1
 pg4         4          4              7
 pg5         5          5              8
 pg6         6          6              9
 pg7         7          7             10
 pg8         8          8             11     -2     -4     -6     -7     -8     -9    -10     15

 ufl         9          9             12      1
 uf2        10         10             12      5     -1
 uf3        11         11             12      3     -1
 vod        12         12              1    -12
 fil        13         13             13     -2     -4     -6     -7     -8     -9    -10    -11

                       14     or      13     11    -15     -9
 rfl        14         15             14    -13
number of input zones     14
number of  code zones     15
length of integer array  620
```

Figure M9.B.6 (continued)

```
 code zone     input zone     zone data loc.     no. of bodies    region no.    media no.    box input zone    box code zone
      1             1              106                6              1             2              0                0
      2             2              137                4              1             2              0                0
      3             3              158                4              1             2              0                0
      4             4              179                1              1             2              0                0
      5             5              185                1              1             2              0                0
      6             6              191                1              1             2              0                0
      7             7              197                1              1             2              0                0
      8             8              203                9              1             2              0                0
      9             9              249                2              1             1              0                0
     10            10              260                3              1             1              0                0
     11            11              276                3              1             1              0                0
     12            12              292                2              1          1000              0                0
     13            13              303                9              1             3              0                0
     14            13              349                4              1             3              0                0
     15            14              370                2              1             0              0                0

    i    krl(i)    kr2(i)
    1        1         1
    2        2         2
    3        3         3
    4        4         4
    5        5         5
    6        6         6
    7        7         7
    8        8         8
    9        9         9
   10       10        10
   11       11        11
   12       12        12
   13       13        14
   14       15        15
0
         morse region in input zone(i) array  (mriz(i),i=1, 14)

            1    1    1    1    1    1    1    1    1    1    1    1    1    1
0
         morse media in input zone(i) array (mmiz(i),i=1, 14)

            2    2    2    2    2    2    2    2    1    1    1 1000    3    0
0
         morse universe in input zone(i) array (nbiz(i),i=1, 14)

            0    0    0    0    0    0    0    0    0    0    0    0    0    0
1 option 0 was used in calculating volumes, for  1 regions
 0-set volumes = 1, 1-concentric spheres, 2-slabs, 3-inputvolumes.


          volumes ( cc ) used in collisions density and track length estimators.
    reg         1
 volume  1.000E+00


 array data requires         8 locations, leaving     13921 locations
```

Figure M9.B.6 (continued)

COMBINATORIAL GEOMETRY ZONE TRANSFER SUMMARY TABLES

EXIT ZONE	EXIT BODY	LOC. IN MA ARRAY	ENTERING ZONE	NO* OF ENTRIES	LOC. FOR NEXT ZONE
1	2				
		109	13	755	411
		411	8	89	0
1	-1				
		114	12	508	396
		396	9	491	0
1	-4				
		119	3	153	0
1	-6				
		124	2	188	0
1	-7				
		129	4	138	0
1	-8				
		134	0	0	0
2	6				
		140	13	437	405
		405	8	80	408
		408	1	77	0
2	-5				
		145	10	580	0
2	-10				
		150	7	57	0
2	-1				
		155	9	74	0
3	4				
		161	13	320	399
		399	1	177	402
		402	8	73	420
		420	2	33	0
3	-3				
		166	11	612	0
3	-9				
		171	0	0	0
3	-1				
		176	9	152	0
4	7				
		182	13	467	438
		438	14	83	0
5	8				
		188	13	566	0
6	9				
		194	13	409	414
		414	3	253	423
		423	11	181	426
		426	8	7	0
7	10				

Figure M9.B.6 (continued)

COMBINATORIAL GEOMETRY ZONE TRANSFER SUMMARY TABLES

EXIT ZONE	EXIT BODY	LOC. IN MA ARRAY	ENTERING ZONE	NO* OF ENTRIES	LOC. FOR NEXT ZONE
7	10				
		200	13	182	444
		444	14	12	0
8	11				
		206	13	893	0
8	-2				
		211	1	44	0
8	-4				
		216	3	114	0
8	-6				
		221	2	90	0
8	-7				
		226	0	0	0
8	-8				
		231	0	0	0
8	-9				
		236	0	0	0
8	-10				
		241	7	1	0
8	15				
		246	0	0	0
9	12				
		252	0	0	0
9	1				
		257	4	258	381
		381	2	186	384
		384	1	157	387
		387	10	75	390
		390	3	52	393
		393	11	36	0
10	12				
		263	0	0	0
10	5				
		268	7	165	429
		429	13	151	432
		432	2	94	435
		435	8	48	0
10	-1				
		273	9	8	0
11	12				
		279	0	0	0
11	3				
		284	3	176	417
		417	6	70	0
11	-1				
		289	9	23	0

Figure M9.B.6 (continued)

COMBINATORIAL GEOMETRY ZONE TRANSFER SUMMARY TABLES

EXIT ZONE	EXIT BODY	LOC. IN MA ARRAY	ENTERING ZONE	NO. OF ENTRIES	LOC. FOR NEXT ZONE
12	1				
		295	1	218	0
12	-12				
		300	9	241	0
13	13				
		306		300	0
13	-2				
		311		2033	0
13	-4				
		316	3	1016	0
13	-6				
		321	2	1050	0
13	-7				
		326	4	377	0
13	-8				
		331	5	509	0
13	-9				
		336	6	939	0
13	-10				
		341	7	334	0
13	-11				
		346	8	1504	447
		447	14	147	0
14	13				
		352	0	0	0
14	11				
		357	13	176	441
		441	7	17	0
14	-15				
		362	0	0	0
14	-9				
		367	6	11	0
15	14				
		373	0	0	0
15	-13				
		378	13	6976	0

Figure M9.B.6 (continued)

Special attention should be given to:

1. This model does not use the MARS array feature; therefore, Input Requirement A.9 is not entered. Input A.8 consisted only of the terminating zero input.

2. All input zones are in the absolute universe, and no other input zones are described.

M9.C COMBINATORIAL GEOMETRY ZONE SUMMARY TABLE DESCRIPTION

Input zones are described by one or more code zones. The code zone description consists of the union or the intersection of bodies. If a body is totally included in a code zone, then a particle could exit the zone by exiting the body. If a body is an excluded body referenced with a negative sign in a code zone description, then a particle could exit the zone by entering the body. Every time a particle exits a zone, it does so by entering or leaving one or more bodies used in the zone description. To save time in determining the next zone of entry, combinatorial geometry builds a table of the zones entered when a particle exits a given zone by way of a specific body in the zone description. To make this process more useful, combinatorial geometry counts the number of times it enters a given zone from a given body in an adjacent zone. At the end of a batch or generation of particles, this table is sorted in order of the most frequent zone of entry. This sorting enables the geometry tracking system to check the more probable zones of entry before checking the less probable zones of entry. For most problems, this process will not accelerate the tracking significantly. It will, however, provide the user with a detailed account of where his tracking took place and with how much frequency. The zone transfer summary table is printed out at the end of each calculation. It is a good way to check geometry models for inconsistencies. The zone summary table gives the frequency of each zone transfer and by what body the zone transfer took place.

The following zone transfers are from the plexiglas pipe (Sect. M9.B.3). The exit and entry zone refers to code zones. We shall discuss the transfers out of Code Zone 3. This code zone's body description is 4-3-9-1. For each body in Zone 3's description, there will be an exit table giving the zones entered upon exiting Zone 3 from each body and the frequency each was entered. For example, histories exiting Code Zone 3 by way of Body 4 entered Code Zone 13 320 times; Zone 1 was entered 177 times; Zone 8 was entered 73 times; Zone 2 was entered 33 times. All of these entries were exits from Code Zone 3 by way of exiting Body 4. The user should examine his zone summary table and decide if the transfers were correct for the model he intended to design. Very often the intended model is not the model input. It is easy in three-dimensional (3-D) geometry modeling to leave a small crack in the model. The code zone transfer summary table is designed to verify and assist in the proper construction of a geometry model.

M9.D INTERFACING THE MARS SUBROUTINES MODULE TO OTHER COMPUTER CODES

MARS has been developed in a modularized system so that it may be easily adapted with minimal effort into other computer codes. There are only a very few subroutines the user needs to communicate with inside the MARS system. For input the user will have to call subroutines JOMIN1, JOMIN2, and AZIP in MARS. Examples of this may be found in Subroutine RINPUP in the SCALE SAS3 control program, and in Subroutine RINPU1 in MORSE-SGC. For asking the location of a particle given a coordinate in the absolute universe, Level 0 of the geometry model, the user needs to call Subroutine CALI. Examples of this can be found in Subroutines SOURCE and GETNT in MORSE-SGC. Knowing a particle location, trajectory, and distance it may travel, the user needs to call Subroutine PILOT to determine the next zone of entry. Examples of calls to PILOT may be found in Subroutines GOMST and EUCLID in MORSE-SGC. Notice that labeled common ARAR contains NAR, the number of arrays in a model and NLEV, the number of geometry levels present in a model. Occasionally, the user will have the nesting table for a particle and need the particle coordinate either in a lower or higher geometry level. Subroutine RISK was written to take a particle coordinate in Geometry Level NL1 and translate it to Geometry Level NL2, given the nesting array. For calling RISK, NL2 must be greater than or equal to NL1. The opposite may be accomplished by calling Subroutine CLEV. That is, CLEV takes a coordinate in Level NL1 and translates the coordinate to Level NL2. CLEV is in the MARS subroutine library. PILOT in MARS and GETNT in MORSE call CLEV.

The user should be careful in using MARS to protect the particle nesting table during tracking. The user should be aware that, when a particle enters a rotated coordinate system, the particle direction cosines, WB in labeled common PAREM, are automatically rotated.

M9.E MARS DATA STORAGE AND PROGRAM LOGIC

Subroutine CALI answers the question: What is the particle location? It is given particle coordinates, usually in the absolute universe, although this is not a requirement. It proceeds to determine if the particle is in an array or in a valid material media. If the particle is in a valid media, it determines this and returns. If the particle is in an array, it then checks the next level of the geometry as described in the array description. It repeats the process until it determines a valid positive material media the particle coordinates are inside. In this process, it starts from a lower, more global level of the geometry hierarchy, and checks from there to a higher, more local geometry level. The process is completed when the particle is located in a positive real media.

During the process of checking successive levels of a geometry model, the nesting table is always updated as the particle coordinates are translated. Therefore, as MARS goes from a lower global level to a higher, local geometry level, MARS always maintains the knowledge of where the particle is located relative to the lower, more global geometry levels.

Subroutine PILOT goes through the same process during tracking, except it has the logic to translate from higher levels to lower levels as well as from lower levels to higher levels. This is necessary for tracking. PILOT uses the nesting table generated by CALI when the particle initial location was determined. Both PILOT and CALI call Subroutine STORA to update the nesting table.

M9.E.1 MARS SUBROUTINE DESCRIPTIONS

ABEND - ABEND is called for an abnormal termination of a calculation. It calls RCOVER.

ABOX - ABOX is called from JOMIN1. It reads the BPP and WPP body data and converts the data to the BOX and WED body input format. The BPP and WPP are alternative ways of describing the BOX and WED.

ALBERT - ALBERT is called from GENI to construct the floating-point data to be stored in the FPD table for the ARB body, the arbitrary polyhedron body.

ARGEN - ARGEN is called from AZIP. It generates the size of each array from the array content tables and NLV table. It must compute the size of the simplest arrays first. These arrays are the arrays that contain only universes that do not contain subarrays. ARGEN comes from the term "array generator." The x-width, y-length, and z-height of each array is stored in the WLH array. This array is not needed in tracking or particle locating. It is needed to verify the fit of each array in each reference location.

AZIP - AZIP reads the combinatorial MARS array size and content input. It calls several other subroutines and generates a series of tables from the input data that are needed for MARS array tracking. It is called after JOMIN2 and GENI have set up the combinatorial data tables in memory. It uses much of the combinatorial input data from memory to construct the MARS data tables.

BOD - BOD is called from CELL after the lattice cell position of a particle has been determined. It returns the cell contents. If the contents of a cell is vacant, it sets a flag. This is legal for exiting an array but fatal for entering an array. A particle cannot enter a vacant lattice position of an array.

CALI - CALI is called from outside the MARS subroutine module to determine a particle location. It first determines the universe and array the particle is inside. Frequently this requires checking several levels of the geometry model. CALI calls LOOKZ to determine the combinatorial geometry input zone a particle is inside for each universe or array. When CALI has checked several levels of geometry logic and determines the positive media the particle is inside, it then returns the information in labeled common PAREM, with the nesting table set by calls to STORA.

CELL - CELL is called from both CALI and PILOT. It is the guts of entering or exiting an array. It is called for a particle inside of or moving through an array. It returns the lattice cell position and content for the current particle position. CELL serves a dual role. It indicates the location of a particle in an array when the particle is not moving, and it says the next cell the particle will enter when the particle is moving. CELL calls subroutines SORT and BOD.

CLEV - CLEV is called from PILOT to translate a particle coordinate from a larger level, more local coordinate system to a lower, more global geometry level number given the nesting table. Because of the presence of several labeled commons in CLEV, it changes quite a few variables in a few commons. The user should be careful before calling CLEV so as not to inadvertently change some important information needed for tracking.

CORNER - CORNER is called from TRENTE and RTEXIT. It returns the origin or vertex for a reference body. This information is essential to particle translation for both entering and exiting a universe or an array.

CTRAN - CTRAN is called to determine the particle coordinate relative to either a lattice cell in an array or given the lattice position and the particle coordinate, it can determine the coordinate of the particle relative to the origin of the array. It requires the array number, the lattice position, and the particle coordinate to perform the proper translation. The argument NX determines the proper translation to perform.

DELTA - DELTA is called from ARGEN. It computes the size of each dimension of each lattice cell from the reference body of the cell. This dimension is summed in ARGEN to compute the total array size on each dimension.

DIPR - DIPR is called from several subroutines to dump MARS array information after an error has been detected. It calls DUPR. DIPR is called to simplify the call to DUPR from the error detecting coding.

DUPR - DUPR is called from DIPR. It dumps the MARS array tables from memory and the nesting table of the current particle location. It generates quite a bit of output and should not be called frequently during debugging. The argument IXD in DUPR can suppress much of the geometry dump to allow frequent printouts of the nesting array during model debugging.

FINEFI - FINEFI is called from AZIP. It checks the MARS array input with the combinatorial input for snug fit. Most of the MARS input error messages regarding array content, reference, or fit comes from FINEFI. It is essential to have exact geometry fits before successful tracking can be initiated.

GENI - GENI is called from JOMIN2. It reads the binary file generated by JOMIN1 and stores the data into memory in the combinatorial geometry array tables. It edits and prints the output edit of the combinatorial input.

GG - GG is called from LOOKZ and G1. It is the guts and essence of the combinatorial geometry system. It computes, given the body number, the RIN and ROUT for the body.

GTVLIN - GTVLIN is called from JOMIN2 to calculate input zone volumes. If IVOPT = 0, it sets all the volumes equal to 1.

G1 - G1 is called from PILOT to determine the next input zone a particle may enter. It is in three parts. The first part of G1 determines the distance to exit the present zone if the zone will be exited. The second part of G1 determines the next zone of entry by checking those previous zones the particles entered when exiting the current zone by way of the body causing the particle to exit. If a new zone of entry is not determined from this table, then the third part of G1 proceeds to check all other possible zones of entry in the current universe. Errors in combinatorial geometry tracking come from G1.

IPACK - IPACK is called from JOMIN1 to pack several integers into one integer.

JOMIN1 - JOMIN1 reads the free-form combinatorial input for the body data, zone description data, region data, universe data, and media data. The input is written on a scratch file for later use by GENI.

JOMIN2 - JOMIN2 is called during combinatorial geometry input processing. It sets up the combinatorial geometry array pointers from information determined by JOMIN1. It then calls GENI, and the input data are stored in the proper arrays. JOMIN2 can call GTVLIN but usually does not.

LEVEL - LEVEL is called from AZIP. It determines the highest level number each array is referenced inside. These data are placed in the NLV table for later use in AZIP. The NLV table is not used for tracking or locating a particle.

LOOKZ - LOOKZ is called from CALI and PILOT to determine the particle location in a universe. It calls GG to determine RIN and ROUT for each body in a zone description table. It then determines the code and input zone the particle is inside. This information is returned in labeled common PAREM.

ORTHOM - ORTHOM is called from AZIP. It computes the rotational matrices of each BOX body, which references either an array or a universe. A BOX can be arbitrarily positioned in space. When a particle enters a universe or an array and when the reference body is a BOX, then both the particle coordinates and direction cosines must be rotated. Subroutine ROTA is the only routine that makes use of these matrices constructed by ORTHOM.

PILOT - PILOT is called from outside the MARS subroutine module to determine the next input zone a particle may enter. The first zone the particle enters with a positive media number is returned. PILOT cannot be called without first knowing the particle location as determined by calling CALI.

PR - PR is called from combinatorial geometry errors discovered in LOOKZ or G1. It generates even more output.

RCOVER - RCOVER is called from ABEND. If MORSE is the program being run, RCOVER calls NRUN to normalize and print results for the batches completed prior to the error, and then executes a 'STOP 6135'. If PICTURE is being run, only the 'STOP 6135' is executed.

RESTOR - RESTOR is called by JOMIN when RINPU2 calls JOMIN. When executed in SCALE, the geometry and array data are written out on a binary file for later recovery. RESTOR reads labeled commons REPEAT, ARAR, GOMLOC, and PAREM. It also reads the MA, FPD arrays and all of the MARS array storage from the binary file. The file read by RESTOR is written by RINPUP in the SAS3 control module in SCALE or by RINPU1 in MORSE-SGC.

RISK - RISK translates coordinates defined on geometry level NL1 to geometry level NL2 using the nesting table stored in array LP. This translation is from a global coordinate to a local coordinate system. NL2 must be greater than NL1.

ROTA - ROTA performs particle and direction cosine rotation upon entering or exiting a coordinate system defined by a BOX reference body. It is called from TRENTE and RTEXIT. It uses the rotational matrices constructed by ORTHOM during input processing.

RTEXIT - RTEXIT is called on exiting either a universe or an array. The "RT" means rotate, then translate. The rotation must be performed first, and then the translation can occur. RTEXIT is given the reference body for the universe or the array. If the body is an RPP, only translation of coordinates is required. If the body is a BOX, then both rotation and translation are required.

SAZAR - SAZAR is called by JOMIN if NDSN, the number of array analysis collision edits (input in MORSE-SGC) required, is > 0. SAZAR reads the location, media, and response criteria for each edit. This allows the user to selectively sample specific collisions.

SKPBLK - SKPBLK is called from JOMIN1 to skip blanks while reading free-form input cards.

SORCER - SORCER is called after completion of a batch of histories. It sorts the next zone of entry table in the order of most probable entry. This is a simple, fast routine used to speed up tracking through a complex geometry model.

SORT - SORT is called from CELL. It is called for each dimension of an array. It determines the cell position on each dimension for the particle location. It determines when a particle is exiting an array lattice and sets a flag for CELL to take appropriate action.

STORA - STORA is called from CALI and PILOT. It updates the nesting table during array tracking and locating. This is one of the most important aspects of array nesting logic. It is essential to the MARS logic.

TRENTE - TRENTE is called on entering either a universe or an array. The "TR" means translate, then rotate. The translation of the particle coordinate must occur and then the rotation. TRENTE is the opposite of RTEXIT. It requires the reference body of the universe or the array to determine the appropriate coordinate transformation.

UNIS - UNIS is called by AZIP to read, to verify, and to edit the universe type input. If a universe is erroneously declared simple, UNIS changes the universe type specification to combinatorial and writes warnings to the user.

ZEXITS - ZEXITS is called to dump the combinatorial summary of zone transfers at the end of a calculation. In MORSE-SGC, it is called by NRUN.

Table M9.E.1 MARS subroutine

Model			
Input routines		Tracking routines	
Combinatorial	MARS array input	Combinatorial	MARS array tracking
JOMIN1	AZIP	LOOKZ	CALI
JOMIN2	LEVEL	G1	PILOT
GENI	ARGEN	GG	CELL
ABOX	DELTA	PR	SORT
GTVLIN	ORTHOM	SORCER	BOD
	FINEFI	ZEXITS	ROTA
	UNIS	ALBERT	CORNER
	SAZAR	NORML	RTEXIT
			TRENTE
			CTRAN
			STORA
			CLEV
			RISK
			DIPR
			DUPR

Table M9.E.2 MARS storage requirements

Address pointer	Array name	Length of the array	Description
IP(NP)	NLV	NAR	Largest level each array is referenced inside; there are NAR arrays in a model
IP(NP+1)	WLH	3*NAR	The width on X, the length on Y, and the height on Z of each array
IP(NP+2)	-----	INACTIVE	------
IP(NP+3)	NCMAX	3*NAR	The size of each array lattice $NXMAX_i$ by $NYMAX_i$ by $NZMAX_i$
IP(NP+4)	NI4	NAR	Pointer for the array content description for each array
IP(NP+5)	NBN	$\sum_{j=1}^{NAR} NXMAX_j*NYMAX_j*NZMAX_j$	Lattice cell content for each array as pointed to by NI4
IP(NP+6)	NBOD	IBOD	Body No. that defines each universe; there are IBOD universes
IP(NP+7)	NCN	NAR*3	Address for the cell boundaries for each array in each dimension
IP(NP+8)	RBY	$\sum_{j=1}^{NAR} NXMAX_j+NYMAX_j+NZMAX_j+3$	The lattice cell boundary for each array as pointed to by NCN
IP(NP+9)	NBA	NUMB	Address for BOX rotation matrices for all BOX bodies that reference either arrays or universes
IP(NP+10)	ORT	NF	Rotation matrices as pointed to by NBA
IP(NP+11)	LP	6*NLEV+4	Particle nesting table for tracking

Table M9.E.3 Layout of combinatorial geometry data

Starting location	Information	Size
NGEOM=NADD	Length of geometry array	1
KMA	MA - Integer array	LTMA
KFPD	FPD - Floating point array	LFPD
KLCR	LOCREG - Indices to correlate MA array data with code zone data	NUMR
KNBD	NUMBOD - Number of bodies for each code zone	NUMR
KIOR	IROR - Indices to correlate input zone to code zone	NUMR
KRIZ	MRIZ - Indices to correlate MORSE region to input zone	IRTRU
KRCZ	MRCZ - Indices to correlate MORSE region to code zone	NUMR
KBIZ	NGIZ - Indices to correlate MORSE universe to input zone	IRTRU
KBCZ	NGCZ - Indices to correlate MORSE universe to code zone	NUMR
KMIZ	NMIZ - Indices to correlate MORSE media to input zone	IRTRU
KMCZ	NMCZ - Indices to correlate MORSE media to code zone	NUMR
KKR1	KR1 - Indices to correlate first code zone to input zone	IRTRU
KKR2	KR2 - Indices to correlate last code zone to input zone	IRTRU
KNSR	NSOR - Indices of code zones in which source particles have been found	NUMR
KVOL	VNOR - Volume of each MORSE region	NIR
IP(1)	Array storage for MARS	IP(12)-IP(1)

Table M9.E.4 Detailed layout of the FPD array[a]

Position in Blank Common	Information stored	Size	Description
KFPD	RIN for Body 1	1	Path length data for last trajectory in Body 1
KFPD + 1	ROUT for Body 1	1	
KFPD + 2	First six words of real data for Body 1	6	Read from first card of Body 1 card set
KFPD + 8	Remaining words of real data for Body 1	N_1	N_1 depends on body type (see Table M9.A.1)
KFPD + 8 + N_1	RIN for Body 2	1	
	ROUT for Body 2	1	Same information as above but for Body 2
	Remaining data for Body 2 (N_2 words) Repeat for NUMB bodies	N_2	

[a]NOTE: Eight words are set aside at the end of the FPD array but are not used.

Table M9.E.5 Detailed layout of the MA array

Position in Blank Common	Information stored	Size	Description
KMA	Body 1		
KMA + 1	LOOP for Body 1		
KMA + 2	Body type (ITYPE)		
KMA + 3	LRI	7	Body 1 data (each body requires seven words of information)
KMA + 4	LRO		
KMA + 5	LL - Last universe body was referenced inside		
KMA + 6	Beginning location in FPD body data on		
KMA + 7	Body 2	7	Same information and order as for Body 1
KMA + 14			
KMA + (L-1)*7	Body (L)	7	Body L is the last body
KMA + L*7	Code Zone 1	1	Beginning of code zone information
	Number of first body in this zone		Beginning of information about bodies defining Code Zone 1. Integer data location is given by: 7*(body number) - 6
	Location of integer data for this body	5 words per body per code zone reference	
	First zone to search upon exiting this body		
	Number of entries into the zone		
	Location of next zone to be searched		

Table M9.E.5 (continued)

Position in Blank Common	Information stored	Size	Description
	Data on second body in this zone	5	The last three words in each set of body data initiate the "leap frog" process by which the code stores possible zones which can be entered upon exiting this body in that particular zone. These zones are checked by the code when the next zone entered is being determined. If the next zone is not located from this stored data, all zones are searched.
	Data on last body is the zone	5	
	Zone 2 Body information	1	Same information as above except for Code Zone 2
	Zone data of the last zone		Code zone information about the last zone input on cards
KMA + LDATA	Code search information KMA+LTMA - 1	2*NAZT	Storage set aside for determining the zone to be searched and where the next zone number is located

Table M9.E.6 Definitions of variables in common GOMLOC

Variable	Definition
KMA	Starting location for the array MA containing integer data for each code zone
KFPD	Starting location for the array FPD containing real data for each code zone
KLCR	Starting location for the array LOCREG(I) that contains the starting location in the MA array for the I*th* code zone data
KNBD	Starting location for the array NUMBOD(I) that contains the number of bodies for the I*th* code zone
KIOR	Starting location for the array IROR(I) that contains the index of the corresponding input zone for the I*th* code zone
KRIZ	Starting location for the array MRIZ(I) that contains the index of the MORSE region corresponding to the I*th* geometry input zone
KRCZ	Starting location for the array MRCZ(I) that contains the index of the MORSE region corresponding to the I*th* geometry code zone
KMIZ	Starting location for the array MMIZ(I) that contains the index of the MORSE media corresponding to the I*th* geometry input zone
KMCZ	Starting location for the array MMCZ(I) that contains the index of the MORSE media corresponding to the I*th* code zone
KKR1	Starting location for the array KR1(L) contains the first code zone which was made from the L*th* input zone
KKR2	Starting location for the array KR2(L) contains the last code zone which was made from the L*th* input zone
KNSR	Starting location for array NSOR that contains the code zones in which source particles have been found
KVOL	Starting location for the array VNOR(I) which contains the volume for MORSE region (I)
NADD	Starting location for the geometry data and changed in JOMIN2 to the total number of words required for geometry data
LDATA	Length of the integer data in the MA array excluding the words set aside for zone search information
LTMA	Total length of the MA array
LFPD	Length of the FPD array
NUMR	Number of code-produced zones
IRTRU	Number of input zones
NUMB	Number of bodies
NIR	Number of MORSE geometry regions
KBIZ	Starting location for the array NGIZ(I) that contains index of the MORSE universe corresponding to the Ith geometry input zone
KBCZ	Starting location for the array NGCZ(I) that contains index of the MORSE universe corresponding to the Ith geometry code zone

Table M9.E.7 Definitions of variables in common PAREM as found in combinatorial geometry

Variable	Definition
XB(3)	Coordinates of the starting point of the present path. Changed in EUCLID, GOMST, and LOOKZ
WB(3)	Direction cosines of particle trajectory. Equal to U, V, and W. Changed in EUCLID, GOMST, and LOOKZ
WP(3)	Temporary storage of WB(3)
XP(3)	Temporary storage of XB(3). Changed in NORML
RIN	Distance to entry calculated in GG
ROUT	Distance to exit calculated in GG
PINF	Machine infinity (1.0E + 20)
DIST	Distance from XB(3) to present point
IR	Combinatorial zone of present particle position
IDBG	Set nonzero to initialize a debug printout
IRPRIM	Next region to be entered after a call of G1
NASC	Body number of last calculated intersection. Set negative to indicate source or collision point not on a body surface
LSURF	Surface of body NASC where intersection occurred. Positive if particle is entering the body and negative when exiting
NBO	Body number and a sign used to define zones. Input in zone description as positive when zone is contained in body and as negative if zone is outside body
LRI	Entry surface calculated in GG
LRO	Exit surface calculated in GG
KLOOP	Trajectory index of present path incremented in G1
LOOP	Index of last trajectory calculated for body NBO. If LOOP is equal to KLOOP, GG returns immediately with old values in RIN, ROUT, LRI, and LRO
ITYPE	Body type of Body NBO (indicated BOX, SPH, etc.)
NOA	Not used

Table M9.E.8 Definitions of variables in common ORGI[a]

Variable	Definition
DIST0	Distance from point XB(3) to next scattering point. Used in G1 to avoid calculating the next zone if a scattering event occurs before the intersection
MARKG	Set 1 in G1 if trajectory end point is reached before next intersection. Otherwise set to 0
NMEDG	Input zone number for current collision from a LOOKZ call
NBLZ	Packed word containing both input zone and code zone numbers for current collision stored in LOOKZ
BLZOLD	Packed word containing code and input zone numbers for previous collisions
IRPOLD	Input zone number for previous collision

[a]Variable names are not the same in all routines.

Table M9.E.9 Definitions of variables in common TAPE

Variable name	Definition
INT	Logical number of standard input unit
IOT	Logical number of standard output unit
IOUT	Logical number of scratch unit for geometry data
IOU2	Logical number of second scratch unit
IDM(4)	Not used at present

Table M9.E.10 Definitions of variables in common MGOMV

Variable	Definition
MUS	Pointer for array indicating type of universe - simple or comjom
MUZ	Pointer for array indicating last zone for a given universe
LL	Current universe number
IPRET	Signal - when = 1 PILOT returns at every boundary crossing rather than tracking until media changes
IFLOW	Signal indicating direction of crossing. Inward if =0, outward if =1
IECT	Error counter - prints messages first 10 times. MORSE-SGC abends on error number 11
NLO	Signal when changing levels - = 0 means same level = –1 means down one level = +1 means up one level
IGX	Signal indicating entry to array if 0, or exit from array if 1

Table M9.E.11 Definitions of variables in common ARAR

Variable	Definition
NBY	Body number
NLEV	Number of geometry levels
NAR	Number of arrays
NQ	= 1 for MORSE
IAW	Number of universes
IAY	Length of lattice cell array
NF	Maximum size of array lattice
NX1(1)	Current x lattice position
NX1(2)	Current y lattice position
NX1(3)	Current z lattice position
	NX1(1-3) = 0 if outside of array

Table M9.E.12 Definitions of variables in common ARK

Variable	Definition
LM	Content of lattice position of current array > 0 for a universe; < 0 for an array
NLU	Current array number
NBB	Reference body for current array
NZY(1-3)	Current lattice position in array NLU (i.e., X, Y, Z position)
XD(1-3)	Current X, Y, Z of particle

M9.F COMBINATORIAL GEOMETRY TRACKING

M9.F.1. COMJOM TRACKING THEORY

Tracking a particle in MARS consists of:

1. determining the array, universe, and code zone in which a point is located,

2. finding the distance along a given direction to the exit point from this code zone,

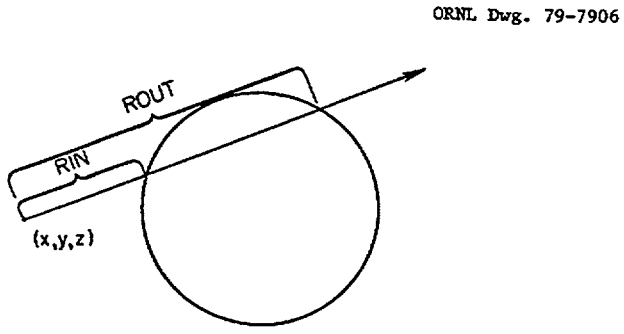
3. determining the next code zone the ray will enter in the same universe, and

4. finding the distance to the exit point of this code zone.

This process is continued until the next collision point is encountered, the particle leaks from the system, or an albedo surface is encountered.

Given a starting point (x, y, z) a direction (specified by direction cosines u, v, and w) and a body (one of the basic geometric shapes mentioned earlier), the basic tracking Subroutine GG in the combinatorial geometry package will determine whether the ray from the starting point and the specified direction will intersect the given body. If it does, the subroutine will calculate RIN, the distance to the entry point into the body, and ROUT, the distance to the exit point from the body. A number of orientations are possible:

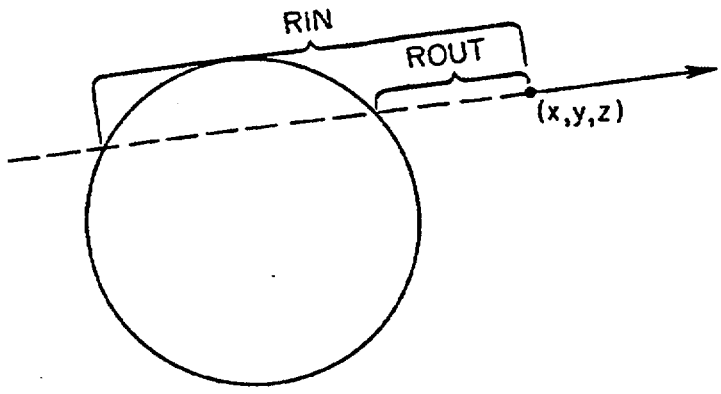
1. The ray starts at a point outside the body and intersects the body in the positive direction.



In this case, ROUT ≥ RIN > 0. (ROUT) may equal RIN if the ray grazes the body.

2. The ray starts at a point outside the body and intersects the body in the negative direction.

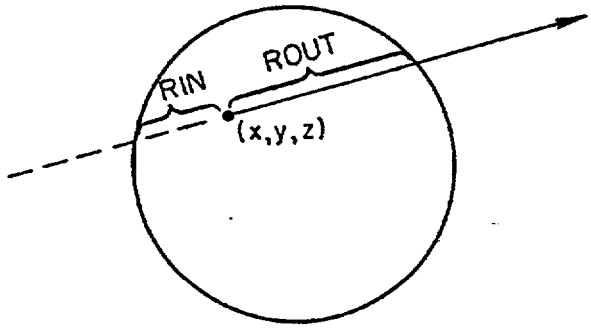
ORNL Dwg. 79-7907



In this case, 0 > ROUT ≥ RIN.

3. The ray starts at a point inside the body.

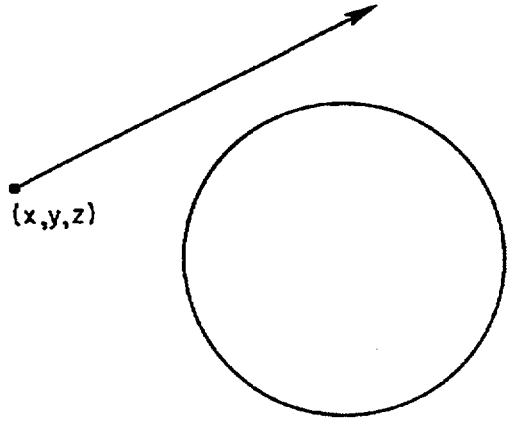
ORNL Dwg. 79-7908



In this case, ROUT > 0 > RIN.

4. The ray misses the body.

ORNL Dwg. 79-7909



In this case, ROUT is set equal to –PINF, and RIN is usually set equal to PINF, where PINF is a large number (the computer's approximation of infinity).

To demonstrate how tracking is performed, as shown in Fig. M9.F.1, consider the following description:

Bodies

1. RPP $-1.0 \le x \le 0.5$, $-1.0 \le y \le 1.0$, $-1.0 \le z \le 1.0$
2. RPP $-0.5 \le x \le 1.0$, $-1.0 \le y \le 1.0$, $-1.0 \le z \le 1.0$
3. RPP $-2.0 \le x \le 2.0$, $-2.0 \le y \le 2.0$, $-2.0 \le z \le 2.0$
4. RPP $-3.0 \le x \le 3.0$, $-3.0 \le y \le 3.0$, $-3.0 \le z \le 3.0$

Input Zones

1. 1 -2 , media 1, region 1
2. 2 +1 , media 2, region 1
3. -1 +2 , media 3, region 1
4. 3 -1 -2, media 1000, region 1
5. 4 -3 , media 0, region 1

Since all input zones in this example are described without OR operators, the input zones and code zones will be the same. Let 'a' be the starting point (-1.5, 1.0, 0.0) with direction cosines (.8, –.6, 0).

ORNL Dwg. 79-7910

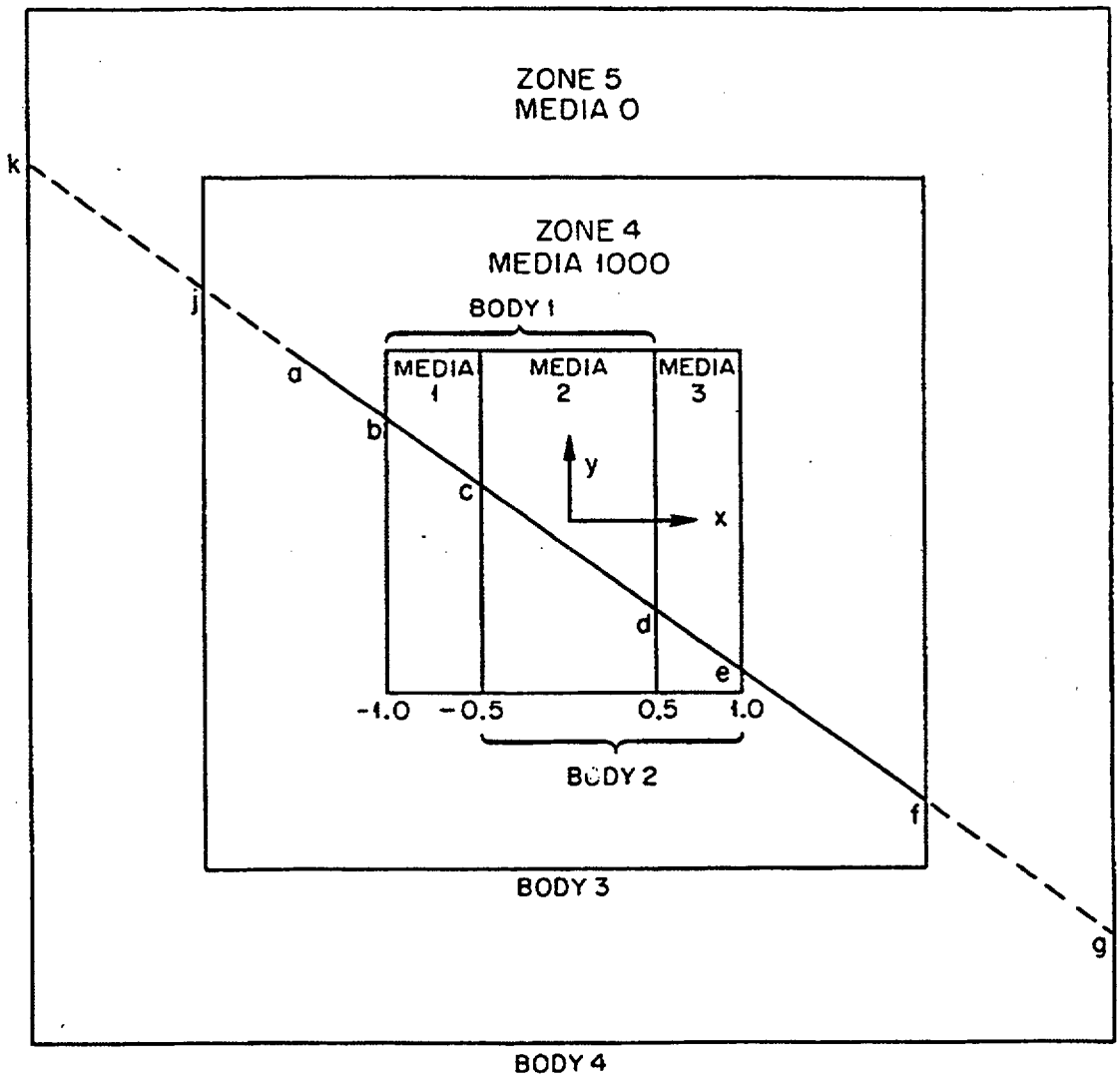


Figure M9.F.1 A simple demonstration of particle tracking

The determination of the location of the starting point is made by attempting to calculate an exit distance for each code zone. If a valid distance is found for a code zone, then the point is in that code zone. The code zones are initially examined in the order of their description.

To see if the starting point is in Code Zone 1, the bodies in the zone are tested. Body 1 is the first body in Zone 1. RIN and ROUT for Body 1 are calculated giving

$$\text{RIN} = .625, \text{ROUT} = 2.5 \ .$$

Since RIN > 0, the point is not in Body 1 and therefore cannot be in Zone 1. The next body in Zone 1 does not need to be checked. To check Zone 2, the first body is Body 2. (The bodies are checked in the order given in the input description.) RIN and ROUT for Body 2 are calculated giving

$$\text{RIN} = 1.25, \text{ROUT} = 3.125 \ .$$

Again, RIN > 0, and the point is not in Body 2 and cannot be in Zone 2. To check Zone 3, the first body is Body –1. RIN and ROUT are retrieved for Body 1 giving

$$\text{RIN} = .625, \text{ROUT} = 2.5 \ .$$

Since RIN > 0, the point is not in Body 1 and therefore is in Body -1. The next body in Zone 3 must then be checked. The data for Body 2 are retrieved giving

$$\text{RIN} = 1.25, \text{ROUT} = 3.125 \ .$$

Since RIN > 0, the point is not in Body 2 and is not in Zone 3. To check Zone 4, the first body is Body 3. RIN and ROUT for Body 3 are calculated giving

$$\text{RIN} = .625, \text{ROUT} = 4.375 \ .$$

Since RIN < 0 and ROUT > 0, the point is in Body 3. The next body in Zone 4 is Body –1. RIN and ROUT are retrieved for Body 1 giving

$$\text{RIN} = .625, \text{ROUT} = 2.5 \ .$$

Since RIN > 0, the point is not in Body 1 and therefore is in Body –1. The next body in Zone 4 is Body –2. RIN and ROUT are retrieved for Body 2 by giving

$$\text{RIN} = 1.25, \text{ROUT} = 3.125 \ .$$

Since RIN > 0, the point is not in Body 2 and therefore is in Body –2. The point is in all the bodies in Zone 4 and therefore is in Zone 4.

At the same time that the RINs and ROUTs are checked to see if the point is in the various bodies of a zone, the exit distance, DIST, is also calculated. The exit distance from the zone is the smallest of the distances to leave Body 3 (ROUT = 4.375); to enter Body 1 (RIN = .625), or to enter Body 2 (RIN = 1.25); therefore,

$$\text{DIST} = .625 \ .$$

Once the exit distance for a given zone is found, the number of mean-free paths that the particle travels in the zone is calculated to see if a collision occurs in the zone, and if so, at what point. The total number of mean-free paths traveled to the next collision point will have previously been selected. For this example, it will be assumed that the number of mean-free paths selected is large enough so that a collision will not occur, and the particle will leak from the system.

The next step then is to determine which code zone the particle enters next. Zone 1 will be checked first. The first body in Zone 1 is Body 1. RIN and ROUT are retrieved for Body 1 giving

$$\text{RIN} = .625, \ \text{ROUT} = 2.5 \ .$$

If the particle is to be in (or enter) Body 1 after traveling this far, then DIST $\geq$ RIN and DIST $<$ ROUT. Since DIST = RIN = .625 and DIST = RIN $<$ ROUT, the tests are passed and the particle has entered the Body 1. The next body in the zone is Body –2. RIN and ROUT are retrieved for Body 2 giving

$$\text{RIN} = 1.25, \ \text{ROUT} = 3.125 \ .$$

If the particle is to be in Body –2 (not in Body 2), then either DIST $<$ RIN or DIST $\geq$ ROUT. Since DIST $<$ RIN, the particle is in Body –2. The particle has therefore entered Zone 1.

The exit distance from Zone 1 is found next by picking the smallest of the ROUTs for the positive bodies and the RINs of the bodies which are negative. For Body 1 ROUT = 2.5, and for Body 2 (which is negative in the zone) RIN = 1.25. Therefore, the exit distance from Zone 1 is

$$\text{DIST} = 1.25 \ .$$

The total distance in mean-free paths is again calculated and compared against the predetermined number of mean-free paths which the particle is to travel to see if a collision occurs in Zone 1. If not, then tracking continues as above to determine the next zone the particle enters and the exit distance from that zone. When the particle reaches Zone 5, the medium number of 0 is used as a flag to indicate that the particle has leaked, and the tracking can be terminated. If a collision occurs, then the weight of the particle will be multiplied by the nonabsorption probability, a new energy is selected, a new direction is selected, etc. The tracking of the particle then continues from this point in the new direction if it has not been killed by some process such as Russian roulette or an energy cutoff (where the particle has scattered down to an energy range that is not of interest in the problem). If an albedo surface is encountered during tracking (this is determined by specifying a special medium number to indicate an albedo surface), then a problem-dependent subroutine will be called which will specify the new particle parameter needed for continuation of the tracking.

M9.G DIAGNOSTIC MESSAGES FROM MARS

Numerous error messages are printed out by the MARS geometry package. These messages aid the user in determining the cause of the trouble when an error is detected by MARS during the input step or during particle tracking. Sections M9.G.1 and M9.G.2 give the actual message that is printed, the subroutine name where the error was detected, and an explanation of the message and/or its cause.

M9.G.1 DIAGNOSTIC MESSAGES FROM MARS INPUT MODULE

Subroutine printing message	Message	Meaning
ARGEN	ARRAY NO __ IS IMPROPERLY DEFINED - FATAL ERROR IN ARGEN	The array size exceeds the size of the array lattice (NCMAX)
ARGEN	ARGEN IXY= __ IX= __ MR= __ NA= __ NE= __ NMAX= __	Error was detected in DELTA. See message from DELTA.
AZIP	FATAL ERROR - UNIVERSE NO. __ IS NOT DEFINED	Either the universe number is incorrect or the media number is not -1000.
DELTA	IN DELTA.UNIVERSE REFERENCE BODY TO RPP OR BOX IBOD= __ IBO= __ MA INDEX= ITYPE= __ ND= __	Self-explanatory. Check the input data. IBO is body number.
FINEFI	WARNING - IN FINEFI NO REFERENCE WAS MADE TO ARRAY NO. __	One of the arrays specified is not referenced.
FINEFI	IN FINEFI INVALID ARRAY REFERENCE IN ARRAY __ POSITION __ TO NONEXISTENT ARRAY __	Array number exceeds maximum (NAR).
FINEFI	FINEFI FATAL ERROR - ARRAY POSITION __ REFERS TO AN INVALID OR UNDEFINED UNIVERSE -	Universe number exceeds number of universes (IBOD) in system.
FINEFI	IN FINEFI ARRAY NO. __ POSITION __ REFERS TO UNIVERSE __ DEFINED BY BODY __ WHICH IS NOT AN RPP OR BOX __ FATAL ERROR	The reference body for an array must be either a BOX or an RPP. Check input data.
FINEFI	FINEFI - FATAL ERROR IN ARRAY __ ELEMENT POSITION __ CONTAINS UNIVERSE __ MISFIT IN POSITION	Self-explanatory. Check input.
FINEFI	IN FINEFI ARRAY __ HAS NO VALID ELEMENTS - VERY FATAL	This message is usually in addition to one of the others from FINEFI. All lattice cell positions have been checked for fits prior to this message.

Subroutine printing message	Message	Meaning
FINEFI	FINEFI - CODE ZONE __ CONTAINS ARRAY BUT IS DEFINED WITH MORE THAN ONE BODY __ WARNING __ FIRST BODY WILL BE REFERENCE BODY	Self-explanatory. Check input.
FINEFI	FINEFI FATAL ERROR - CODE ZONE __ REFERENCES AN INVALID ARRAY __	The array number is > number of arrays (NAR) in the system.
FINEFI	FINEFI FATAL ERROR - CODE ZONE __ CONTAINS ARRAY __ INSIDE BODY __ REFERENCED BODY IS NOT AN RPP OR BOX	The reference body for an array must be either a BOX or an RPP. Check input data.
FINEFI	FINEFI FATAL ERROR - ARRAY __ IN BODY __ REFERENCED IN CODE ZONE __ DOES NOT FIT	The overlap of lattice cell boundary and input zone boundary is too large.
FINEFI	FINEFI FATAL ERROR - YOU HAVE AT LEAST ONE ARRAY BUT NO ARRAY WAS REFERENCED IN A LEVEL ZERO ZONE	Self-explanatory. Probable input error
GTVLIN	**********ERROR IN VOLUME CALCULATION********* JF= __ NIR= __	The number of regions for which volumes were calculated does not equal the number in the geometry.
JOMIN1	ITYPE __ DOES NOT EQUAL ANY OF THE FOLLOWING _____	The body type given does not exist in the code.
JOMIN1	EXCEEDED CORE DURING CG INPUT ISTR= __ N= __ NADD= LIM= LTMA= __ LFPD= __ NUMR= __ IRTRU= __ NAZT= __ IBODT= __	The space allocated for the data is insufficient. ISTR + N + 1 is amount required up to this point. LIM is space available.
SAZAR	NMOST INCREASED TO __ BY SUBROUTINE SAZAR	An array edit was requested, but there was inadequate space to save it. Space was added.
UNIS	WARNING -- UNIVERSE __ IS NOT SIMPLE CODE ZONE __ CONTAINS ARRAY __	A negative media number was found in a simple universe. UNIS changes it to combinatorial universe.
UNIS	CODE ZONE __ IN UNIVERSE __ CANNOT BE A SIMPLE UNIVERSE	The number of bodies in this code zone is >2, so it is not simple. UNIS changes it.
UNIS	BODY __ IN UNIVERSE __ IS NOT REFERENCED POSITIVE IN THE UNIVERSE	Fatal error.

M9.G.2 DIAGNOSTIC MESSAGES FROM MARS TRACKING EVENTS

Subroutine printing message	Message	Meaning
CALI	CALI NL,NLU,IR,IRPRIM,NMED,NLEV__	Printed only if debug switch IDBG is on (>0).
CALI	ERROR IN CALI FROM CELL * LZ= __ LU= __ IER= __	Either CELL has set the error signal IER>0 or lattice cell is vacant (LZ>0) on entering array.
CALI	ERROR IN CALI * NMED,IPS,LZ,IER,LU,IR,IRPRIM,LM,LL,NL __	When this message follows one above see that explanation. If IPS>2, there is error on exiting array.
CLEV	ERROR IN CLEV * NL1= __ NL2= __ NGY= __	Level NL1 is lower than level NL2. It should be higher because code translates from a higher to a lower level.
G1	NO VALID DISTANCE IN G1 * IR,XB,WB,DIST= __	G1 could not determine the next body that the ray will intersect. There is a probable error in user's geometry specifications, or he may have written over his geometry data.
G1	********** GEOMETRY SEARCH ARRAY FULL **********	In order to same some computer time, user may want to increase the value of NAZ in his input. Only harm done is an increase in computer time which is often insignificant.
G1	IR= __ XB= __,__,__ WB= __,__,__ DIST= __ LL= __ MA ARRAY Entire MA array printed. FPD ARRAY Entire FPD array printed. ****EXIT BEING CALLED FROM G1. NEXT ZONE NOT FOUND	G1 could not find the next zone that the particle would enter. It checked all zones and is saying that the particle won't enter any of them. Probable error in zone specifications. Subroutine PR called to print values from commons GOMLOC, DBG, and PAREM. Among the variables printed the following apply to the maximum body number and therefore have no significance - NBO,N,NUM,ITYPE,SIN,IRP, and LOCAT. The most important variable is NASC which is the number of the next body the ray will intersect. That is, the code cannot find what zone this body is in. Check zone specification for this body.

Subroutine printing message	Message	Meaning
GG	IN GG ITYPE= __ IR= __ NBO= __ .	ITYPE is not one of the body types (1-9) allowed. User has either overstored MA array or has used a body number out of range in the zone description.
LOOKZ	IR= __ XB= __,__,__ WB= __,__,__ DIST= __ LL= __ MA ARRAY Entire MA array printed. FPD ARRAY Entire FPD array printed. ****EXIT BEING CALLED FROM LOOKZ	Zone has not been found. Check the zone specifications for error.
NORML	INVALID REGION OR BODY IN NORMAL. IR= __ NASC= __	NASC is not in region IR. Check whether IR or NASC has been overwritten.
NORML	ROUND-OFF ERROR IN NORMAL NBO= __ LSURF= __ XP= __,__,__	Self-explanatory. Applies only to ELL and BOX.
PILOT	PROBLEM ENCOUNTERED IN ARRAY PROCESSING, PARTICLE WILL BE TERMINATED AS ESCAPE.	Printed when PILOT is in a loop when processing an array. Particle is probably unable to enter or leave an array. May be input error.
PILOT	PILOT CRASH	Printed only if debug switch IDBG is on (>0).
PILOT	ERROR IN PILOT ON ENTERING ARRAY	If IER>0, previous error message from SORT explains error. If LZ>0 or LM=0, lattice cell is vacant or cell position is out of range (<0 or > maximum).
PILOT	ERROR IN PILOT ON EXITING ARRAY	If IER>0, previous error message from SORT explains error. IF IEXIT=1 or LM=0, lattice position is out of range. NL<0 means error in level number.
SORT	FATAL ERROR IN SORT *** PARTICLE LOST ON ENTERING OR EXITING ARRAY. M,NMAX,IGX,LX1,LX2,NXY __ XB,RBY(LX2),SML,SMALL	On entering array, particle position is ot at a lattice cell boundary (RBY) for array; on exiting array, either lattice position is > size of array lattice or is < 0 or particle position is not at lattice cell boundary.
STORA	IN STORA EITHER AN ILLEGAL LEGAL TRANSFER WAS ATTEMPTED OR AN INCORRECT ARRAY REQUEST WAS MADE *NLO= __ NL= __ NLU= __ LM= __ .	The level number NL is wrong. Either it is greater than the number of levels (NLEV) or it is 0.

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FIDO INPUT SYSTEM

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ABSTRACT

This document provides a description of the FIDO input system being used in conjunction with several SCALE functional modules. The FIDO system is a widely used method of entering or modifying large data arrays with minimum effort. Special advantage is taken of patterns of repetition or symmetry whenever possible.

CONTENTS

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M10.1 INTRODUCTION

The FIDO input method is specially devised to allow entering or modifying large data arrays with minimum effort. Advantage is taken of patterns of repetition or symmetry wherever possible. The FIDO system was patterned after the input method used with the FLOCO coding system at Los Alamos and was first applied to the DTF-II code. Since that time, numerous features requested by users have been added, a free-field option has been developed, and the application of FIDO has spread to innumerable codes.

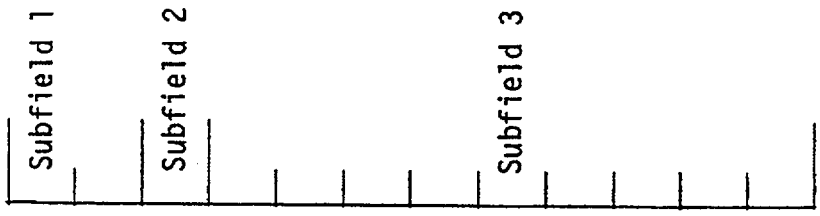
The data are entered in units called "arrays." An array comprises a group of contiguous storage locations that are to be filled with data at the same time. These arrays usually correspond on a one-to-one basis with FORTRAN arrays used in the program. A group of one or more arrays read with a single call to the FIDO package forms a "block," and a special delimiter is required to signify the end of each block. Arrays within a block may be read in any order with respect to each other, but an array belonging to one block must not be shifted to another. The same array can be entered repeatedly within the same block. For example, an array could be filled with "0" using a special option, and then a few scattered locations could be changed by reading in a new set of data for that array. If no entries to the arrays in a block are required, the delimiter alone satisfies the input requirement.

Three major types of input are available: fixed-field input, free-field input, and user-field input.

M10.2 FIXED-FIELD INPUT

The fixed-field input option is documented here for completeness. **The use of fixed-field input is NOT recommended. Use the free-field input option documented in Sect. M10.3.**

Each card is divided into six 12-column data fields, each of which is divided into three subfields. The following sketch illustrates a typical data field. The three subfields always comprise 2, 1, and 9 columns, respectively.



To begin the first array of a block, an array originator field is placed in any field on a card:

Subfield 1: An integer array identifier <100 specifying the data array to be read in.

Subfield 2: An array-type indicator:
"$" if the array is integer data
"*" if the array is real data
"#" if the array is double-precision data

Subfield 3: Blank

Data are then placed in successive fields until the required number of entries has been accounted for.

In entering data, it is convenient to think of an "index" or "pointer" as a designator that is under the control of the user and which specifies the position in the array into which the next data entry is to go. The pointer is always positioned at array location #1 by entering the array originator field. The pointer subsequently moves according to the data operator chosen. Blank fields are a special case in that they do not cause any data modification and do not move the pointer.

A data field has the following form:

Subfield 1: The data numerator, an integer <100. We refer to this entry as N_1 in the following discussion.

Subfield 2: One of the special data operators listed below.

Subfield 3: A nine-character data entry, to be read in F9.0 format. It will be converted to an integer if the array is a "$" array or if a special array operator such as Q is being used. Note that an exponent is permissible but not required. Likewise, a decimal is permissible but not required. If no decimal is supplied, it is assumed to be immediately to the left of the exponent, if any; and otherwise to the right of the last column. This entry is referred to as N_3 in the following discussion.

A list of data operators and their effect on the array being input follows:

"Blank" indicates a single entry of data. The data entry in the third subfield is entered in the location indicated by the pointer, and the pointer is advanced by one. However, an entirely blank field is ignored.

"+" or "–" indicates exponentiation. The data entry in the third field is entered and multiplied by $10^{\pm N_1}$, where N_1 is the data numerator in the first subfield, given the sign indicated by the data operator itself. The pointer advances by one. In cases where an exponent is needed, this option allows the entering of more significant figures than the blank option.

"&" has the same effect as "+".

"R" indicates that the data entry is to be repeated N_1 times. The pointer advances by N_1.

"I" indicates linear interpolation. The data numerator, N_1, indicates the number of interpolated points to be supplied. The data entry in the third subfield is entered, followed by Nj interpolated entries equally spaced between that value and the data entry found in the third subfield of the next nonblank field. The pointer is advanced by $N_1 + 1$. The field following an "I" field is than processed normally, according to its own data operator. The "I" entry is especially valuable for specifying a spatial mesh. In "$" arrays, interpolated values will be rounded to the nearest integer.

"L" indicates logarithmic interpolation. The effect is the same as that of "I" except that the resulting data are evenly separated in log-space. This feature is especially convenient for specifying an energy mesh.

"Q" is used to repeat sequences of numbers. The length of the sequence is given by the third subfield, N_3. The sequence of N_3 entries is to be repeated N_1 times. The pointer advances by N_1*N_3. If either N_1 or N_3 is 0, then a sequence of $N_1 + N_3$ is repeated one time only, and the pointer advances by $N_1 + N_3$. This feature is especially valuable for geometry specification.

The "N" option has the same effect as "Q," except that the order of the sequence is reversed each time it is entered. This feature is valuable for the type of symmetry possessed by S_n quadrature coefficients.

"M" has the same effect as "N," except that the sign of each entry in the sequence is reversed each time the sequence is entered. For example, the entries

1 2 3 2M2

would be equivalent to

1 2 3 -3 -2 2 3.

This option is also useful in entering quadrature coefficients.

"Z" causes $N_1 + N_3$ locations to be set at 0. The pointer is advanced by $N_1 + N_3$.

"C" causes the position of the last array entered to be printed. This is the position of the pointer, less 1. The pointer is not moved.

"O" causes the print trigger to be changed. The trigger is originally off. Successive "O" fields turn it on and off alternately. When the trigger is on, each card image is listed as it is read.

"S" indicates that the pointer is to skip N_1 positions leaving those array positions unchanged. If the third subfield is blank, the pointer is advanced by N_1. If the third subfield is nonblank, that data entry is entered following the skip, and the pointer is advanced by $N_1 + 1$.

"A" moves the pointer to the position, N_3 specified in the third subfield.

"F" fills the remainder of the array with the datum entered in the third subfield.

"E" skips over the remainder of the array. The array length criterion is always satisfied by an E, no matter how many entries have been specified. No more entries to an array may be given following an "E," except that data entry may be restarted with an "A."

The reading of data to an array is terminated when a new array origin field is supplied, or when the block is terminated. If an incorrect number of positions has been filled, an error edit is given; and a flag is set which will later abort execution of the problem. FIDO then continues with the next array if an array origin was read. Otherwise, control is returned to the calling program.

A block termination consists of a field having "T" in the second subfield. Entries following "T" on a card are ignored, and control is returned from FIDO to the calling program.

Comment cards can be entered within a block by placing an apostrophe (') in column 1. Then columns 2–80 will be listed, with column 2 being used for printer carriage control. Such cards have no effect on the data array or pointer.

M10.3 FREE-FIELD INPUT

With free-field input, data are written without fixed restrictions as to field and subfield size and positioning on the card. The options used with fixed-field input are available, although some are sightly restricted in form. In general, fewer data cards are required for a problem, the interpreting print is easier to read, a card listing is more intelligible, the cards are easier to keypunch, and certain common keypunch errors are tolerated without affecting the problem. Data arrays using fixed- and free-field input can be intermingled at will within a given block,

The concept of three subfields per field is still applicable to free-field input; but if no entry for a field is required, no space for it need be left. Only columns 1-72 may be used, as with fixed-field input. A field may not be split across cards.

The array originator field can begin in any position. The array identifiers and type indicators are used as in fixed-field input. The type indicator is entered twice to designate free-field input (i.e., "$$," "**," or "##"). The blank third subfield required in fixed-field input is not required. For example,

```
31**
```

indicates that array 31, a real-data array, will follow in free-field format.

Data fields may follow the array origin field immediately. The data field entries are identical to the fixed-field entries with the following restrictions:

1. Any number of blanks may separate fields, but at least one blank must follow a third subfield entry if one is used.

2. If both first- and second-subfield entries are used, no blanks may separate them (i.e., 24S, but not 24 S).

3. Numbers written with exponents must not have imbedded blanks (i.e., 1.0E+4, 1.0-E4, 1.0+4, or even 1+4, but *not* 1.0 E4). A zero should never be entered with an exponent. For example, 0.00-5 or 0.00E-5 will be interpreted as -5×10^{-2}.

4. In third-subfield data entries only 9 digits, including the decimal but not including the exponent field, can be used (i.e., 123456.89E07, but *not* 123456.789E07).

5. The Z entry must be of the form: 738Z, *not* Z738 or 738 Z.

6. The + or - data operators are not needed and are not available.

7. The Q, N, and M entries are restricted: 3Q4, 1N4, M4, but *not* 4Q, 4N, or 4M.

M10.4 USER-FIELD INPUT

If the user follows the array identifier in the array originator field with the character "U" or "V," the input format is to be specified by the user. If "U" is specified, the FORTRAN FORMAT to be used must be supplied in columns 1–72 of the next card. The format must be enclosed by the usual parentheses. Then the data for the entire array must follow on successive cards. The rules of ordinary FORTRAN input as to exponents, blanks, etc., apply. If the array data do not fill the last card, the remainder must be left blank.

"V" has the same effect as "U," except that the format read in the last preceding "U" array is used.

M10.5 CHARACTER INPUT

If the user wishes to enter character data into an array, at least three options are available. The user may specify an arbitrary format using a "U" and reading in the format. The user may follow the array identifier by a "/". The next two entries into subfield 3 specify the beginning and ending indices in the array into which data will be read. The character data are then read starting with the next data card in an 18A4 format.

Finally, the user may specify the array as a free-form "*" array and then specify the data entries as "nH" character data where n specifies how many characters follow H.

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PICTURE: A 2-D PLOTTING PROGRAM FOR MARS GEOMETRIES

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ABSTRACT

The PICTURE program was written to provide aid in preparing correct input data for the MARS geometry package, which is a multiple-array system using combinatorial geometry. It provides a printed view of arbitrary two-dimensional slices through the geometry. By inspecting these pictures one may determine if the geometry specified by the input cards is indeed the desired geometry. This report describes PICTURE, its options, and its input.

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ACKNOWLEDGMENTS

The PICTURE program makes use of two freeware packages, PBMPLUS and GD, in generating a color display. The following copyright notices apply to these packages.

The PBMPLUS package:
** Based on GIFENCOD by David Rowley <mgardi@watdscu.waterloo.edu>. A
** Lempel-Zim compression based on "compress".
**
** Modified by Marcel Wijkstra <wijkstra@fwi.uva.nl>
**
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*/

The GD package:

gd 1.2 is copyright 1994, 1995, Quest Protein Database Center, Cold Spring Harbor Labs. Permission granted to copy and distribute this work provided that this notice remains intact. Credit for the library must be given to the Quest Protein Database Center, Cold Spring Harbor Labs, in all derived works. This does not affect your ownership of the derived work itself, and the intent is to assure proper credit for Quest, not to interfere with your use of gd. If you have questions, ask. ("Derived works" includes all programs that utilize the library. Credit must be given in user-visible documentation.)

M13.1 INTRODUCTION

The PICTURE program was written to help the user determine whether his MARS input data correctly describe his geometry. PICTURE displays, as printed output or on the computer screen, two-dimensional (2-D) slices through the specified geometry. A regularly spaced array of points is generated, and each point is plotted as a symbol or a color related to either media, region, or zone, depending on the option selected by the user. By printing out this array, a rough picture of one view of the geometry is produced. The user may then look at the picture and determine if the geometry is as intended. A sample problem is described in Sect. M13.5.

Running PICTURE requires the routines described in this report plus those making up the MARS geometry package described in Sect. M9. MARS also uses routines from the SCALE subroutine library and the SCALE unix library. The color plot display requires the LEGEND program described in Appendix A, and the freeware package PBMPLUS, which includes PPMTOGIF and RAWTOPPM, is also used. Both LEGEND and PBMPLUS are distributed with the SCALE package. In order to look at the color display, a plot viewer such as XV on workstations or LVIEW on PCs is required.

M13.2 ROUTINES

M13.2.1 Main Programs

The executive routine for the PICTURE program, MAIN or O0O016, sets the dimension for blank common, the I/O unit numbers, the signal indicating what type of PICTURE run, and the ratio of the number of characters per inch down the page to the number across the page for printer plots, and calls subroutine PICTUR. See Table M13.2.1 for content of common PNIT which contains I/O unit numbers.

Subroutines called: PICTUR, OPNFIL, IONUMS, MESAGE

Commons required: Blank, PNIT

Variables changed: INT, IOT, RAYX, NDIM, N16, N17, N93, N95, KTYPE

IOT, RAYX, NDIM, N16, N17, N93 and N95 are the same for both cases.

KTYPE = 0 for standalone PICTURE (MAIN)

KTYPE = 1 for PICTURE run from within SAS4 (O0O016)

INT = 5 set by MAIN

INT = 93 set by O0O016

Table M13.2.1 Definition of variables in common PNIT

Variable	Definition
INT	Input unit number
IOT	Standard output unit
N16	Scratch unit used by MARSLIB
N17	Scratch unit used by MARSLIB
N93	Input unit for PICTURE data if KTYPE = 1
N95	Binary input unit for MARS data if data was preprocessed

M13.2.2 Subroutines

Subroutine PRINT (KXX, KYY, ATABLE, IOT)

This routine controls the printing of the picture or the writing of a GIF-format file. First some variables are initialized depending on whether this is a screen plot or a printer plot. If it's a screen plot, a command is passed to the operating system to execute the programs in the freeware PBMPLUS that are necessary to produce the final GIF-format plot. The code determines if the picture is more than one "page" (130 columns) wide. Then for each line of the picture the information to be printed is determined by calling "MESH" and is printed with a 130A1 format for printer plots or written to unit I1 for a screen plot. This process continues until that "page" is finished. Note that a page refers to the width, not length. Thus as much detail as necessary may be obtained in both directions by piecing together printer output.

Screen plots contain a legend identifying the color used for each material (or zone or region). PRINT determines the legend by sorting the materials used and counting them. After writing the plot to a file on unit I1 and calculating the materials used, the unit is closed; a new dataset containing the title of the plot, the number of materials used, the name of the gif picture to which the legend is added, the external and internal voids, and the material numbers and corresponding red, green, and blue components is written to the same unit. The output plot data file is then closed, and the system is called to execute the RAWTOPPM program which pipes its output to the PPMTOGIF program which then pipes its output to the LEGEND program.

Called from: PICTUR

Subroutine called: MESH, SYSTEM, OPNFIL

Commons required: PICT, PCOLOR, JOMN2, GOMLOC, blank

Variables required:

KXX - number of intervals in the U direction (direction of paper movement through the printer),

KYY - number of intervals in the V direction (line),

LTYPE - logical variable which is a signal indicating type of plot,
True = screen plot; False = printer plot

X0, Y0, Z0 - coordinates

ATABLE - table of characters to be printed,

IOT - output logical unit.

Variables changed:

MTRLUSED - array of material numbers used,

MAXMATRL - maximum number of materials used.

Significant internal variable:

NPAGES - number of subpictures required to cover the width of the total picture,

NV - number of characters per line (characters/page width).

Subroutine MESH (XS, YS, ZS, NV)

Subroutine MESH is used by the PICTURE package to set up one line of print in the array NSTOR. Both for efficiency and to debug the MARS array geometry data, this version has been modified to work exactly like particle tracking. CALI is first called to determine the zone of the first grid point. A trajectory to the last grid point is then initialized, and successive calls to PILOT, which calls 'G1,' "track" a particle to the last point, setting the region of each grid point in NSTOR. By setting IRG negative, zero, or positive, either NREG, IR, or NMED will be stored in the print array NSTOR.

Called from: PRINT

Subroutines called: CALI, RESET, PILOT

Commons required: PICT, GOMLOC, PAREM, ORGI, REPEAT, ARAR, MGOMV, SS, JOMN2, blank.

Variables required:

XS, YS, ZS - coordinates of first grid point,

NV - number of grid points,

DELV - distance between grid points,

IRG - flag to print NREG, IR, or NMED if IRG is negative, zero, or positive.

Variables changed: NSTOR - print array.

Significant internal variables:

J - grid point index,

ISTOR - value to be stored in NSTOR between successive boundary crossings,

IROLD - present input zone number,

SUMS1 - distance traveled on current line (DIST),

DLINE - total distance to end of current line (DIST0).

Subroutine PICTUR (NDIM, RAYX, KTYPE)

Subroutine PICTUR reads in the input, calculates the coordinates of the picture to be plotted, and controls the calls to other routines. There are several different ways in which a 2-D slice through the geometry may be obtained. These different options are discussed in Sect. M13.4 with discussions of the input. For printer plots, the characters to be printed for corresponding media or regions may be changed by altering the values in ATABLE as given in the data statement. For screen plots, the default colors may be changed by specifying new colors using the CLR= option on input.

Called from: Main Program (MAIN or O0O016)

Subroutines called: JOMIN, PRINT, AREAD, IREAD, FREAD, CLEAR, SCANON, SCANOF, RCOLOR, CLRNIT

Commons required: PICT, MGOMV, JOMN2, JOMK, PCOLOR, Blank, PNIT (see Table M13.2.1)

Variables required: Input data is read based on the value of KTYPE which indicates whether PICTURE is being run from MAIN or from O0O016.

Variables changed: All variables in common PICT (see Table M13.2.2) except MTRLUSED and NSTOR

IPRET in MGOMV

RAYX - reset to "1" if it's a screen plot,

LTYPE - logical variable denoting type of plot.

If IXS is read in, the direction cosines required are set equal to 1; otherwise, cosines are part of input data.

Significant internal variables:

NADD(1) - first location in blank common for storage of geometry data,

NCK - flag to indicate which set of input options was used to define the 2-D slice.

Subroutine RCOLOR(RED, GREEN, BLUE, IRET, BNDX, ENDX)

This routine reads the input data specifying the red, green, and blue components of the colors being selected for the current plot. When IRET is not equal to 0, RCOLOR reads the keyword "END COLOR" or "END" that terminates this part of the input data.

Called from: PICTUR

Subroutines called: AREAD, IREAD

Variables required:

IRET - signal indicating whether more integer data is to be read. If IRET > 0, then the next data is character data,

BNDX - integer indicating lower limit of range of RED, GREEN, BLUE,

ENDX - integer indicating upper limit of range of RED, GREEN, BLUE

Variables changed: RED, GREEN, BLUE

Subroutine CLRNIT

This routine sets up the default colors for a screen plot as indicated in Table M13.3.1.

Called from: PICTUR

Commons required: PICT, PCOLOR

Variables changed: RED, GREEN, BLUE

Table M13.2.2 Definition of variables in common PICT

Variable	Definition
X0,Y0,Z0	The coordinates in geometry units defining the first point (upper-left-hand corner) of the picture.
X1,Y1,Z1	The coordinates in geometry units defining the last point (lower-right-hand corner) of the picture.
XU,YU,ZU	The length (in direction U) of the picture in geometry units.
XV,YV,ZV	The width (in direction V) of the picture in geometry units.
DELU	The increment in geometry units between lines in the picture in the U direction.
DELV	The increment in geometry units between lines in the picture in the V direction.
IRG	A flag indicating that region, zone, or medium geometry parameter should be printed if IRG is negative, zero, or positive, respectively.
NU	Number of intervals to print along U axis.
NV	Number of intervals to print along V axis.
ICNT	A flag indicating whether this is last plot (and if not, whether next plot is of a different geometry).
LTYPE	Logical variable indicating printer plot if "FALSE" or plot to screen if "TRUE."
TITLE(18)	Title for plot.
MTRLUSED(256)	An array of material or region or zone numbers used in the picture.
NSTOR(2048)	An array used to store the medium, region, or zone number for one line of the picture.

M13.3 INPUT DATA

The format of the input data for PICTURE has been revised to use free form with a system of keywords to identify the variables. Following is a description of the data.

1. Card PA:

   NUSE: The number of characters to be read on Card B to replace the standard values of ATABLE. Specify a 0 and omit Card B if the standard ATABLE is desired or for a screen plot. NUSE ≤ 50.

2. Card PB: Format (50A1) (omit if NUSE = 0)

   ATABLE(I), I=1, NUSE: The list of characters that are to be printed for each medium. For medium N, ATABLE (N+1) is printed. If N ≥ 47, ATABLE (48) is printed. The standard values of ATABLE are:

Medium Number	Character Printed
0 (external void)	
1 through 9	1 through 9
10 through 35	A through Z
36 through 46	Various special characters
≥47 (including internal voids)	(blank)

3. GEOM input: MARS combinatorial geometry input.[1]

4. Remaining data uses keywords, and multiple values can appear on a line.

   TTL = title in 18A4 format
   TITLE(I),I=1,18 72 characters to be printed as a title.

   ICN = inam(18) ICNT
   - = −1 There is only one plot. Default.
   - = 0 After this picture, return to step 4 for another picture with the same geometry.
   - = 1 After this picture, read in a new GEOM input. (step3 above)

   IRG = inam(17) IRG
   - = −1 Display the region geometry.
   - = 0 Display the zone geometry.
   - = 1 Display the material geometry. Default.

[1]See description of geometry input in Sect. M9.A.

IXS = inam(22) option to allow code to set the direction cosines for a plot.

IXS
- = 'xy' plot x vs y; x-axis across screen or page; y-axis down
- = 'xz' plot x vs z; x-axis across screen or page; z-axis down
- = 'yz' plot y vs z; y-axis across screen or page; z-axis down

The corresponding direction cosines are set equal to 1.

Enter X0, Y0, and Z0 the X, Y, and Z coordinates in the combinatorial geometry of the upper left corner of the picture. Data must be entered for all three coordinates unless all three values from the previous plot are to be used.

XUL = fnam(1)

YUL = fnam(2)

ZUL = fnam(3)

Enter X1, Y1, and Z1 the X, Y, and Z coordinates in the combinatorial geometry of the lower-right corner of the picture.

XLR = fnam(4)

YLR = fnam(5)

ZLR = fnam(6)

Note: These six coordinates partially describe the plane of the slice by defining two points in the plane and designate the top, bottom, left and right sides of the picture. Default values are those from the previous plot.

Enter XU, YU, and ZU the direction numbers proportional to the direction cosines for the U axis of the picture. The U axis points down the printed page in the direction the page moves through the printer.

UAX = fnam(7)

VAX = fnam(8)

WAX = fnam(9)

Enter XV, YV, and ZV the direction numbers for the V axis of the picture. The V axis points to the right across the page.

UDN = fnam(10)

VDN = fnam(11)

WDN = fnam(12)

Note: These values complete the description of the plane of the slice by giving a line in the plane and also specify the orientation of the picture on the output.

Enter DELU, DELV, NU, and NV the spacing and number of intervals.

DLX = fnam(13)	DELU:	Spacing (in GEOM units) of intervals along the U axis.
DLD = fnam(14)	DELV:	Spacing (in GEOM units) of intervals along the V axis.
NAX = inam(15)	NU:	Number of intervals to print along the U axis (overrides DELU).
NDN = inam(16)	NV:	Number of intervals to print along the V axis (overrides DELV).

For printer plots, NV, which is input as keyword NDN, is the number of characters across the page (i.e., along the V axis); for a 132-character-per-line printer, NDN=130 is a good choice. NU, which is input as keyword NAX, is the number of characters down the page (along theU axis). For screen plots, NV is the number of pixels across the screen. The lower the value, the faster the program executes, but the smaller the picture is. NV should be chosen based on the resolution of the monitor being used. NDN=640 will produce a good picture in most cases.

Note: All four entries are not required as input; see Sect. M13.4 for an explanation.

Enter SCR the method of plot display.

SCR= wrd The plot display method is specified by entering either **YES** or **NO** for wrd. The default value is NO. SCR=NO utilizes the printer plot display method. SCR=YES utilizes the color plot display method. If SCR is entered more than once for a plot, the last value entered is the one that is used. Also, if more than one plot is being done in a run and SCR is not specified for the second or subsequent plots, the value for the previous plot will be used.

NOTE: It is possible to mix printer plots and color plots in the same run; however, SCR must be defined for each one (i.e., the default value will not be implemented except for the first plot in the run).

Enter CLR if SCR=YES and colors other than the default are desired.

CLR= num(i) red(num(i)) green(num(i)) blue(num(i)) **END COLOR**
enter only if plots are to be made utilizing the color plot display method (**SCR=YES**).

After entering the keyword **CLR=**, 4 numbers are entered i times.
The first number, num(i), represents a media (mixture) number, region number, or zone number. The next three numbers, whose values can range from 0 through 255, define the red, green, and blue components of the color that will represent this num(i) in the plot. The sequence num(i) red(num(i)) green(num(i)) blue(num(i)) is repeated until the colors associated with all of the media (mixture) numbers, region numbers, or zone numbers used in the problem are defined. The smallest number that can be entered for num(i) is -1, representing the internal void. A num(i) of 0 represents the external void, num(i) of 1 represents the smallest numbered media, region or zone, num(i) of 2 represents the next larger numbered

media, region or zone used in the problem, etc. The color plot definition data is terminated by entering the keywords **END COLOR** or **END**. A total of 256 default colors are provided in Table M13.3.1. Two of those colors represent void regions, num(-1) as gray for internal voids (media 1000); and num(0) as black for external void (media 0). The remaining 254 colors represent the default values for mixtures, regions, or zones used in the problem.

If **num** is entered as **-1** or **1000** , the next three numbers define the color that will be used to represent internal void regions of the plot. The default color for internal void is gray, represented as 200 200 200. If **num** is entered as **0**, the next three numbers define the color that will represent external void regions in the plot. The default color for external void is black, represented by 0 0 0.

For example, suppose a color plot is to be made for a problem that utilizes void regions and media numbers 1, 3, and 5. By default, the internal void regions (Index -1) will be gray; external void regions (Index 0) will be black; the first mixture, mixture 1 (Index 1), will be medium blue; the next larger mixture, mixture 3 (Index 2), will be turquoise; and the last mixture, mixture 5 (Index 3) will be green2. If these values are acceptable, data need not be entered for **CLR=**. If the user decides to define internal void to be white (255 255 255), mixture 1 to be red (255 0 0), mixture 3 to be bright blue (0 0 255), and mixture 5 to be green (0 255 0), the following data could be entered:

```
CLR=1000 255 255 255  1 255 0 0  2 0 0 255  3 0 255 0 END COLOR
                          or
CLR=-1 255 255 255  1 255 0 0  2 0 0 255  3 0 255 0 END
```

In this example, the first number (1000 or -1) defines the internal void and the next three numbers are the red, green and blue components that combine as the color white. The fifth number (1) represents the smallest mixture number (mixture number (mixture 1) and the next three numbers are the red, green, and blue components of red. The ninth number (2) represents the next larger mixture number (mixture 3), and the next three numbers are the red, green, and blue components of bright blue. The thirteenth number (3) represents the next larger mixture number (mixture 5), and the next three numbers are the red, green, and blue components of green. The END COLOR or END terminates the color definition data. Because color data were not entered for num(i) of 0, external void regions will be represented by the color black, the default specification from Table M.13.3.1. The red, green, and blue components of some bright colors are listed below.

Display Color	red	green	blue
black	0	0	0
white	255	255	255
"default void gray"	200	200	200
red	255	0	0
green	0	255	0
brightest blue	0	0	255
yellow	255	255	0
brightest cyan	0	255	255
magenta	255	0	255

The 256 default colors are listed in Table M13.3.1.

Signal the end of data for this plot.

END

If there are more plots, set up the data according to the value of ICNT and specify parameters that need changing. REMINDER: See the note on the SCR parameter above.

Table M13.3.1 Default color specifications for the color plot display method

Index	Red	Green	Blue	Color Name(s)
-1	200	200	200	default void gray
0	0	0	0	black gray0 grey0
1	0	0	205	medium blue MediumBlue blue3
2	0	229	238	turquoise2
3	0	238	0	green2
4	205	205	0	yellow3
5	238	0	0	red2
6	145	44	238	purple2
7	150	150	150	gray59 grey59
8	240	200	220	white gray100 grey100
9	0	191	255	deep sky blue DeepSkyBlue DeepSkyBlue1
10	224	255	255	light cyan LightCyan LightCyan1
11	0	255	127	spring green SpringGreen SpringGreen1
12	255	255	224	light yellow LightYellow LightYellow1
13	255	0	0	red red1
14	255	0	255	magenta magenta1
15	67	110	238	RoyalBlue2
16	174	238	238	PaleTurquoise2
17	180	238	180	DarkSeaGreen2
18	238	220	130	LightGoldenrod2
19	238	99	99	IndianRed2
20	238	122	233	orchid2
21	25	25	112	midnight blue MidnightBlue
22	0	0	128	navy navy blue NavyBlue
23	100	149	237	cornflower blue CornflowerBlue
24	72	61	139	dark slate blue DarkSlateBlue
25	106	90	205	slate blue SlateBlue
26	123	104	238	medium slate blue MediumSlateBlue
27	30	144	255	dodger blue DodgerBlue DodgerBlue1
28	135	206	235	sky blue SkyBlue
29	135	206	250	light sky blue LightSkyBlue
30	70	130	180	steel blue SteelBlue
31	176	196	222	light steel blue LightSteelBlue
32	176	224	230	powder blue PowderBlue
33	0	206	209	dark turquoise DarkTurquoise
34	72	209	204	medium turquoise MediumTurquoise
35	95	158	160	cadet blue CadetBlue
36	102	205	170	medium aquamarine MediumAquamarine aquamarine3
37	127	255	212	aquamarine aquamarine1
38	0	100	0	dark green DarkGreen
39	85	107	47	dark olive green DarkOliveGreen
40	143	188	143	dark sea green DarkSeaGreen
41	60	179	113	medium sea green MediumSeaGreen
42	32	178	170	light sea green LightSeaGreen
43	152	251	152	pale green PaleGreen
44	0	255	0	green green1
45	127	255	0	chartreuse chartreuse1
46	0	250	154	medium spring green MediumSpringGreen
47	173	255	47	green yellow GreenYellow
48	50	205	50	lime green LimeGreen
49	154	205	50	yellow green YellowGreen OliveDrab3
50	34	139	34	forest green ForestGreen
51	107	142	35	olive drab OliveDrab
52	189	183	107	dark khaki DarkKhaki
53	240	230	140	khaki
54	238	232	170	pale goldenrod PaleGoldenrod
55	250	250	210	light goldenrod yellow LightGoldenrodYellow
56	255	255	224	light yellow LightYellow LightYellow1
57	255	255	0	yellow yellow1
58	255	215	0	gold gold1
59	238	221	130	light goldenrod LightGoldenrod
60	184	134	11	dark goldenrod DarkGoldenrod

Table M13.3.1 (continued)

Index	Red	Green	Blue	Color Name(s)	Index	Red	Green	Blue	Color Name(s)
61	188	143	143	rosy brown	97	138	43	226	blue violet
				RosyBrown					BlueViolet
62	205	92	92	indian red	98	160	32	240	purple
				IndianRed	99	147	112	219	medium purple
63	139	69	19	saddle brown					MediumPurple
				SaddleBrown	100	216	191	216	thistle
				chocolate4	101	238	233	233	snow2
64	160	82	45	sienna	102	238	229	222	seashell2
65	205	133	63	peru	103	238	223	204	AntiqueWhite2
				tan3	104	238	213	183	bisque2
66	222	184	135	burlywood	105	238	203	173	PeachPuff2
67	245	245	220	beige	106	238	207	161	NavajoWhite2
68	245	222	179	wheat	107	238	233	191	LemonChiffon2
69	244	164	96	sandy brown	108	238	232	205	cornsilk2
				SandyBrown	109	238	238	224	ivory2
70	210	105	30	chocolate	110	224	238	224	honeydew2
71	178	34	34	firebrick	111	238	224	229	LavenderBlush2
72	165	42	42	brown	112	238	213	210	MistyRose2
73	233	150	122	dark salmon	113	224	238	238	azure2
				DarkSalmon	114	122	103	238	SlateBlue2
74	250	128	114	salmon	115	67	110	238	RoyalBlue2
75	255	160	122	light salmon	116	0	0	238	blue2
				LightSalmon	117	28	134	238	DodgerBlue2
				LightSalmon1	118	92	172	238	SteelBlue2
76	255	165	0	orange	119	0	178	238	DeepSkyBlue2
				orange1	120	126	192	238	SkyBlue2
77	255	140	0	dark orange	121	164	211	238	LightSkyBlue2
				DarkOrange	122	185	211	238	SlateGray2
78	255	127	80	coral	123	188	210	238	LightSteelBlue2
79	240	128	128	light coral	124	178	223	238	LightBlue2
				LightCoral	125	209	238	238	LightCyan2
80	255	99	71	tomato	126	174	238	238	PaleTurquoise2
				tomato1	127	142	229	238	CadetBlue2
81	255	69	0	orange red	128	0	238	238	cyan2
				OrangeRed	129	141	238	238	DarkSlateGray2
				OrangeRed1	130	118	238	198	aquamarine2
82	255	0	0	red	131	180	238	180	DarkSeaGreen2
				red1	132	78	238	148	SeaGreen2
83	255	105	180	hot pink	133	144	238	144	light green
				HotPink					lightGreen
84	255	20	147	deep pink					PaleGreen2
				DeepPink	134	0	238	118	SpringGreen2
				DeepPink1	135	0	238	0	green2
85	255	192	203	pink	136	118	238	0	chartreuse2
86	255	182	193	light pink	137	179	238	58	OliveDrab2
				LightPink	138	188	238	104	DarkOliveGreen2
87	219	112	147	pale violet red	139	238	230	133	khaki2
				PaleVioletRed	140	238	220	130	LightGoldenrod2
88	176	48	96	maroon	141	238	238	209	LightYellow2
89	199	21	133	medium violet red	142	238	238	0	yellow2
				MediumVioletRed	143	238	201	0	gold2
90	208	32	144	violet red	144	238	180	34	goldenrod2
				VioletRed	145	238	173	14	DarkGoldenrod2
91	238	130	238	violet	146	238	180	180	RosyBrown2
92	221	160	221	plum	147	238	99	99	IndianRed2
93	218	112	214	orchid	148	238	121	66	sienna2
94	153	50	204	dark orchid	149	238	197	145	burlywood2
				DarkOrchid	150	238	216	174	wheat2
95	148	0	211	dark violet	151	238	154	73	tan2
				DarkViolet	152	238	118	33	chocolate2
96	186	85	211	medium orchid	153	238	44	44	firebrick2
				MediumOrchid	154	238	59	59	brown2

Table M13.3.1 (continued)

Index	Red	Green	Blue	Color Name(s)	Index	Red	Green	Blue	Color Name(s)
155	238	130	98	salmon2	198	202	225	255	LightSteelBlue1
156	238	149	114	LightSalmon2	199	191	239	255	LightBlue1
157	238	154	0	orange2	200	224	255	255	light cyan
158	238	118	0	DarkOrange2					LightCyan
159	238	106	80	coral2					LightCyan1
160	238	92	66	tomato2	201	187	255	255	PaleTurquoise1
161	238	64	0	OrangeRed2	202	152	245	255	CadetBlue1
162	238	0	0	red2	203	0	245	255	turquoise1
163	238	18	137	DeepPink2	204	151	255	255	DarkSlateGray1
164	238	106	167	HotPink2	205	127	255	212	aquamarine
165	238	169	184	pink2					aquamarine1
166	238	162	173	LightPink2	206	193	255	193	DarkSeaGreen1
167	238	121	159	PaleVioletRed2	207	84	255	159	SeaGreen1
168	238	48	167	maroon2	208	154	255	154	PaleGreen1
169	238	58	140	VioletRed2	209	0	255	127	spring green
170	238	0	238	magenta2					SpringGreen
171	238	122	233	orchid2					SpringGreen1
172	238	174	238	plum2	210	127	255	0	chartreuse
173	209	95	238	MediumOrchid2					chartreuse1
174	178	58	238	DarkOrchid2	211	192	255	62	OliveDrab1
175	145	44	238	purple2	212	202	255	112	DarkOliveGreen1
176	159	121	238	MediumPurple2	213	255	246	143	khaki1
177	238	210	238	thistle2	214	255	236	139	LightGoldenrod1
178	255	250	250	snow	215	255	255	224	light yellow
				snow1					LightYellow
179	139	137	137	snow4					LightYellow1
180	255	245	238	seashell	216	255	215	0	gold
				seashell1					gold1
181	255	228	196	bisque	217	255	193	37	goldenrod1
				bisque1	218	255	185	15	DarkGoldenrod1
182	255	218	185	peach puff	219	255	193	193	RosyBrown1
				PeachPuff	220	255	106	106	IndianRed1
				PeachPuff1	221	255	130	71	sienna1
183	255	250	205	lemon chiffon	222	255	211	155	burlywood1
				LemonChiffon	223	255	231	186	wheat1
				LemonChiffon1	224	255	165	79	tan1
184	255	248	220	cornsilk	225	255	127	36	chocolate1
				cornsilk1	226	255	48	48	firebrick1
185	255	255	240	ivory	227	255	64	64	brown1
				ivory1	228	255	140	105	salmon1
186	240	255	240	honeydew	229	255	160	122	lightsalmon
				honeydew1					LightSalmon
187	255	240	245	lavender blush					LightSalmon1
				LavenderBlush	230	255	165	0	orange
				LavenderBlush1					orange1
188	255	228	225	misty rose	231	255	127	0	DarkOrange1
				MistyRose	232	255	114	86	coral1
				MistyRose1	233	255	99	71	tomato
189	240	255	255	azure					tomato1
				azure1	234	255	69	0	orangered
190	131	111	255	SlateBlue1					OrangeRed
191	72	118	255	RoyalBlue1					OrangeRed1
192	30	144	255	dodger blue	235	255	20	147	deep pink
				DodgerBlue					DeepPink
				DodgerBlue1					DeepPink1
193	99	184	255	SteelBlue1	236	255	110	180	HotPink1
194	0	191	255	deep sky blue	237	255	181	197	pink1
				DeepSkyBlue	238	255	174	185	LightPink1
				DeepSkyBlue1	239	255	130	171	PaleVioletRed1
195	135	206	255	SkyBlue1	240	255	52	179	maroon1
196	176	226	255	LightSkyBlue1	241	255	62	150	VioletRed1
197	198	226	255	SlateGray1	242	255	131	250	orchid1

Table M13.3.1 (continued)

Index	Red	Green	Blue	Color Name(s)	Index	Red	Green	Blue	Color Name(s)
243	255	187	255	plum1	250	139	0	0	dark red
244	224	102	255	MediumOrchid1					darkRed
245	191	62	255	DarkOrchid1					red4
246	155	48	255	purple1	251	0	139	0	green4
247	171	130	255	MediumPurple1	252	0	0	139	dark blue
248	255	225	255	thistle1					darkBlue
249	139	0	139	dark magenta					blue4
				darkMagenta	253	0	139	139	dark cyan
				magenta4					darkCyan
									cyan4
					254	139	139	0	yellow4

M13.4 OPTIONS

1. $X_{LR} = Y_{LR} = Z_{LR} = 0$.

For this case, NU and NV must be specified. In addition, either DELU or DELV must be specified. If the other is left blank, the code will produce an undistorted picture. If both DELU and DELV are specified, the picture is likely to be distorted. Because printers typically give more characters per inch across a line than down the page, DELU = RAYX*DELU is necessary to produce an undistorted picture (see Sect. M13.2.1).

2. X_{LR} or Y_{LR} or $Z_{LR} \neq 0$.

If any one of the variables X_{LR}, Y_{LR}, or Z_{LR} is specified, the code will calculate the others to produce an undistorted picture.

If both NU and DELU (or both NV and DELV) are specified, DELU (or DELV) will be ignored.

The U and V axes may have arbitrary orientation. (If they are not orthogonal, the resulting picture will be distorted.) In Option 1, the first point will be at $(X, Y, Z)_{UL}$, and the remaining points in the directions and at the distances specified. In Option 2, the range from X_{UL} to X_{LR} is divided into intervals and the calculated points will be at the midpoints of the intervals. The first point will be 1/2 interval past $(X, Y, Z)_{LR}$ and the final point will be within 1/2 interval of $(X, Y, Z)_{LR}$. If $(X, Y, Z)_{LR}$ does not lie on the U-V plane, or if the U and V axes are not orthogonal, the location of the final point is not readily predictable.

The simplest method to obtain the correct results is to specify two diagonal corners of the plane of the slice, with the top having the short dimension. Then specify the U axis to be parallel to the edge of the slice with the large dimension (left or right side), and the V axis to be parallel to the edge of the slice with the small dimension (top or bottom). Finally, do not specify NU, DELU, or DELV, but let NV be equal to the maximum number of characters per line on your printer; this arrangement will provide the largest undistorted picture.

M13.5 PICTURE SAMPLE PROBLEM

This problem illustrates the use of the PICTURE program for looking at the geometry of a given problem. Two geometries are being demonstrated, one as a printer plot and the other as a color display.

The first geometry being illustrated is a tank. This tank model was constructed purely as an illustration of the combinatorial geometry and is in no way accurate or detailed. The use of the OR operator and the ARB body is demonstrated in a plot of the **zone** geometry. The input data for the printer plot option are listed in Fig. M13.5.1, and the output and picture produced by this option are shown in Fig. M13.5.2.

The second geometry being illustrated is a spent fuel shipping cask with 7 assemblies. This geometry model which demonstrates the use of arrays is from sample problem 4 for the SAS4 code. The input data for a color plot display of the **material** geometry are listed in Fig. M13.5.3. The printer output produced by the color display option is contained in Fig. M13.5.4. Figure M13.5.5 is a black and white copy of the color screen display. To see the colors, users should view the GIF file on a color monitor.

```
=picture
    7
.1eta0
combinatorial geometry tank sample problem
 0 0 0 10
  arb      1.25      -1.25      .5        1.25      -2.0      0.0
           1.25      2.0        0.0       1.25      1.25      .5
           -1.25     -1.25      .5        -1.25     -2.0       0.0
           -1.25     2.0        0.0       -1.25      1.25      .5
           1234.     4158.      6587.     2673.     5621.     4378.
  ell      0.0       -.5        .5        0.0       .5        .5
           1.5
  trc      0.0       0.0        .8        0.0       2.5       0.0
           .1        .05
  arb      1.25      -2.0       0.0       1.25      -1.8      -.8
           1.25       2.0       0.0       1.25       1.8      -.8
          -1.25       2.0       0.0      -1.25       1.8      -.8
          -1.25      -2.0       0.0      -1.25      -1.8      -.8
           1243.     7135.      8756.     2864.     7821.     3465.
  box      1.25      -1.979     -.6895    0.0       .358      .179
           0.0       -.2        .4        -2.5      0.0       0.0
  box      1.25      1.979      -.6895    0.0       -.358     .179
           0.0       .2         .4        -2.5      0.0       0.0
  rcc      1.25      -2.0       -.2       -2.5      0.0       0.0
           .2
  rcc      1.25      -1.8       -.6       -2.5      0.0       0.0
           .2
  rcc      1.25       2.0       -.2       -2.5      0.0       0.0
           .2
  rcc      1.25      1.80       -.6       -2.5      0.0       0.0
           .2
  rcc      1.25      -.9        -.6       -2.5      0.0       0.0
           .2
  rcc      1.25      -.45       -.2       -2.5      0.0       0.0
           .2
  rcc      1.25      0.0        -.6       -2.5      0.0       0.0
           .2
  rcc      1.25      .45        -.2       -2.5      0.0       0.0
           .2
  rcc      1.25      .9         -.6       -2.5      0.0       0.0
           .2
  rpp      -10.      10.        -10.      10.       -10.      10.
  end
   z1          +1
   z2          +2      -1
   z3          +3      -2
   z4    or    +4      -7      -8      -9     -10     -11     -12     -13     -14
              -15or    +5       -7      -8or    +6      -9     -10
   z5    or    +7or    +8or    +9or   +10or   +11or   +12or   +13or   +14or   +15
   z6         +16      -1      -2      -3      -4      -5      -6      -7      -8
               -9     -10
  end
    1    1    1    1    1    1
6*0
    1    2    3    4    5 1000
0
ttl=
  this is a combinatorial geometry tank.
icn= 1  irg= 0
yul= -3.  zul= -2. ylr= 3. zlr= 2. vax= 1.  wdn= 1.
ndn= 130  end
```

Figure M13.5.1 Input data for PICTURE sample problem printer plot option

```
        combinatorial geometry tank sample problem

                 ivopt = 0          idbg = 0


                                                    body data
 arb    1  0.1250000E+01 -0.1250000E+01  0.5000000E+00  0.1250000E+01 -0.2000000E+01  0.0000000E+00
           0.1250000E+01  0.2000000E+01  0.0000000E+00  0.1250000E+01  0.1250000E+01  0.5000000E+00
          -0.1250000E+01 -0.1250000E+01  0.5000000E+00 -0.1250000E+01 -0.2000000E+01  0.0000000E+00
          -0.1250000E+01  0.2000000E+01  0.0000000E+00 -0.1250000E+01  0.1250000E+01  0.5000000E+00
           0.1234000E+04  0.4158000E+04  0.6587000E+04  0.2673000E+04  0.5621000E+04  0.4378000E+04
                              -0.1000000E+01  0.0000000E+00  0.0000000E+00  0.1250000E+01
                               0.0000000E+00  0.0000000E+00 -0.1000000E+01  0.5000000E+00
                               0.1000000E+01  0.0000000E+00  0.0000000E+00  0.1250000E+01
                               0.0000000E+00  0.0000000E+00  0.1000000E+01  0.0000000E+00
                               0.0000000E+00  0.5547002E+00 -0.8320503E+00  0.1109400E+01
                               0.0000000E+00 -0.5547002E+00 -0.8320503E+00  0.1109400E+01
                               0.9013878E+00  0.6000000E+01
 ell    2  0.0000000E+00 -0.5000000E+00  0.5000000E+00  0.0000000E+00  0.5000000E+00  0.5000000E+00
           0.1500000E+01
 trc    3  0.0000000E+00  0.0000000E+00  0.8000000E+00  0.0000000E+00  0.2500000E+01  0.0000000E+00
           0.1000000E+00  0.5000000E-01
 arb    4  0.1250000E+01 -0.2000000E+01  0.0000000E+00  0.1250000E+01 -0.1800000E+01 -0.8000000E+00
           0.1250000E+01  0.2000000E+01  0.0000000E+00  0.1250000E+01  0.1800000E+01 -0.8000000E+00
          -0.1250000E+01  0.2000000E+01  0.0000000E+00 -0.1250000E+01  0.1800000E+01 -0.8000000E+00
          -0.1250000E+01 -0.2000000E+01  0.0000000E+00 -0.1250000E+01 -0.1800000E+01 -0.8000000E+00
           0.1243000E+04  0.7135000E+04  0.8756000E+04  0.2864000E+04  0.7821000E+04  0.3465000E+04
                              -0.1000000E+01  0.0000000E+00  0.0000000E+00  0.1250000E+01
                               0.0000000E+00  0.0000000E+00 -0.1000000E+01  0.0000000E+00
                               0.1000000E+01  0.0000000E+00  0.0000000E+00  0.1250000E+01
                               0.0000000E+00  0.0000000E+00  0.1000000E+01  0.8000000E+00
                               0.0000000E+00  0.9701425E+00  0.2425356E+00  0.1940285E+01
                               0.0000000E+00 -0.9701425E+00  0.2425356E+00  0.1940285E+01
                               0.8246211E+00  0.6000000E+01
 box    5  0.1250000E+01 -0.1979000E+01 -0.6895000E+00  0.0000000E+00  0.3580000E+00  0.1790000E+00
           0.0000000E+00 -0.2000000E+00  0.4000000E+00 -0.2500000E+01  0.0000000E+00  0.0000000E+00
 box    6  0.1250000E+01  0.1979000E+01 -0.6895000E+00  0.0000000E+00 -0.3580000E+00  0.1790000E+00
           0.0000000E+00  0.2000000E+00  0.4000000E+00 -0.2500000E+01  0.0000000E+00  0.0000000E+00
 rcc    7  0.1250000E+01 -0.2000000E+01 -0.2000000E+00 -0.2500000E+01  0.0000000E+00  0.0000000E+00
           0.2000000E+00
 rcc    8  0.1250000E+01 -0.1800000E+01 -0.6000000E+00 -0.2500000E+01  0.0000000E+00  0.0000000E+00
           0.2000000E+00
 rcc    9  0.1250000E+01  0.2000000E+01 -0.2000000E+00 -0.2500000E+01  0.0000000E+00  0.0000000E+00
           0.2000000E+00
 rcc   10  0.1250000E+01  0.1800000E+01 -0.6000000E+00 -0.2500000E+01  0.0000000E+00  0.0000000E+00
           0.2000000E+00
 rcc   11  0.1250000E+01 -0.9000000E+00 -0.6000000E+00 -0.2500000E+01  0.0000000E+00  0.0000000E+00
           0.2000000E+00
 rcc   12  0.1250000E+01 -0.4500000E+00 -0.2000000E+00 -0.2500000E+01  0.0000000E+00  0.0000000E+00
           0.2000000E+00
 rcc   13  0.1250000E+01  0.0000000E+00 -0.6000000E+00 -0.2500000E+01  0.0000000E+00  0.0000000E+00
           0.2000000E+00
 rcc   14  0.1250000E+01  0.4500000E+00 -0.2000000E+00 -0.2500000E+01  0.0000000E+00  0.0000000E+00
           0.2000000E+00
 rcc   15  0.1250000E+01  0.9000000E+00 -0.6000000E+00 -0.2500000E+01  0.0000000E+00  0.0000000E+00
           0.2000000E+00
 rpp   16 -0.1000000E+02  0.1000000E+02 -0.1000000E+02  0.1000000E+02 -0.1000000E+02  0.1000000E+02

number of bodies      16
length of fpd-array  252


                                                    input zone data
      input zone    code zone        body numbers
 z1          1          1             1
 z2          2          2             2     -1
 z3          3          3             3     -2
 z4          4          4             4     -7     -8     -9    -10    -11    -12    -13    -14
                                    -15
                        5     or      5     -7     -8
                        6     or      6     -9    -10
 z5          5          7             7
                        8     or      8
                        9     or      9
                       10     or     10
                       11     or     11
                       12     or     12
                       13     or     13
                       14     or     14
                       15     or     15
 z6          6         16            16     -1     -2     -3     -4     -5     -6     -7     -8
                                     -9    -10
number of input zones      6
number of  code zones     16
length of integer array  453
```

Figure M13.5.2 Output of PICTURE sample problem printer plot option

```
 code zone    input zone    zone data loc.    no. of bodies   region no.   media no.    box input zone   box code zone
      1            1             113               1             1            1              0               0
      2            2             119               2             1            2              0               0
      3            3             130               2             1            3              0               0
      4            4             141              10             1            4              0               0
      5            4             192               3             1            4              0               0
      6            4             208               3             1            4              0               0
      7            5             224               1             1            5              0               0
      8            5             230               1             1            5              0               0
      9            5             236               1             1            5              0               0
     10            5             242               1             1            5              0               0
     11            5             248               1             1            5              0               0
     12            5             254               1             1            5              0               0
     13            5             260               1             1            5              0               0
     14            5             266               1             1            5              0               0
     15            5             272               1             1            5              0               0
     16            6             278              11             1         1000              0               0

    i    kr1(i)    kr2(i)
    1       1         1
    2       2         2
    3       3         3
    4       4         6
    5       7        15
    6      16        16
0
         morse region in input zone(i) array  (mriz(i),i=1,  6)

            1    1    1    1    1    1
0
         morse media in input zone(i) array (mmiz(i),i=1,  6)

            1    2    3    4    5 1000
0
         morse universe in input zone(i) array (nbiz(i),i=1,  6)

            0    0    0    0    0    0
1 option 0 was used in calculating volumes, for  1 regions
 0-set volumes = 1, 1-concentric spheres, 2-slabs, 3-inputvolumes.


          volumes ( cc ) used in collisions density and track length estimators.
   reg       1
volume  1.000E+00


 array data requires         8 locations, leaving     13889 locations

1this is a combinatorial geometry tank.
0zone geometry
0the selected atable values are
         .   1   e   t   a   0
0      upper  left        lower right
       coordinates        coordinates
0x      0.0000E+00         0.0000E+00
 y     -0.3000E+01         0.3000E+01
 z     -0.2000E+01         0.2000E+01
0          u axis       v axis
           (down)       (across)
0x         0.00000       0.00000
 y         1.00000       0.00000
 z         0.00000       1.00000
0nu=  157   nv=  130     delu= 0.3846E-01     delv= 0.3077E-01
```

Figure M13.5.2 (continued)

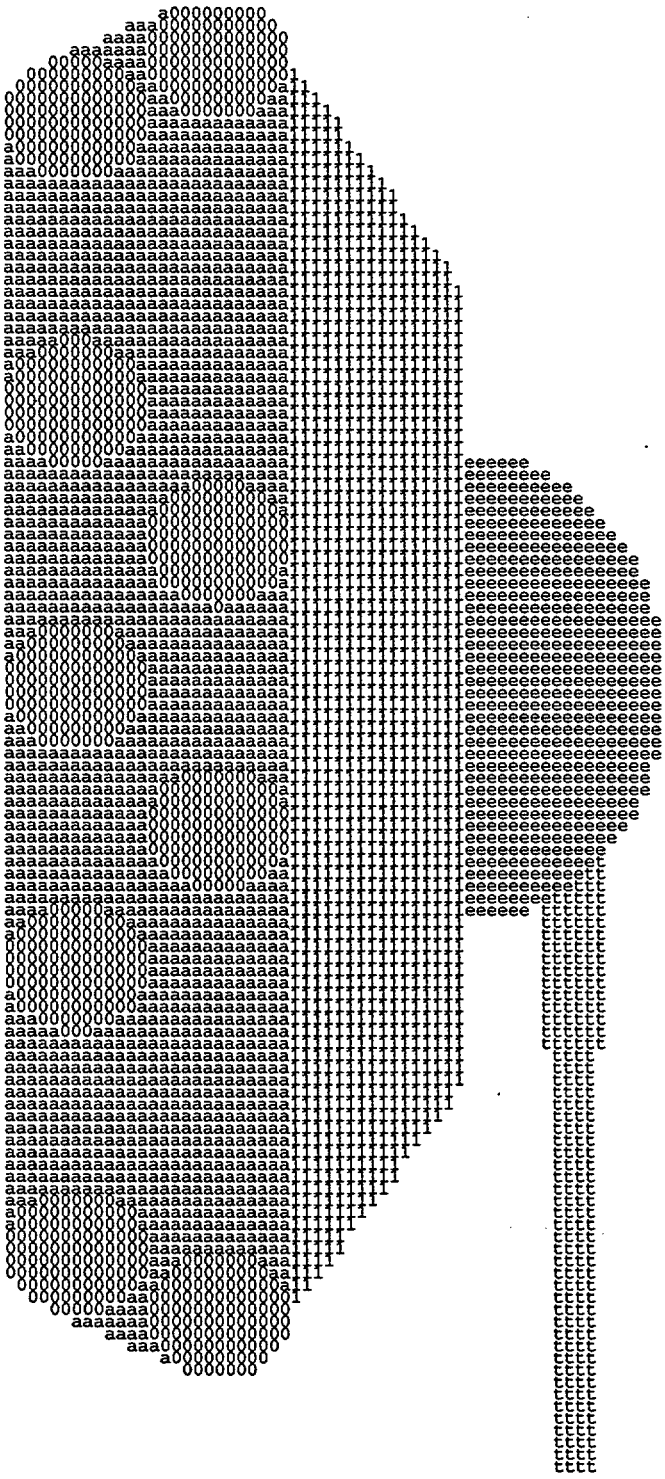

Figure M13.5.2 (continued)

```
sas4d shipping cask with 7 heterogeneous fuel assemblies
    0     0     1    20
rcc     1 0.00 0.00  -2.29870e+02 0.00 0.00   4.59740e+02   4.58200e+01
rcc     2 0.00 0.00  -2.37490e+02 0.00 0.00   4.74980e+02   5.34400e+01
rcc     3 0.00 0.00  -2.37490e+02 0.00 0.00   4.74980e+02   5.34410e+01
rcc     4 0.00 0.00  -2.37490e+02 0.00 0.00   4.74980e+02   5.34420e+01
rcc     5 0.00 0.00  -2.41300e+02 0.00 0.00   4.82600e+02   5.72500e+01
rcc     6 0.00 0.00  -2.41270e+02 0.00 0.00   4.82540e+02   5.72600e+01
rcc     7 0.00 0.00  -2.41280e+02 0.00 0.00   4.82560e+02   5.72700e+01
rcc     8 0.00 0.00  -2.37490e+02 0.00 0.00   4.74980e+02   4.58200e+01
rcc     9 0.00 0.00  -2.37491e+02 0.00 0.00   4.74982e+02   4.58200e+01
rcc    10 0.00 0.00  -2.37492e+02 0.00 0.00   4.74984e+02   4.58200e+01
rcc    11 0.00 0.00  -2.41310e+02 0.00 0.00   4.82620e+02   5.72600e+01
rcc    12 0.00 0.00  -2.41290e+02 0.00 0.00   4.82580e+02   5.72600e+01
rcc    13 0.00 0.00  -2.37492e+02 0.00 0.00   4.74984e+02   5.34420e+01
rcc    14 0.00 0.00  -3.41310e+02 0.00 0.00   6.82620e+02   1.57270e+02
rcc    15 0.00 0.00  -4.41310e+02 0.00 0.00   8.82620e+02   2.57270e+02
rcc    16 0.00 0.00  -5.41310e+02 0.00 0.00   1.08262e+03   3.57270e+02
rcc    17 0.00 0.00  -2.24131e+03 0.00 0.00   4.48262e+03   2.05727e+03
rcc    18 0.00 0.00  -2.34131e+03 0.00 0.00   4.68262e+03   2.15727e+03
rcc    19 0.00 0.00  -2.28600e+02 0.00 0.00   4.57200e+02   4.45500e+01
rcc    20 0.00 0.00  -2.28599e+02 0.00 0.00   4.57198e+02   4.45490e+01
rcc    21 0.00 0.00  -1.82880e+02 0.00 0.00   3.65760e+02   3.99349e-01
rcc    22 0.00 0.00  -1.82880e+02 0.00 0.00   3.65760e+02   4.26660e-01
rcc    23 0.00 0.00  -1.82880e+02 0.00 0.00   3.65760e+02   4.53971e-01
rcc    24 0.00 0.00   0.00000e+00 0.00 0.00   1.82890e+02   4.53971e-01
rcc    25 0.00 0.00  -1.82890e+02 0.00 0.00   1.82890e+02   4.53971e-01
rpp    26 -6.3000e-01  6.3000e-01 -6.3000e-01  6.3000e-01 -1.8288e+02
          1.8288e+02
rpp    27 -6.3000e-01  6.3000e-01 -6.3000e-01  6.3000e-01  1.8288e+02
          1.8289e+02
rpp    28 -6.3000e-01  6.3000e-01 -6.3000e-01  6.3000e-01 -1.8289e+02
         -1.8288e+02
rpp    29 -1.0710e+01  1.0710e+01 -1.0710e+01  1.0710e+01 -1.8289e+02
          1.8289e+02
rpp    30 -1.0715e+01  1.0715e+01 -1.0715e+01  1.0715e+01 -1.8289e+02
          1.8289e+02
rpp    31 -1.0725e+01  1.0725e+01 -1.0725e+01  1.0725e+01 -1.8289e+02
          1.8289e+02
rpp    32 -1.2325e+01  1.2325e+01 -1.2325e+01  1.2325e+01 -1.8289e+02
          1.8289e+02
rpp    33 -2.4650e+01  2.4650e+01 -3.6975e+01 -1.2325e+01 -1.8289e+02
          1.8289e+02
rpp    34 -3.6975e+01  3.6975e+01 -1.2325e+01  1.2325e+01 -1.8289e+02
          1.8289e+02
rpp    35 -2.4650e+01  2.4650e+01  1.2325e+01  3.6975e+01 -1.8289e+02
          1.8289e+02
  end
inn      1  -19
rs1      2  -10
rs2      3   -2
rs3      4   -3
our      5  -13
wtr      6   -5
jac      7   -6   -5
as1      8   -1
as2      9   -8
as3     10   -9
imp     11   -5  -12
hol     13   -4  -10
de2  or    14   -5   -7  -11 or    12   -5   -7
de3     15  -14
de4     16  -15
inv     17  -16
exv     18  -17
cav     19  -20
ins     20  -33  -34  -35
fue     21
gap     22  -21
cla     23  -22
fcl     26  -23
uv1     18  -26
```

Figure M13.5.3 Input data for PICTURE sample problem color display option

```
hr2     24  -23
hc2     27  -24
uv2     18  -27
hr3     25  -23
hc3     28  -25
uv3     18  -28
ar1     29
spa     30  -29
can     31  -30
unt     32  -31
uv4     18  -32
ar2     33
ar3     34
ar4     35
  end
12r1 2 1 2  23r1
19*0  5*1 3*2 3*3 5*4 3r0
    4     5 1000 1000     4 1000 1000     5 1000 1000 1000 1000  4*1000
      0   1000   1000       1       2       2   1000  -1000   1000   1000
  -1000   1000   1000  -1000      -1   1000   1000   1000
 -1000     -2     -3     -4
   17    17     3     2     1     1     3     1     1     2     1     1     0     0
  289*3     289*1     289*2  7*4
4r0
 ttl= sas4d sample problem
  icn= -1   irg=1
 scr=yes
 clr= 1 255 0 0  2 0 255 0  3 0 0 255 1000 0 0 205 end color
  xul=-75.0  yul= 58.0 zul=0.0  xlr=75.0  ylr=-58.0 zlr=0.0
  uax=1 vax=0 wax=0 udn=0 vdn=-1 wdn=0
  ndn=600 end
end
```

Figure M13.5.3 (continued)

```
sas4d shipping cask with 7 heterogeneous fuel assemblies

          ivopt = 0          idbg = 0

                                                    body data
 rcc     1  0.0000000E+00  0.0000000E+00 -0.2298700E+03  0.0000000E+00  0.0000000E+00  0.4597400E+03
            0.4582000E+02
 rcc     2  0.0000000E+00  0.0000000E+00 -0.2374900E+03  0.0000000E+00  0.0000000E+00  0.4749800E+03
            0.5344000E+02
 rcc     3  0.0000000E+00  0.0000000E+00 -0.2374900E+03  0.0000000E+00  0.0000000E+00  0.4749800E+03
            0.5344100E+02
 rcc     4  0.0000000E+00  0.0000000E+00 -0.2374900E+03  0.0000000E+00  0.0000000E+00  0.4749800E+03
            0.5344200E+02
 rcc     5  0.0000000E+00  0.0000000E+00 -0.2413000E+03  0.0000000E+00  0.0000000E+00  0.4826000E+03
            0.5725000E+02
 rcc     6  0.0000000E+00  0.0000000E+00 -0.2412700E+03  0.0000000E+00  0.0000000E+00  0.4825400E+03
            0.5726000E+02
 rcc     7  0.0000000E+00  0.0000000E+00 -0.2412800E+03  0.0000000E+00  0.0000000E+00  0.4825600E+03
            0.5727000E+02
 rcc     8  0.0000000E+00  0.0000000E+00 -0.2374900E+03  0.0000000E+00  0.0000000E+00  0.4749800E+03
            0.4582000E+02
 rcc     9  0.0000000E+00  0.0000000E+00 -0.2374910E+03  0.0000000E+00  0.0000000E+00  0.4749820E+03
            0.4582000E+02
 rcc    10  0.0000000E+00  0.0000000E+00 -0.2374920E+03  0.0000000E+00  0.0000000E+00  0.4749840E+03
            0.4582000E+02
 rcc    11  0.0000000E+00  0.0000000E+00 -0.2413100E+03  0.0000000E+00  0.0000000E+00  0.4826200E+03
            0.5726000E+02
 rcc    12  0.0000000E+00  0.0000000E+00 -0.2412900E+03  0.0000000E+00  0.0000000E+00  0.4825800E+03
            0.5726000E+02
 rcc    13  0.0000000E+00  0.0000000E+00 -0.2374920E+03  0.0000000E+00  0.0000000E+00  0.4749840E+03
            0.5344200E+02
 rcc    14  0.0000000E+00  0.0000000E+00 -0.3413100E+03  0.0000000E+00  0.0000000E+00  0.6826200E+03
            0.1572700E+03
 rcc    15  0.0000000E+00  0.0000000E+00 -0.4413100E+03  0.0000000E+00  0.0000000E+00  0.8826200E+03
            0.2572700E+03
 rcc    16  0.0000000E+00  0.0000000E+00 -0.5413100E+03  0.0000000E+00  0.0000000E+00  0.1082620E+04
            0.3572700E+03
 rcc    17  0.0000000E+00  0.0000000E+00 -0.2241310E+04  0.0000000E+00  0.0000000E+00  0.4482620E+04
            0.2057270E+04
 rcc    18  0.0000000E+00  0.0000000E+00 -0.2341310E+04  0.0000000E+00  0.0000000E+00  0.4682620E+04
            0.2157270E+04
 rcc    19  0.0000000E+00  0.0000000E+00 -0.2286000E+03  0.0000000E+00  0.0000000E+00  0.4572000E+03
            0.4455000E+02
 rcc    20  0.0000000E+00  0.0000000E+00 -0.2285990E+03  0.0000000E+00  0.0000000E+00  0.4571980E+03
            0.4454900E+02
 rcc    21  0.0000000E+00  0.0000000E+00 -0.1828800E+03  0.0000000E+00  0.0000000E+00  0.3657600E+03
            0.3993490E+00
 rcc    22  0.0000000E+00  0.0000000E+00 -0.1828800E+03  0.0000000E+00  0.0000000E+00  0.3657600E+03
            0.4266600E+00
 rcc    23  0.0000000E+00  0.0000000E+00 -0.1828800E+03  0.0000000E+00  0.0000000E+00  0.3657600E+03
            0.4539710E+00
 rcc    24  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.1828900E+03
            0.4539710E+00
 rcc    25  0.0000000E+00  0.0000000E+00 -0.1828900E+03  0.0000000E+00  0.0000000E+00  0.1828900E+03
            0.4539710E+00
 rpp    26 -0.6300000E+00  0.6300000E+00 -0.6300000E+00  0.6300000E+00 -0.1828800E+03  0.1828800E+03

 rpp    27 -0.6300000E+00  0.6300000E+00 -0.6300000E+00  0.6300000E+00  0.1828800E+03  0.1828900E+03

 rpp    28 -0.6300000E+00  0.6300000E+00 -0.6300000E+00  0.6300000E+00 -0.1828900E+03 -0.1828800E+03

 rpp    29 -0.1071000E+02  0.1071000E+02 -0.1071000E+02  0.1071000E+02 -0.1828900E+03  0.1828900E+03

 rpp    30 -0.1071500E+02  0.1071500E+02 -0.1071500E+02  0.1071500E+02 -0.1828900E+03  0.1828900E+03

 rpp    31 -0.1072500E+02  0.1072500E+02 -0.1072500E+02  0.1072500E+02 -0.1828900E+03  0.1828900E+03

 rpp    32 -0.1232500E+02  0.1232500E+02 -0.1232500E+02  0.1232500E+02 -0.1828900E+03  0.1828900E+03

 rpp    33 -0.2465000E+02  0.2465000E+02 -0.3697500E+02 -0.1232500E+02 -0.1828900E+03  0.1828900E+03

 rpp    34 -0.3697500E+02  0.3697500E+02 -0.1232500E+02  0.1232500E+02 -0.1828900E+03  0.1828900E+03

 rpp    35 -0.2465000E+02  0.2465000E+02  0.1232500E+02  0.3697500E+02 -0.1828900E+03  0.1828900E+03

number of bodies      35
length of fpd-array  305
```

Figure M13.5.4 Printer output from color display option

input zone data

	input zone	code zone		body numbers			
inn	1	1		1	-19		
rs1	2	2		2	-10		
rs2	3	3		3	-2		
rs3	4	4		4	-3		
our	5	5		5	-13		
wtr	6	6		6	-5		
jac	7	7		7	-6	-5	
as1	8	8		8	-1		
as2	9	9		9	-8		
as3	10	10		10	-9		
imp	11	11		11	-5	-12	
hol	12	12		13	-4	-10	
de2	13	13		14	-5	-7	-11
		14	or	12	-5	-7	
de3	14	15		15	-14		
de4	15	16		16	-15		
inv	16	17		17	-16		
exv	17	18		18	-17		
cav	18	19		19	-20		
ins	19	20		20	-33	-34	-35
fue	20	21		21			
gap	21	22		22	-21		
cla	22	23		23	-22		
fcl	23	24		26	-23		
uv1	24	25		18	-26		
hr2	25	26		24	-23		
hc2	26	27		27	-24		
uv2	27	28		18	-27		
hr3	28	29		25	-23		
hc3	29	30		28	-25		
uv3	30	31		18	-28		
ar1	31	32		29			
spa	32	33		30	-29		
can	33	34		31	-30		
unt	34	35		32	-31		
uv4	35	36		18	-32		
ar2	36	37		33			
ar3	37	38		34			
ar4	38	39		35			

number of input zones 38
number of code zones 39
length of integer array 1319

code zone	input zone	zone data loc.	no. of bodies	region no.	media no.	box input zone	box code zone
1	1	246	2	1	4	0	0
2	2	257	2	1	5	0	0
3	3	268	2	1	1000	0	0
4	4	279	2	1	1000	0	0
5	5	290	2	1	4	0	0
6	6	301	2	1	1000	0	0
7	7	312	3	1	1000	0	0
8	8	328	2	1	5	0	0
9	9	339	2	1	1000	0	0
10	10	350	2	1	1000	0	0
11	11	361	3	1	1000	0	0
12	12	377	3	1	1000	0	0
13	13	393	4	2	1000	0	0
14	13	414	3	2	1000	0	0
15	14	430	2	1	1000	0	0
16	15	441	2	2	1000	0	0
17	16	452	2	1	1000	0	0
18	17	463	2	1	0	0	0
19	18	474	2	1	1000	0	0
20	19	485	4	1	1000	0	0
21	20	506	1	1	1	1	1
22	21	512	2	1	2	1	1
23	22	523	2	1	2	1	1
24	23	534	2	1	1000	1	1
25	24	545	2	1	-1000	1	1
26	25	556	2	1	1000	2	2
27	26	567	2	1	1000	2	2
28	27	578	2	1	-1000	2	2
29	28	589	2	1	1000	3	3
30	29	600	2	1	1000	3	3
31	30	611	2	1	-1000	3	3
32	31	622	1	1	-1	4	4
33	32	628	2	1	1000	4	4
34	33	639	2	1	1000	4	4
35	34	650	2	1	1000	4	4
36	35	661	2	1	-1000	4	4
37	36	672	1	1	-2	0	0
38	37	678	1	1	-3	0	0
39	38	684	1	1	-4	0	0

Figure M13.5.4 (continued)

```
    i    kr1(i)    kr2(i)
    1         1         1
    2         2         2
    3         3         3
    4         4         4
    5         5         5
    6         6         6
    7         7         7
    8         8         8
    9         9         9
   10        10        10
   11        11        11
   12        12        12
   13        13        14
   14        15        15
   15        16        16
   16        17        17
   17        18        18
   18        19        19
   19        20        20
   20        21        21
   21        22        22
   22        23        23
   23        24        24
   24        25        25
   25        26        26
   26        27        27
   27        28        28
   28        29        29
   29        30        30
   30        31        31
   31        32        32
   32        33        33
   33        34        34
   34        35        35
   35        36        36
   36        37        37
   37        38        38
   38        39        39
0
         morse region in.input zone(i) array  (mriz(i),i=1, 38)

            1    1    1    1    1    1    1    1    1    1    1    1    2    1    2    1    1    1    1    1    1    1

            1    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1
0
         morse media in input zone(i) array (mmiz(i),i=1, 38)

            4    5 1000 1000    4 1000 1000    5 1000 1000 1000 1000 1000 1000 1000 1000    0 1000 1000    1    2    2

          1000-1000 1000 1000-1000 1000 1000-1000   -1 1000 1000 1000-1000   -2   -3   -4
0
         morse universe in input zone(i) array (nbiz(i),i=1, 38)

            0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    1    1    1

            1    1    2    2    2    3    3    3    4    4    4    4    4    0    0    0
1 option 0 was used in calculating volumes, for  2 regions
 0-set volumes = 1, 1-concentric spheres, 2-slabs, 3-inputvolumes.


          volumes ( cc ) used in collisions density and track length estimators.
    reg       1           2
 volume  1.000E+00   1.000E+00
1              array no.    1     array size is   17 by   17 by    3

               level     1 of array no.     1

     x =   1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17
   y

   17      3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3

   16      3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3

   15      3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3

   14      3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3

   13      3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3

   12      3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3

   11      3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3

   10      3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3

    9      3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3

    8      3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3

    7      3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3
```

Figure M13.5.4 (continued)

```
 6       3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3
 5       3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3
 4       3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3
 3       3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3
 2       3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3
 1       3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3

             level     2 of array no.     1

   x =   1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17
 y
17       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
16       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
15       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
14       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
13       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
12       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
11       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
10       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 9       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 8       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 7       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 6       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 5       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 4       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 3       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 2       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 1       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1

             level     3 of array no.     1

   x =   1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17
 y
17       2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
16       2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
15       2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
14       2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
13       2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
12       2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
11       2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
10       2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
 9       2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
 8       2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
 7       2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
 6       2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
 5       2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
 4       2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
 3       2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
 2       2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
 1       2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
1            array no.    2     array size is    2 by    1 by    1
```

Figure M13.5.4 (continued)

```
                level     1 of array no.     2

     x =   1  2
   y

    1       4  4
1               array no.    3     array size is    3 by    1 by    1


                level     1 of array no.     3

     x =   1  2  3
   y

    1       4  4  4
1               array no.    4     array size is    2 by    1 by    1


                level     1 of array no.     4

     x =   1  2
   y

    1       4  4
1

                    universe specifications

               universe          1-simple/0-comjom


                   1                    0

                   2                    0

                   3                    0

                   4                    0

 array data requires      1152 locations, leaving     11449 locations

1sas4d sample problem
0material geometry
0       upper  left        lower right
        coordinates         coordinates
0x      -0.7500E+02          0.7500E+02
 y       0.5800E+02         -0.5800E+02
 z       0.0000E+00          0.0000E+00
0           u axis       v axis
            (down)       (across)
0x          1.00000       0.00000
 y          0.00000      -1.00000
 z          0.00000       0.00000
0nu=  776   nv=  600     delu= 0.1933E+00     delv= 0.1933E+00
```

Figure M13.5.4 (continued)

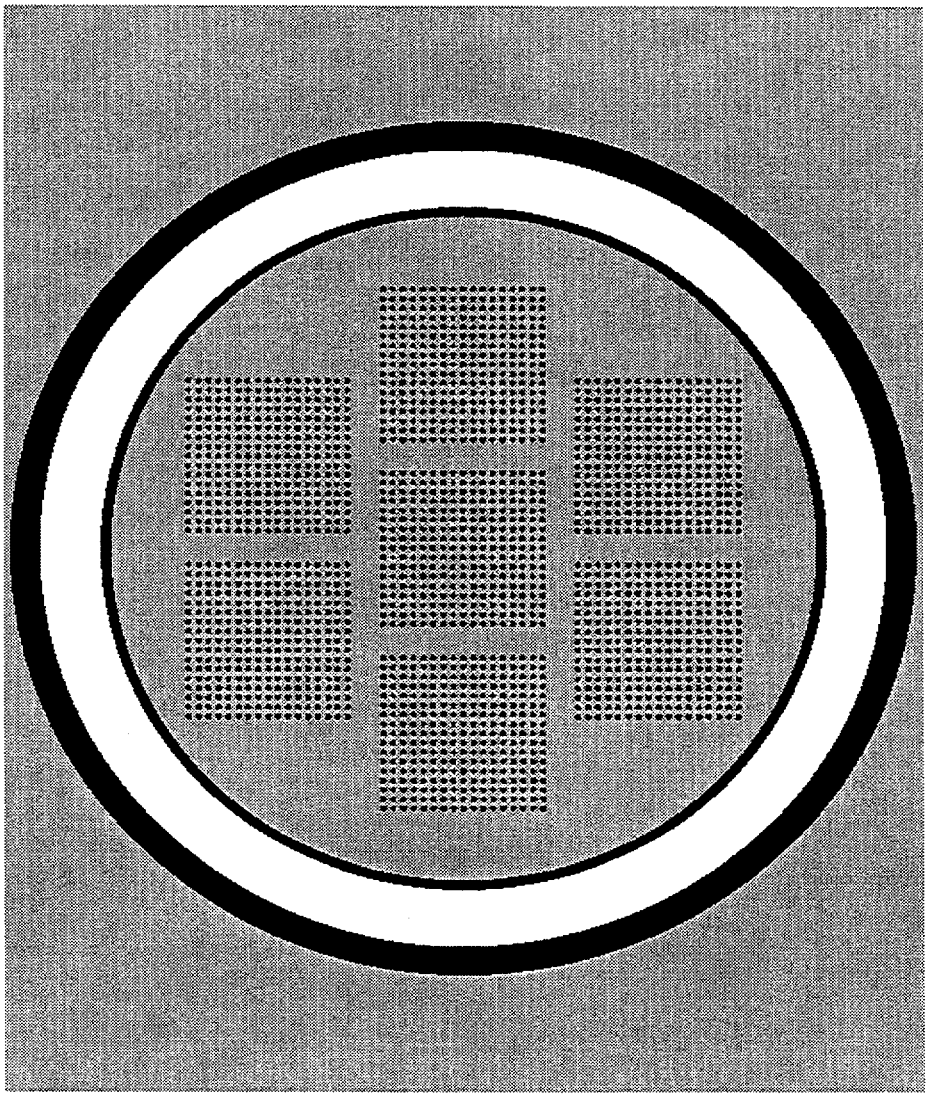

Figure M13.5.5 Black and white print of color display

APPENDIX M13.A

THE LEGEND PROGRAM

LEGEND is a C program that receives a GIF-formatted two-dimensional (2-D) plot piped through a standard input buffer. LEGEND uses routines from the GD freeware package. LEGEND also accesses a data file containing information to be added to the plot in the form of a legend in the upper right corner of the plot. A larger GIF-formatted plot is generated that includes this legend.

LEGEND has been compiled, linked, and executed on the IBM RS/6000, HP and SUN workstations, and on a PC. This program is distributed with the SCALE package.

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Computational Physics and Engineering Division

COMPOZ DATA GUIDE

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ABSTRACT

The COMPOZ program used to create the Standard Composition Library is described. Of particular importance is documentation of the COMPOZ input data file structure. Knowledge of the file structure allows users to edit the data file and subsequently create their own site-specific composition library.

CONTENTS

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M14.1 INTRODUCTION

COMPOZ is the program that creates (writes) the SCALE Standard Composition Library (see Sect. M8). Data are input in free form using the AREAD, FREAD, and IREAD functions in SCALE (see Sects. M2–M3). A card-image data file containing the input to COMPOZ (and the Standard Composition Library) is available with the SCALE system. Execution of COMPOZ using this data file creates the Standard Composition Library currently available with the SCALE package. This section provides documentation of the data file structure. Knowledge of the data file structure allows users to edit the data file and subsequently create their own site-specific or user-specific composition library.

COMPOZ is intended to create or make *permanent changes* to and/or to print the composition library and should not be used for any other purpose. To avoid confusion with the Standard Composition Library provided with SCALE, it is strongly recommended that only *new* keywords and compositions be used in any site-specific or user-specific library.

M14.2 INPUT DATA DESCRIPTION

COMPOZ input data are entered in free form (see Sect. M3). All data must be followed by at least one blank. The COMPOZ input data file contains *five* data records or blocks:

1. COMPOZ mode flag selects whether a new standard composition library will be created, or an old standard composition library will be listed. Only if a new library is being created are the following data records entered.

2. The head record contains the library identification, a set of parameters describing the size of the library, and a three-line library title with 80 characters per line.

3. The standard composition table contains the name, theoretical density, number of elements, and other information about each standard composition. Individual nuclides, mixtures, and compounds are all included in the table.

4. The nuclide information table contains the nuclide identification number, atomic mass, resonance energy cross sections, and a resonance flag for each nuclide.

5. The isotopic distribution table contains the nuclide identification number and the atom percent of each isotope used in specifying the default enrichment.

Note that for executing COMPOZ via SCALE, an =COMPOZ is required in the first eight columns of a record preceding the mode flag, and an END is required in the first three columns of a record inserted after the last data record.

M14.2.1 COMPOZ MODE SELECTOR

1 LGEN = 0 - create a new library and list it

1 - list an existing library

If LGEN is 0, then input the following data to create a new standard composition library.

M14.2.2 LIBRARY HEADING INFORMATION

1 IDT - library identification number

2 NSC - number of standard compositions

3 NNUC - number of entries in the Nuclide Information Table

4 NELV - number of variable isotope definitions

5 MXELSC - maximum number of elements in a standard composition

6 MXISEL - maximum number of isotopes in a variable isotope element definition

7 AVOGAD - Avogadro's constant (atoms/b-cm)

8 TITLE - 3 lines of 80 characters used to identify the library

M14.2.3 STANDARD COMPOSITION TABLE

1. SCID Composition name, maximum of 12 characters.

2. NEL Number of elements.

3. ROTH Theoretical density, gm/cm^3.

4. IVIS Does first element have variable isotope distribution? (As of the current version of SCALE, this is no longer used, but a value must be present.)
   0, no;
   1, yes.

5. ICP 0 for a mixture,
   1 for a compound.

6. IRS No longer used, but a value must be present.
   0 for no resonance data,
   1 for resonance data in any constituent.

7. NCZA Element or nuclide ID

8. ATPM Weight percent if ICP = 0. Number of atoms per molecule if ICP = 1.

For each composition, items 7 and 8 are repeated until all components of the composition are described. There should be NEL pairs of entries. Items 1 through 8 are entered in a similar fashion for all compositions. There should be a total of NSC composition descriptions. The number of elements per composition can not exceed MXELSC.

M14.2.4 NUCLIDE INFORMATION TABLE

1. NZA Nuclide ID. This should be the mass number + 1000 * the atomic number.

2. AM Atomic mass, C-12 scale.

3. SIGS Resonance energy scattering cross section, barns.

4. SIGT Resonance energy total cross section, barns.

5. JRS Resonance nuclide identification. Not used, but must be present.
   0, no resonance data;
   1, resonance data.

6. MTS Multiple thermal scatter identifier. Enter 1. Not used, but must be present.

The resonance energy cross sections are averaged over the appropriate energy range for the nuclide. Items 1–6 are repeated for all nuclides. There should be a total of NNUC sets of entries. Entries should be made in order of increasing nuclide ID.

M14.2.5 ISOTOPIC DISTRIBUTION TABLE

1. NZN 1000 * atomic number of variable isotope elements.

2. NISO Number of isotopes in the default abundance.

3. ISZA Isotope ID.

4. ABWP Default abundance, atom percent.

The default abundance is generally the naturally occurring abundance. For each element, items 3 and 4 are repeated until 100% total abundance is described, making a set for this element. The next element is described in the same fashion in the next set, etc. There should be a total of NELV sets. The number of isotopes per element cannot exceed MXISEL.

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USER'S GUIDE FOR AMPX UTILITY MODULES

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ABSTRACT

The purpose of this section is to document selected AMPX-77 modules that can benefit the analyst interested in editing, converting, or combining cross-section libraries normally used by the SCALE system modules.

CONTENTS

M15.1 INTRODUCTION

Previous releases of the SCALE system did not include the utility modules discussed in this section, although in practice they perform invaluable operations for edit and special use of cross-section libraries in the SCALE system. For example, AIM is absolutely necessary to move the binary-formatted cross sections between different computer hardware. AJAX and WAX are modules to extract and combine sets of data from different libraries. ALE produces listings of data on cross-section libraries. ALPO converts SCALE cross sections to ANISN formats, whereas LAVA performs the reverse operation. RADE is a cross-section checking module that makes simple tests on SCALE cross-section libraries.

All of the modules in this section are shared by the SCALE and AMPX systems. Their input uses the FIDO procedures described in Sect. M10. In the descriptions on the following pages, the number of items to be input into an array is given in square brackets, []; the default values for parameters are given in parentheses, ( ). As with SCALE input data for its various calculational sequences, the input data for a module must be terminated by an "END" on a separate line.

M15.2 AIM—MODULE TO CONVERT MASTER CROSS-SECTION LIBRARIES FROM BCD TO BINARY FORMAT (OR VICE VERSA)

AIM (AMPX Interchangeable Masters) is a module whose primary purpose is to be able to pass AMPX master cross-section libraries between computers. All AMPX cross-section files are written in binary formats, which are not compatible between machines of different manufacturers. AIM has the capability to either read a binary-formatted master library and to "unload" it to the card image format or to read a file written in this same card image format and create a master library. Because all machines can read textual files, this file serves to transmit data between computers. Alternatively, it is possible, though not necessarily efficient, to use AIM to create a master library using card image input because a user can independently create data in the special card image format.

M15.2.1 AIM Input Data

Block 1

0$ Logical Unit Assignments [2]*
1. MBIN – Binary master (1)**
2. MBCD – BCD master (18)

1$ Option Selection Trigger [1]
1. IOPT
   0 – Binary to BCD conversion
   1 – BCD to binary conversion

2$ Data Edit Triggers [4]
1. IP1D (0)
   0 – No 1-D edit
   1 – Edit 1-D cross sections

2. IP2D (-1)
   -1 – No 2-D edit
   L – Edit through P_L of 2-D arrays

3. IPRES (0)
   0 – FIDAS print master library data as processed
   1 – FIDAS print suppressed

4. IPBOND Not used, enter zero (0)

T Terminate Block 1.

---

*The number of entries in the array is given in square brackets.
**Default values are given in parentheses.

If, and only if, the BCD data are to be read from cards, continue with the following input; otherwise, the input to AIM is complete. Note that the following input corresponds to the AMPX master interface specification (see Sect. F2.3.8).

Block M1

2$ Tape Identification [10]

1. IID – Library identification number
2. NNUC – Number of nuclides in this library
3. IGM – Number of neutron energy groups
4. IFTG – First thermal group
5. MSN – Nordheim treatment revision level required for this library. (A value of 2 is used when the cross sections are intended for NITAWL-II.)
6. IPM – Number of gamma-ray energy groups
7. I7 – Zero
8. I8 – Zero
9. I9 – Zero
10. I10 – Zero

T Terminate Block M1.

Five Title Cards, each in (20A4) format. The five cards of Hollerith information can be used to describe the library.

Block M2

Input Block M2 NNUC times.

TITLE card in (18A4) format. This information is the title for the nuclide.

3$ ID(19–50) Refer to the following table for a description of the ID(19), ID(20, ..., ID(50) entries. Note that floating-point entries can be entered using the 3* designation, whereas the integers are input in a 3$ array. Simply input both 3$ and 3* arrays, and use the "skip" or "address" options to make the input to the proper place in the array.

Word(s)	Item
1–18	18 words of text describing the set
19	Identifier of the set
20	Number of 6-parameter sets of resolved resonance data
21	Zero
22	Number of 1-D neutron processes
23	Number of 2-D neutron processes
24	Zero
25	Number of 1-D gamma processes
26	Number of 2-D gamma processes
27	Number of 2-D neutron-to-gamma processes

28	(Maximum order of scattering)*32768 + (total number of separate 2-D arrays for this set)
29	A - neutron equivalent mass number
30	ZA - 1000*Z + A
31	Zero
32	Zero
33	Zero
34	Power per fission in watt-s/fission
35	Energy release per capture in watt-s/capture
36	Maximum length of any 2-D record in the set
37	Number of sets of Bondarenko data
38	Number of σ_0s in Bondarenko data (the σ_0s are the background cross-section values)
39	Number of temperatures available in Bondarenko data
40	Maximum number of groups in Bondarenko data
41	Zero
42	Zero
43	σ_p–potential scattering cross section
44	Zero
45	ENDF MAT for fast neutron data
46	ENDF MAT for thermal neutron data
47	ENDF MAT for gamma data
48	ENDF MAT for gamma production data
49	Nuclide symbol (4 characters of text)
50	Number of records in this set

T Terminate Block M2.

Block M3

7* Neutron energy group boundaries. [IGM + 1] The group boundaries are input high to low in eV.

8* Gamma-ray group boundaries. [IPM + 1] The group boundaries are input high to low in eV.

T Terminate Block M3.

Follow with NNUC sets of Blocks M4–M15 data described as follows:

Block M4

TITLE card in (18A4) format. Use the same title card entered in data block M2 above for the nuclide title.

3$ ID(19–50) Enter the same data for the appropriate nuclide as described in block M2 above.

T Terminate Block M4.

Blocks M5, M6. Bondarenko data

If ID(37) > 0, enter the Bondarenko data.
In the following arrays, the array dimensions are taken from the ID values (3$ array).

ID(37) = NBOND, number of Bondarenko processes
ID(38) = NSIG0, number of σ_0 values
ID(39) = NTEMP, number of temperatures

Block M5

9* Bondarenko Table Ordinates [NTEMP + NSIG0 + 2]

Specify NSIG0 σ_0 values (high-to-low), followed by NTEMP temperatures in K (low-to-high), followed by ELO and EHI, the lower and upper limits of the energy range for which Bondarenko factors apply, respectively.

10$ Bondarenko Table Directory [6* NBOND]

The directory array consists of six strings of numbers, stacked one after the other. The first NBOND numbers are the process identifiers (MT-numbers); for example, 2 for elastic scattering and 18 for fission. (See Sect. F3.B for list of MT identifiers.) The next NBOND numbers are the first energy groups for which Bondarenko factors are given for each of the processes; the next NBOND numbers are the last energy group for which the factors are given. The fourth string will contain all zeroes, except for the case of self-shielding transfer matrices, in which case it contains the order of scattering for the process (i.e., 0 for P_0 terms, 1 for P_1, etc.). The fifth string will contain all zeroes except for transfer matrix shielding, in which case it contains the position of the term to be shielded, relative to the "magic word" in the transfer matrix array (e.g., for the case of only downscatter, a 1 would normally point to the within-group term, a 2 to the first downscatter term). The sixth string contains zeroes.

T Terminate Block M5.

Block M6

This data block will be repeated NBOND times. It consists of two arrays: the infinite dilution values for the process and the corresponding Bondarenko factors. Let NF be the first group for which Bondarenko data are given and NL be the last group. (These groups are taken from the second and third strings from the directory array discussed earlier.)

11* Infinite Dilution Cross Sections [NL – NF + 1]
(σ_{ID}(i), i = NF, NL)

12* Bondarenko Factors [NSIG0*NTEMP*(NL – NF + 1)]
(((BF(i,j,k),i = 1,NSIG0),j = 1,NTEMP),k = NF,NL)

T Terminate Block M6.

Block M7. Resonance Parameter and Other Neutron Cross-Section Data

In this block, the following definitions are used:

NRES = ID(20) = number of resolved resonances
N1D = ID(22) = number of temperature-independent averaged neutron cross sections
N2D = ID(23) = number of neutron-neutron scattering processes

13* Resonance data array; enter if NRES is nonzero
[6*NRES + 9]

The first nine words contain parameters used in both the resolved and unresolved resonance calculations:

1. A, the mass ratio for the isotope or mixture of isotopes
2. σ_p, the potential scattering cross section
3. Zero
4. NRES, the number of six-parameter resonance sets
5. s, a factor used in the Nordheim calculation to determine the range over which the calculation will be made
6. Zero
7. Zero
8. Zero
9. Zero

The next 6*NRES words consist of six-word sets of data used in the Nordheim calculation. The first six words are:

1. Zero
2. NBLK, the number of blocks of resolved data
3. Zero
4. Zero
5. TREF, the reference temperature at which the infinite dilution arrays on this library were calculated
6. Zero

Following these six words are NBLK six-word groups that are used to specify information concerning blocks of resonance data that apply to, for example, different isotopes, different energy regions, different kinds of data (s-wave or p-wave resonances), etc. These groups are stacked as follows:

1. AWRI, the mass ratio associated with the block of data
2. ABUN, the abundance for the block of data
3. NRE, the number of resonances in the block
4. ℓ, the value of spin for the resonances in the block
5. EL, the low-energy cut-off for resonances in the block
6. EH, the upper-energy cut-off for resonances in the block

After these NBLK groups of six words, the six-word sets of resonance parameters are arranged as follows:

1. E_0, the resonance energy
2. Γ_n, the neutron width of the resonance
3. Γ_γ, the gamma width of the resonance
4. Γ_f, the fission width of the resonance
5. r, a factor used in the Nordheim treatment for determining the range of calculation
6. g_J, the statistical factor for the resonance

The following chart illustrates the structure just described schematically:

	1	2	3	4	5	6
	0	NBLK	0	0	TREF	0
	$AWRI_1$	$ABUN_1$	NRE_1	ℓ_1	EL_1	EH_1
	$AWRI_2$	$ABUN_2$	NRE_2	ℓ_2	EL_2	EH_2
	.					
	.					
	.					
	$AWRI_{NBLK}$	$ABUN_{NBLK}$	NRE_{NBLK}	ℓ_{NBLK}	EL_{NBLK}	EH_{NBLK}
	E_0	Γ_n	Γ_γ	Γ_f	r	g
first	.	.	.	.	.	.
block	.	.	.	.	.	.
	.	.	.	.	.	.

14* Averaged neutron cross sections [N1D*(IGM + 1)]

Enter process identifier for first process followed by averaged cross sections for all groups (highest energy group to lowest); enter second process identifier followed by its cross sections, etc.

16$ Directory for Neutron-Neutron Scattering Data [N2D*4]

Enter the process identifiers for all processes (N2D values), followed by the corresponding length of the "magic-word" (Sect. M9) compressed arrays, followed by the order of the Legendre fit to each process, followed by the number of temperatures at which the cross sections for each process are given; that is,

$(MT_i, i = 1, N2D)$,
$(L_i, i = 1\ N2D)$,
$(NL_i, i = 1, N2D)$,
$(NT_i, i = 1, N2D)$.

T Terminate Block M7.

Blocks M8 and M9. Neutron-Neutron Scattering Matrices

Each scattering process has an M8 and M9 block. Processes where NL is greater than zero have NL + 1 repeats. When NT $\geq$ 1, the number of repeats is NT*(NL + 1). Data for all arrays for the first temperature are given first, etc.

Block M8. Parameters and Temperatures

17* Temperatures at which the cross sections are given [NT]

18$ Parameters [2]
1. NMW–number of "magic words" embedded in the transfer matrix
2. LPL – length of the compressed scattering matrix (including space for magic words)

T Terminate Block M8.

Block M9. Scattering Matrix

19$ Magic Words [NMW]. Specify the "magic words" that are included in the transfer matrix.

20* Scattering Matrix [LPL]. Specify the transfer matrix as in the master library format described below. Include zeroes in the positions that will contain magic words.

T Terminate Block M9.

Scattering Matrix Structure

This record type is used to store scattering matrix data (sometimes called 2-D data). As will be illustrated, it has provisions for truncating zero and/or impossible elements from the array. It exists in two forms: (1) a self-defining form used for gamma production data on a master library and (2) a form that is not self-defining. The only difference is that the self-defining form has the array length as the first word in the record, while the other does not; that is,

L, (X(I), I = 1, L)

or

(X(I), I = 1, L).

The structure of the X-array is as follows:

magic word for a group,
terms for scattering to the group,
magic word for the next group,
terms for scattering to this group,
etc.

In some cases, a negative or zero magic word is used to specify the end of data in the record.

A magic word is used to define:

1. the sink group number, III,
2. the first group number, JJJ, which scatters to group III, and
3. the last group number, KKK, which scatters to group III.

The magic word is then defined as

$$MW = 1000000*JJJ + 1000*KKK + III$$

such that it is composed of three 3-digit integers:

MW: JJJKKKIII

The scattering terms following a magic word are in reverse order (following the typical practice for transport theory programs); that is, the scattering term for scattering from the last group is first, etc.

MW for group III
σ(KKK → III)
σ(KKK - 1 → III)
.
.
.
σ(JJJ → III)

The scattering matrix record will contain one P_ℓ matrix for a process.

Consider an elastic scattering matrix for hydrogen that will be a full triangular matrix and assume three energy groups. The scattering matrix will look as follows:

1001001
σ(1 → 1)
1002002
σ(2 → 2)
σ(1 → 2)
1003003
σ(3 → 3)
σ(2 → 3)
σ(1 → 3)

Note that the record is a mixture of integer and real terms.

Data Blocks M10, M11, M12. Gamma-Production Data

These blocks are required only when N2DY[= ID(27)] is greater than zero, where N2DY is the number of processes requiring gamma production data.

Block M10. Gamma-Production-Data Directory

21$ Enter the gamma-production process identifiers [N2DY values], followed by the maximum length of the scattering matrices for a process, followed by the order of scattering for the processes, followed by a trigger (0/1-yields/cross sections) that specifies whether the gamma-production matrices are in cross section or yield units; that is,

$(MTY_i, i = 1, N2DY)$,
$(LY_i, i = 1, N2DY)$,
$(NLY_i, i = 1, N2DY)$,
$(NTY_i, i = 1, N2DY)$.

T Terminate Block M10.

Blocks M11, M12. Gamma-Production Data

These blocks are repeated NLY + 1 times for each gamma-production process. (Note that NLY is a function of the process.)

Block M11. Parameters

22$ Gamma-Production Matrix Parameters [2]
1. NWDY – number of magic words in the scattering matrix.
2. LPLY – length of the scattering matrix.

T Terminate Block M11.

Block M12. Scattering Matrix

23$ Magic Words [NMWY]

Specify the magic words that will be placed in the scattering matrix.

24* Scattering Matrix [LPLY]

Specify the scattering matrix. Enter zeroes in the words that will contain magic words.

T Terminate Block M12.

Blocks M13, M14, M15. Gamma-Ray Cross Sections

These blocks will only be used if either of the following two parameters is a nonzero value.

N1DZ = ID(25) = number of gamma-ray averaged cross sections
N2DZ = ID(26) = number of gamma-gamma scattering processes

Block M13. Gamma Cross Sections and Directories

25* Gamma Averaged Cross Sections [N1DZ*(IPM + 1)]

Specify the identifier for the first process, followed by its cross sections, followed by the second process identifier and its cross sections, etc.

26* Gamma-Gamma Scattering Directory [N2DZ*4]

Specify the identifiers of all scattering processes [N2DZ processes], followed by the lengths of the scattering matrices for the corresponding processes, followed by the orders of scattering for the processes, followed by a zero for each process; that is,

$(MTZ_i, i = 1, N2DZ)$
$(LZ_i, i = 1, N2DZ)$
$(NLZ_i, i = 1, N2DZ)$
$(NTZ_i, i = 1, N2DZ)$

T Terminate Block M13.

Block M14, M15. Gamma-Gamma Scattering Matrices

These blocks are repeated NLZ + 1 times for each of the gamma-ray scattering processes.

Block M14. Gamma Parameters

27$ Gamma-Gamma Matrix Size and Order
1. NMWZ – number of magic words in the scattering matrix
2. LPLZ – length of scattering matrix

T Terminate Block M14.

Block M15. Gamma Scattering Matrix

28$ Magic words [NMW2]

Specify the magic words for the scattering matrix.

29* Scattering Matrix [LPL2]

Specify the scattering matrix.

T Terminate Block M15.

M15.3 AJAX—MODULE TO MERGE, COLLECT, ASSEMBLE, REORDER, JOIN, AND/OR COPY SELECTED DATA SETS FROM AMPX MASTER INTERFACES

AJAX (Automatic Joining of AMPX X-Sections) is a module to combine data from AMPX master interfaces. Options are provided to allow merging from any number of files. You can even determine the final nuclide ordering by accessing the same file multiple times. Any form of master interface (neutron, gamma-ray, or neutron-gamma) can be accessed.

M15.3.1 AJAX Input Data

Block 1

-1$ Core Size [1]
1. LENG - Number of words to allocate to AJAX (100,000)

0$ Logical Unit Assignments [2]
1. MMT - Logical number of new library (default = 1)
2. NMAX - Not used

1$ Number of Files [1]
1. NFILE - Number of files to be used in constructing the new library. (When "reordering" operations are performed that required the same file to be accessed several times, each access is counted in determining the value of NFILE.)

T Terminate Block 1.

Blocks 2 and 3 are stacked, one after the other, NFILE times.

Block 2

2$ File and Option Selection [2]
1. NF - Logical unit number of file considered (A negative value for NF says to use the title information from this file on the library which will be written onto logical MMT; otherwise, the title is taken from the first file accessed.)
2. IOPT
   = -N Delete N nuclides from those on logical NF and add the others to the new file.
   = 0 Add all nuclides on logical NF to the new file.
   = +N Add N nuclides from logical NF to the new file.

   Note that in any case, once an identifier is used, all subsequent sets which use that identifier are skipped.

T Terminate Block 2.

Block 3 {Enter only when IOPT ≠ 0}

3$ Nuclides Selected [|IOPT|]

Identifiers of nuclides that are to be added or deleted from NF.

(When IOPT is +N, the use of a zero in the 3$ array says to select all nuclides from the file. If other identifiers are entered, they can be used to change the sets of data with these identifiers.)

4$ New Identifiers [|IOPT|] {Enter only if an identifier is to be changed.}

This array allows changing the identifier given in the 3$ array for the set of data on the new library. If a zero is entered in the 3$ array, a corresponding zero should be entered here.

T Terminate Block 3.

Note that AJAX operates sequentially to construct the new library. Once an identifier is selected for a nuclide on the new file, the occurrence of a set of data with that identifier on any new library will be ignored. Normally, the identifiers will remain the same as those used on the libraries from which data are selected. The 4$ array provides a way to override these identifiers.

M15.3.2 AJAX Input/Output (I/O) Specifications

The following devices are normally needed to execute AJAX:

Logical No.	Purpose
5	Card input
6	Standard output
15	Scratch device
16	Scratch device
18	Scratch device
19	Scratch device
MMT(1)	Master file to be created
NF	File(s) to be merged onto MMT

M15.4 ALE—MODULE TO LIST INFORMATION FROM MASTER OR WORKING LIBRARIES

ALE is a module that will produce listings of information contained on an AMPX master or working library. It also has provisions for controlling the spacing of the output.

M15.4.1 ALE Input Data

Block 1

0$ Logical assignments [2]
1. MMT – master library
2. MWT – working library

1$ Selection option [1]
1. NEDIT – number of nuclides for which listings are to be produced (a zero selects all nuclides on a library).

2$ Block edit option [10]
(A nonzero value selects editing the data.)
1. NLDN – 1-D neutron arrays
2. NLDG – 1-D gamma arrays
3. NRES – resonance data (including Bondarenko data)
4. IOPT4 – not used
5. IOPT5 – not used
6. IOPT6 – not used
7. IOPT7 – not used
8. IOPT8 – not used
9. IOPT9 – not used
10. ICORE – number of words allocated to this module (default = 50000)

3$ Block carriage control characters [25]

The entries have the following effect on how the header line for a particular kind of data is printed: all values are 0, by default, which says to skip a line before printing the block; a 1 can be used to start a block on a new page.)

1. Nuclide directory information
2. One-dimensional cross sections (absorption, fission, etc.)
3. Two-dimensional cross sections (scattering matrices)
4. Bondarenko data
5. Unassigned
6. Unassigned
7. Unassigned
8. Unassigned

9. Unassigned
10. Unassigned
11. Unassigned
12. Unassigned
13. Unassigned
14. Unassigned
15. Unassigned
16. Unassigned
17. Unassigned
18. Unassigned
19. Unassigned
20. Unassigned
21. Unassigned
22. Unassigned
23. Unassigned
24. Unassigned
25. Unassigned

4$ Scattering Matrices to be edited [100]

Enter the MT numbers of the processes for which edits are desired.

5$ Order of Scattering Matrices to be edited [100]

The 4$ and 5$ arrays are entered in one-to-one correspondence. The entries in the 5$ array give the maximum order of Legendre coefficient to be listed (e.g., a value of 2 would cause the P_0, P_1, and P_2 scattering matrices to be listed).

T Terminate Block 1.

Block 2 (Enter only if NEDIT > 0)

11$ Nuclide identifiers [NEDIT]

These are the identifiers for the nuclides for which listings are to be made.

T Terminate Block 2.

M15.4.2 ALE I/O Specifications

ALE requires the following I/O devices.

Logical No.	Purpose
5	Standard input
6	Standard output
MMT	Master library
MWT	Working library

M15.5 ALPO (ANISN LIBRARY PRODUCTION OPTION)

ALPO is a module for producing ANISN libraries from AMPX working libraries. Several working libraries can be accessed in a given run. The ANISN library can be produced in either binary or BCD format.

M15.5.1 ALPO Input Data

Block 1

-1$ Process Identifiers by Position in the ANISN Library [100].

This array can be used to override the normal arrangement of cross-section types in ANISN[1]-formatted libraries or can be used to produce special cross-section sets; for example, dose factor sets that contain several processes. The identifier for the process to be placed in row 1 of the ANISN tables is input first; row 2, second; etc. Note that nuclides that do not contain the processes noted in this table will revert to the normal ANISN ordering, namely, σ_T in position IHT, $\overline{\nu\sigma_f}$ in position IHT-1, etc.

0$ Logical Assignments [2]

1. MAN – logical unit for ANISN library (Use a 7 when a punched card output–textual–is desired.) (default = 20)
2. MAX – not used

1$ Primary Options [8]

1. NFILE – number of working libraries to be accessed
2. IHT – position of the total cross section in the ANISN tables (3)
3. IHS – position of the within-group cross-section in the ANISN tables IHT + IGM – IFTG + 1, where IGM is the number of neutron energy groups, and IFTG is the first thermal group
4. ITL – table length of the ANISN tables, IHS + IGM + IPM – 1, where IPM is the number of gamma-ray groups
5. MAXPL – the maximum order of scattering to be written on the ANISN library (20)
6. IOPT1D – option to print group averaged cross sections (0). A 1 selects printing
7. IOPT2D – option to print scattering matrices (0). A 1 selects printing.
8. ITRANS – transport correction option (0)
   - -N, truncate P_N and higher matrices and correct all lower ordered within-group terms by $2(2\ell + 1) \times \sigma_N(g \rightarrow g')/(2N + 1)$
   - 0, no transport correction
   - 1, replace σ_t with $\sigma_{tr} = \sigma_a + (1 - \mu)\sigma_s$, where μ is calculated by summing the P_1 matrix and dividing by the P_0 sum, or by $2/(3 \times A)$ when P_1 is not given.

   (The within-group term is also adjusted.)

T Terminate Block 1.

Data Blocks 2 and 3 are repeated NFILE times.

Block 2

2$ File Selection Options [2]
1. NF – logical number of the working library
2. IOPT – nuclide selection
   - –N, accept all nuclides from the working library except the N designated in the 3$ array below.
   - 0, accept all nuclides from the working library
   - +N accept all of the N nuclides from the working library that are designated in the 3$ array below.

T Terminate the data block.

Block 3 {IOPT ≠ 0}

3$ Nuclides to be selected or ignored [IIOPTI]

T Terminate the data block.

M15.5.2 ALPO I/O Specifications

The following devices are normally needed to execute ALPO:

Logical No.	Purpose
5	Card input
6	Standard output
7	Punched card output
14	Scratch device
MAN(20)	ANISN binary library
MAX(4)	AMPX working library

M15.6 CORECTOL—MODULE TO CONVERT PRE-AMPX-77 MASTER LIBRARIES TO THE AMPX-77 FORM

Prior to AMPX-77, the implementation of the Nordheim Integral Treatment in the NITAWL module assumed that the cross sections in the master library would be split into two parts:

1. cross sections for the bodies of the resonances (weighted over a reference spectrum), and
2. the wing cross sections, which included correction values, values for ℓ = 1, 2, etc., resonances (i.e., everything in the cross sections which the Nordheim calculation was not going to calculate)

This arrangement allows one to simply add these pieces together if an infinite dilution set is desired, or to perform a resonance self-shielding calculation and add the shielded values to the second set to obtain self-shielded values. This procedure requires that the processing code know exactly where the bodies of the resonances will be located, and, thereby, precludes the use of the Nordheim treatment with libraries not based on this knowledge.

It was recognized that a better way to implement the Nordheim treatment would be to reference the self-shielded values to infinite dilution values. The Nordheim calculation would then have to make two calculations: (1) the regular calculation, just as before, and (2) a calculation to weight the cross sections over a 1/E flux. The difference in the two values is then simply added to a reference infinite dilution set to obtain shielded values. This new approach has several advantages: (1) it allows the Nordheim calculation to be performed with any library that used 1/E weighting in the resonance range, a commonly used scheme; (2) it allows one to always refine (or unrefine) a calculation by adding (for example, ℓ = 1) or deleting resonance parameters; and (3) it inherently makes the procedure more accurate, since the difference is made using the same integration procedures.

Clearly, the library needed for the two approaches is different. The task of taking the earlier AMPX master libraries and converting them to the new format by adding together the resonance body values and the wing values and discarding the wing values is the purpose of the CORECTOL (CORrECT Old Libraries) module. It is a very simple module to use and requires essentially that the user define where the files are located. Obviously, CORECTOL has no counterpart module for converting newer libraries to the older form, as it is this complicated task that the newer procedures have been designed to eliminate.

M15.6.1 CORECTOL Input Data

Block 1.

-1$ Core Assignment [1]
1. ICORE – Number of words of core to assign to this module (100000)

0$ Logical Assignments [4]
1. NT1 – Old AMPX master (1)
2. NT2 – New AMPX master (2)
3. NS – Scratch device (18)
4. NT – Scratch device (19)

T Terminate Block 1.

M15.6.2 CORECTOL I/O Specifications

CORECTOL uses the following I/O devices:

Logical No.	Purpose
5	Card input
6	Printed output
NT1(1)	Old AMPX master library
NT2(2)	New AMPX master library
NS(18)	Scratch device
NT(19)	Scratch device

M15.7 LAVA—AMPX MODULE TO MAKE AN AMPX WORKING LIBRARY FROM AN ANISN LIBRARY

LAVA (Let ANISN Visit AMPX) is a module that can convert an ANISN library (neutron, gamma, or coupled neutron-gamma) to an AMPX working library that can be used in XSDRNPM. ANISN cross sections can be input on cards (fixed- or free-form FIDO format) or on a binary library.

M15.7.1 LAVA Input Data

Block 1

-1$ Core Allocation [1]

1. NWORD – number of words to allocate to LAVA (50000)

0$ Logical Definitions [6]

1. N1 – ANISN library (20)
2. N2 – AMPX working library (4)
3. N3 – Scratch (18)
4. N4 – Scratch (19)
5. N4 – Input (5)
6. N6 – Output (6)

1$ ANISN Library Parameter Data [8]

1. NNUC – Number of isotopes to be put on new library
2. IGM – Number of neutron groups
3. IHT – Position of σ_t
4. IHS – Position of σ_{g-g}
5. IHM – Table length
6. IFTG – First thermal group
7. IPM – Number of gamma groups
8. IFM – Format of ANISN library
   - -1, binary
   - 0, free-form BCD
   - 1, formatted BCD
9. IFLAG – A flag that selects the method for calculating scattering cross sections from scattering matrices–0 or 1 (default = 1). ANISN matrices are the sum of all the individual scattering matrices (elastic, inelastic, n2n, n3n, etc.) for processes possible for the particular nuclide. LAVA attempts to arbitrarily determine values for an elastic (MT = 2) and an n2n (MT = 16) cross section, recognizing that elastic scattering is generally the most dominant scattering process, and that n2n is the most common scattering process that yields more than a single exit neutron. To accomplish this, the absorption cross section in the ANISN data must be the true absorption value (not an energy absorption cross section as in some older gamma-ray sets or whatever alternative value). When IFLAG = 1, requiring the correct absorption, the elastic value is taken as

$$\sigma_{e\ell}^{g} = \sigma_{t}^{g} - \sigma_{a}^{g},$$

but the n2n is taken from

$$\sigma_{n,2n}^{g} = \sum_{g'} \sigma_{0}(g \rightarrow g') - \sigma_{e\ell}^{g} .$$

When IFLAG = 0, no attempt is made to calculate an n2n value and the elastic value is simply

$$\sigma_{\ell}^{g} = \sum_{g'} \sigma(g \rightarrow g') .$$

T Terminate Block 1.

Block 2

2$ Identifiers of the P_0 Block of Data for a Nuclide on the ANISN Library (see Ref. 1). [NNUC]

3$ Order of Scattering For the Nuclide on the ANISN Library [NNUC]

If an order of scattering for a nuclide is negative, the $P_\ell(\ell > 0)$ matrices for the nuclide will be multiplied by $(2\ell + 1)$ when they are written to the working library. This option is needed because Oak Ridge codes include the $(2\ell+1)$ factor in their cross sections, whereas almost no other code does.

4$ AMPX Identifiers for the Nuclides Selected From ANISN Library [NNUC]

5$ MT of each 1-D position in the ANISN Library [IHT]

The order is from position IHT to position 1. Note, MT numbers of frequently used data appearing in the 1-D positions are as follows:

Reaction	MT
σ_t	1
$\overline{\nu\sigma_f}$	1452
σ_a	27
$\bar{\nu}$	452
χ	1018
σ_f	18

6* Fission Spectrum [IGM]

If a nuclide has a nonzero fission cross section and either no fission spectrum (MT = 1018) is specified in the 1-D positions of the ANISN library or the fission spectrum flag for that nuclide has been appropriately set in the 9$ array, then the fission spectrum specified by the 6* array is included for that nuclide.

7* Neutron Energy Group Boundaries* [IGM + 1]

8* Gamma-Ray Energy Group Boundaries* [IPM + 1]

9$ Nuclide CHI Flags [NNUC]

0/1 – Use the fission spectrum from the ANISN library/use the fission spectrum from the 6* array

T Terminate Block 1.

M15.7.2 LAVA I/O Specifications

The following devices are normally needed in running the LAVA module:

Logical No.	Purpose
N2	AMPX working library written by LAVA (4)
N5	Card input (5)
N6	Standard output (6)
N3	Scratch device (18)
N4	Scratch device (19)
N1	ANISN library (20)

*Read high-to-low in energy (eV).

M15.8 MALOCS—MODULE TO COLLAPSE AMPX MASTER CROSS-SECTION LIBRARIES

MALOCS (Miniature AMPX Library Of Cross Sections) is a module to collapse AMPX master cross-section libraries. The module can be used to collapse neutron, gamma-ray, or coupled neutron-gamma master libraries.

M15.8.1 MALOCS Input Data

Block 1

-1$ Core Allocation [1]
1. NWORD – Number of words of core to allocate to MALOCS (100000)

0$ Case Description [6]*
1. NNEUT – Number of neutron fine groups
2. IGMF – Number of neutron broad groups
3. NGAMM – Number of gamma-ray fine groups
4. IPMF – Number of gamma-ray broad groups
5. IWN – Neutron weighting option (0)**
   - N1, Use the 1-D data identified with an MT number of IOPT2 (see 3$ array) from the IOPT1 master data set on logical unit N1 for the neutron weighting spectrum for all neutron data sets being collapsed.
   - 0, Input neutron weighting spectrum in the 5* array.
   - 1, Use MT=1099 1-D neutron data from each fine-group master data set for the neutron weighting spectrum.
6. IWG – Gamma-ray weighting spectrum option (0)
   - N2, Use the 1-D data identified with an MT number of IOPT6 from the IOPT5 master data set on logical unit N2 for the gamma-ray weighting spectrum for all gamma-ray data sets being collapsed.
   - 0, Input gamma-ray weighting spectrum in the 7* array.
   - 1, Use MT=1009 1-D gamma-ray data from each master data set for the gamma-ray weighting spectrum.

2$ Library Logical Unit Numbers [2]
1. NOLD – Logical number of device containing fine-group AMPX master library (1)
2. NNEW – Logical number of device containing broad-group AMPX master library (22)

*Number of entries in array.
**Default values are given in parentheses.

3$ Option Triggers [10]

1. IOPT1 – Auxiliary neutron weighting spectrum trigger (IWN = – N1) (0)
   - 0, No effect
   - ID, Identification number of master data set from which the neutron weighting spectrum (IOPT2 data) will be obtained
2. IOPT2 – Process identifier (MT number) of neutron weighting spectrum in IOPT1 master data set (used when IWN = – N1) (0)
3. IOPT3 – Trigger to print broad-group 1-D cross section (1)
   - 0, Print the data
   - 1, Do not print
4. IOPT4 – Trigger to print broad-group transfer matrices (1)
   - 0, Print the data
   - 1, Do not print
5. IOPT5 – Auxiliary gamma-ray weighting spectrum trigger (used when IWG = – N2) (0)
   - 0, No effect
   - ID, Identification number of master data set from which the gamma-ray weighting spectrum (IOPT6 data) will be obtained.
6. IOPT6 – Process identifier (MT number) of gamma-ray weighting spectrum in IOPT5 master data set (IWN = -N2) (0)
7. IOPT7 – Trigger to collapse out upscatter terms if nonzero (0). (A discussion of the available options is given in Section M15.8.3.)
   - 0, No upscatter truncation (recommended)
   - 1, XSDRNPM method of upscatter truncation
   - 2, ANISN method of upscatter truncation
   - 3, Simple sum method of upscatter truncation
   - 4, Non-negative ANSIN method of upscatter truncation.
8. IOPT8 – Trigger to truncate downscatters to a maximum of IOPT8 terms below the within group if IOPT8 is nonzero (0)
9. IOPT9 – Not used. Enter zero (0)
10. IOPT10 – Not used.

T Terminate Block 1.

Block 2

4$ Neutron broad-group numbers by fine group* [NNEUT]

5* Neutron weighting spectrum [NNEUT] {Enter only if IWN=0}

6$ Gamma-ray broad-group numbers by fine group** [NGAMM]

---

*A zero "suppresses" a fine group.

**When collapsing the gamma groups in a coupled master library, the 6$ entries are the actual group numbers and do not need to include the number of neutron groups.

7* Gamma-ray weighting spectrum [NGAMM] {Enter only if IWG=0}

T Terminate Block 2.

M15.8.2 MALOCS Input/Output Specifications

MALOCS generally requires the following input/output assignments:

Logical No.	Purpose
NOLD(1)	Fine-group AMPX master library
5	Card input
6	Standard output
17	Scratch device
18	Scratch device
19	Scratch device
NNEW(22)	Broad-group AMPX master library produced by MALOCS
N1(0)	Logical number of master library containing data that are to be used as a weighting spectra for neutron cross sections
N2(0)	Logical number of master library containing data that are to be used as weighting spectra for gamma-ray cross sections

M15.8.3 Upscatter Truncation

If one counts the option of "no upscatter truncation", MALOCS provides five different schemes for dealing with upscatters. We will preface our description of these options with the observation that the only desirable procedure is to *not* collapse out upscattering terms. Collapsing out these terms produces cross sections that work well in only two situations:

1. Satisfactory cross sections will be generated when the fluxes that are used to collapse the cross sections are very close to those in which these data will be used. In other words, if your application generates fluxes that are very different from those used to remove the terms, your results will be suspect.

2. If your application is not sensitive to what goes on in the thermal energy region, it may not matter what you do in that region. For example, if you are doing shielding calculations, the thermal range is rarely of any importance, such that carrying upscattering terms, along with the extra computational burden, may make it prudent to collapse out these terms.

MALOCS provides 4 options for upscatter truncation. These options are selected by inputing a value of 1 through 4 in IOPT7 in the 3$ array mentioned above. In describing these options, we will use the

convention of talking of a group i which is higher in energy than a group j. We are, therefore, setting the $\sigma(j \rightarrow i)$ terms to zero.

IOPT7=1 XSDRNPM Method

The rationale of this approach is to note that if we set a $\sigma(j \rightarrow i)$ term to zero, we can account for the loss of the scattering to group i by adjusting the within-group term by an amount $\sigma(j \rightarrow i)\ \phi(j) / \phi(i)$, i.e.;

$$\sigma(i \rightarrow i) * = \sigma(i \rightarrow i) + \sigma(j \rightarrow i)\ \phi(j) / \phi(i)$$

This approach has the advantage of never yielding negative values, so long as all the data used are physical. It also introduces few changes to the scattering matrices. A cosmetic drawback to the approach is that it obviously leaves the cross sections for groups i and j out-of-balance.

IOPT7=2 ANISN-Method

The rationale of this approach is to note that if we set a $\sigma(j \rightarrow i)$ term to zero, we can account for the loss of the scattering to group i by reducing the downscattering term $\sigma(i \rightarrow j)$ term by an amount $\sigma(j \rightarrow i)\ \phi(j) / \phi(i)$, i.e.;

$$\sigma(i \rightarrow j) * = \sigma(i \rightarrow j) - \sigma(j \rightarrow i)\ \phi(j) / \phi(i)$$

Because we have lost the upscattering from j to i, we must make the same adjustment to the within-group term to group i as made by the XSDRNPM method. But now we must also adjust the within-group term for group j to account for the reduction in the scattering from group i to group j.

$$\sigma(j \rightarrow j)* = \sigma(j \rightarrow j) + \sigma(j \rightarrow i)$$

This approach has the advantage of preserving the cross section balance in both energy groups, but sometimes yields negative downscattering values, which makes the numbers unusable for codes, such as the KENO and MORSE multigroup Monte Carlo codes.

IOPT7=3 Simple Sum Method

This is the simplest of the options provided. Here one simply increases the within-group term in group j by the upscattering term; i.e., we use the last expression shown in the ANISN Method just discussed. This has the advantage of preserving cross section balances, but it obviously does nothing to adjust the scattering source to group i for its lost contribution. In this case, the flux in group i is reduced, since it sees no source from group j, and, conversely, the flux in group j is increased, because it sees an additional within-group scattering source. This is, of course, somewhat offset, since the source from group i to group j is also reduced, because the flux in group i is reduced, which will reduce the flux in group j.

IOPT7=4 Non-Negative ANISN Method

This approach is the same as the ANISN approach, except in the case where a downscattering term goes negative. In this case, the downscattering term is set to zero, and the within-group term in group j is set to

$$\sigma(j \rightarrow j)^* = \sigma(j \rightarrow j) + \sigma(i \rightarrow j)\, \phi(i) / \phi(j).$$

This operation obviously does not preserve balance in either group, but it does attempt to adjust the scattering source to group j to account for the new zero term, and it will let Monte Carlo procedures use the data. This argument, along with noting that negative terms are only infrequently encountered in the ANISN scheme, can be used to justify its use.

Re-iteration of Caveat

As stated above, the whole area of truncating upscatters is questionable and should be used as a last resort, to avoid the calculational penalty associated with treating upscatters, or when the thermal region does not contribute to the results of your analysis.

M15.9 PERFUME—MODULE TO CORRECT LEGENDRE POLYNOMIAL FITS TO SCATTERING MATRICES

PERFUME (PERmute FaUlty Moment Expansions) is a module that examines scattering matrices to locate those matrices that yield nonphysical fits and adjusts them to produce acceptable distributions. The procedure involves an examination of the moments of the cross section, as described in Appendix F9.D.2 of the SCALE documentation. With these prescriptions, a range of possible coefficients is determined, after which PERFUME arbitrarily picks the value at the midpoint of the range.

M15.9.1 PERFUME Input Data

-1$ Core Assignment [1]

1. NWORD – Number of words to allocate to PERFUME (100000)

0$ Logical Assignments [3]

1. NTP – Input master library (23)
2. NOP – Output master library (1)
3. NER – Error message output file (6)

   Assign this to a unit other than 6 to suppress the voluminous error message listing that may be produced by some libraries, if you do not wish to view this information.

1$ Output Suppression Factor [1]

1. EPS – Information concerning bad moments is edited when the zeroeth moment of the transfer term (i.e., σ_0) satisfies the following expression (default = 0.0001):

$$\sigma_0 > \epsilon * N^3$$

   where N is the order of Legendre fit to the cross section. [Warning: For a library with a large number of energy groups and nuclides, the amount of output can be substantial.]

T Terminate Block 1.

M15.9.2 PERFUME I/O Specification

PERFUME uses the following I/O assignments:

Logical No.	Purpose
5	Card input
6	Printed output
NTP(23)	Input master library
NOT(1)	Output master library

M15.10 RADE—MODULE TO CHECK AMPX MASTER CROSS-SECTION LIBRARIES

RADE (Rancid AMPX Data Exposer) is provided to check AMPX- and ANISN-formatted multigroup libraries. It will check neutron, gamma, or coupled neutron-gamma libraries.

Some of the more important checks are made to ensure that:

1. $\sigma_t = \sigma_a + \sigma_s$
2. $\sigma_{in} = \Sigma\ \sigma_{in}^{partial}$
3. $\sigma_a = \sigma_c + \sigma_f$
4. $\sigma_c = \sigma_{n\gamma} + \sigma_{n\alpha} + \sigma_{np} + \sigma_{nd} + \ldots$
5. $\sigma_{el}^{g} = \sum_{g'} \sigma_{el,0}(g \rightarrow g')$ (also made on any process with a scattering matrix)
6. $\sigma_{0(g \rightarrow g')} > 0$
7. $\sigma_t, \sigma_a, \sigma_f, \sigma_{n\gamma}, \sigma_{np}, \ldots > 0$
8. $f_\ell^{min} \leq f_\ell(g \rightarrow g') \leq 1.0$

where $f_\ell(g \rightarrow g') = \dfrac{\sigma_\ell(g \rightarrow g')}{(2\ell + 1)\sigma_0(g \rightarrow g')}$

and $f_\ell^{min} = -1.0$ for all odd ℓ, and is given in the following table for even f:

ℓ	f_ℓ^{min}
2	-0.5
4	-
6	-0.419
8	-0.414

In addition to these checks, the code will compute an estimate of the capture-binding energy for each neutron group in a coupled neutron-gamma set. On option, one can request a display of differential cross sections.

M15.10.1 RADE Input Data

Block 1

-1$ Core Assignment [1]

1. NWORD – number of words to allocate RADE (100000)

1$ Checking Commands [4]

1. MMT – Check the AMPX Master Interface on logical MMT. This can be a neutron, gamma, or a coupled neutron-gamma library.
2. MWT – Check the AMPX Working Interface on logical MWT.
3. MAN – Check the ANISN binary-formatted library on logical MAN.
4. IFM – −1, ANISN library is binary formatted.
   0, ANISN library is BCD free form.
   1, ANISN library is BCD fixed form.

2$ Options [20]

1. IOPT1 – Number of angles at which a display of differential cross sections is desired. These angles will be equally spaced in the cosine range, −1 to +1. These edits are for the group-integrated cross sections and not for each group-to-group transfer.
2. IOPT2 – The ϵ, in thousandths of a percent, to which checks are made (e.g., IPT2 = 1) is equivalent to 0.001% checking. This is the default value when IOPT2 is not input or when a zero value is input.
3. IOPT3

   . Future checking options; skip or input zeros

20. IOPT20

3$ ANISN Options [7] {MAN ≠ 0}

1. NSET – Number of ANISN sets to check
2. IHT – Position of σ_t
3. IHS – Position of σ_{gg}
4. ITL – Table length
5. NL – Maximum order of scattering
6. IGM – Number of neutron groups
7. IPM – Number of photon groups

T Terminate Block 1.

Block 2 {Input only when MAN > 0}

4$ Identification Numbers of P_0 Sets on ANISN Binary Library on Logical MAN [NSET]

5$ Order of Scattering of Sets of ANISN Data on Logical MAN [NSET]

7* Neutron Group Structure, high-to-low in eV [IGM + 1]

8* Gamma Group Structure, high-to-low in eV [IPM + 1]

T Terminate Block 2.

M15.10.2 RADE I/O Specifications

RADE requires the following I/O assignments:

Logical unit	Purpose
5	Card input
6	Printed output
18	Scratch device
19	Scratch device
MMT	Master library
MWT	Working library
MAN	ANISN library

M15.11 WAX — MODULE TO MERGE, COLLECT, ASSEMBLE, RE-ORDER, JOIN, COPY SELECTED NUCLIDES FROM AMPX WORKING INTERFACES

WAX (Working Libraries AJAX) is a module to combine data on AMPX working libraries. Options are provided to allow merging from any number of files in a manner which allows the user to determine the final nuclide ordering, if desired.

M15.11.1 WAX Input Data

Block 1

-1$ Core assignment [1]
1. NWORD – Number of words to allocate to WAX (100000)

0$ Logical assignments [2]
1. MWT – Logical number of new library (default = 1)
2. NWAX – Not used

1$ Number of files [1]
1. NFILE – Number of files from which data will be selected from

T Terminate Block 1.

Blocks 2 and 3 are stacked, one after the other, NFILE times.

Block 2

2$ File and option selection [2]
1. NF – Logical number of file considered
2. IOPT* = -N Delete N nuclides from NF to create the new file on MWT
   = 0 Add all nuclides to the new file on MWT
   = N Add N nuclides from NF to create the new file on MWT

T Terminate Block 2.

Block 3 (Enter only when IOPT ≠ 0)

3$ Nuclides selected [|IOPT|]

Identifiers of nuclides which are to be added or deleted from NF

---

*Sets with duplicate identifiers will not be entered on MWT. The first occurrence of an identifier selects that set for the new library.

4$ New identifiers [IIOPTI]

This array allows changing the identifier given in the 3$ array when it is selected for the new library.

T Terminate Block 3.

M15.11.2 WAX I/O Specifications

The following devices are normally needed to execute WAX.

Logical unit	Purpose
5	Card input
6	Standard output
15	Scratch device
16	Scratch device
18	Scratch device
19	Scratch device
MWT(1)	Working file to be created
NF	File(s) to be merged onto MWT

M15.12 REFERENCE

1. W. W. Engle, Jr., *A User's Manual for ANISN*, USAEC Report K-1693, Union Carbide Corp., Nucl. Div., Oak Ridge Gaseous Diffusion Plant, March 1967.

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COMMENT DATA GUIDE

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ABSTRACT

The COMMENT program is a utility program that selectively tailors FORTRAN source code for different machines and operating systems.

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LIST OF TABLES

M16.1 INTRODUCTION

The COMMENT program is used to selectively tailor FORTRAN source code for different machines and operating systems.

M16.2 DESCRIPTION AND INPUT GUIDE

The COMMENT program is a utility program that selectively comments and uncomments lines of FORTRAN source code to provide a source code tailored to different machines and operating systems.

A list of comments and conversion types is given in Table M16.1.

Table M16.1. COMMENT language flags

	Conversion type							
Comment	IBM	VAX	MFE	LANL	UNIX	UNICOS	ULTRIX	AIX
CSHR	X	X			X		X	X
CLNG			X	X		X		
CIBM	X							
CUNI					X	X	X	X
CULT							X	
CUCS						X		
CAIX								X
CLANL				X				
CMFE			X					
CRAY			X	X		X		
CVAX		X						
CQOT	Protects the case of quoted strings between pairs of CQOT lines.							

The input/output (I/O) files utilized by COMMENT are listed below:

I/O File	Function
sysprint	Dataset containing error messages
sysin	Dataset specifying conversion type, ***(type)***
input	Dataset to be converted
output	Converted dataset

type is the desired conversion type, chosen from the following list:

type	Result
IBM	– Produces upper-case source tailored for MVS systems
VAX	– Produces upper-case source tailored for VAX
MFE	– Produces lower-case source tailored for CTSS on LLNL Cray
LANL	– Produces lower-case source tailored for CTSS on LANL Cray
UNIX	– Produces lower-case source tailored for UNIX
UNICOS	– Produces lower-case source tailored for UNICOS
ULTRIX	– Produces lower-case source tailored for ULTRIX
AIX	– Produces lower-case source tailored for AIX

To utilize COMMENT, compile and load the program into an executable and assign the I/O files as appropriate for the operating system.

COMMENT is called automatically when SCALE is made on a Unix workstation. The language flags must be set in the make configuration file. See the Unix README file distributed with SCALE for details.

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MISCELLANEOUS SCALE UTILITY MODULES

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ABSTRACT

This section documents several utility codes for performing different functions within SCALE. GENWGTS and GWAS were developed to generate KENO weights libraries. KMART is a postprocessor for KENOV.a that generates nuclide activity tables and collapses fluxes. Two utility programs, K5TOK6 and C5TOC6, are available for use in converting KENO V.a and CSAS input files to KENO-VI and CSAS6 format, respectively. The Q0RDPN program is a utility program used to convert FIDO-type binary input files to ASCII format. AWL, MAL, and WGT convert AMPX working format libraries, KENO albedo libraries, and KENO weights libraries, respectively, between ASCII and binary formats.

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M17.1 GENWGTS

M17.1.1 INTRODUCTION

GENWGTS is a program to read the balance tables from an XSDRNPM adjoint calculation, and convert the fluxes to weights for use in a KENO reflector. It produces a weighting library by writing the weights in a format suitable for use with the WGT code.

M17.1.2 DESCRIPTION AND INPUT GUIDE

GENWGTS is a functional module written to convert adjoint XSDRNPM fluxes from the balance table into weights for use by KENO. It was written to primarily function as a module under the GWAS control module, but is capable of being run standalone. Because it was primarily designed to perform a single function in a control sequence, it has some limiting assumptions built in. The first two zones must be fuel zones, the second zone is a constant width. The input to GENWGTS consists of a record with three numbers to be read as list directed input. The input/output (I/O) units utilized by GENWGTS are given in the table below.

I/O File Number	Filename	Function
6	_prt*nnnn*[a]	Messages
5	ingenwgt	Program Input
7	_pun*nnnn*[a]	Weights Output
NB	ft*nb*f001[b]	Balance Table Unit Number

[a]"*nnnn*" is numbered sequentially beginning with 0000.
[b]"*nb*" is a two-digit representation of NB.

The input consists of the following three items.

NB	Unit number from which the balance tables are read
NUMINC	Number of intervals for weights
THICK	Thickness of an interval

M17.2 GWAS

M17.2.1 INTRODUCTION

GWAS is a program that creates a set of weights for a reflector for use by the KENO series of codes. It uses input similar to other SCALE control modules, and generates weights for a series of user specified cross section libraries. GWAS generates the weights by running an adjoint XSDRNPM case, and then using the adjoint fluxes to produce the weights.

M17.2.2 DESCRIPTION AND INPUT GUIDE

GWAS is a utility control program for generating sets of reflector weights for the KENO series of codes. It runs an adjoint XSDRNPM, and uses adjoint fluxes to generate the weights. It produces weights for a user specified series of cross section libraries. The input to GWAS starts with a title record, which is followed by a record of data defining the geometry to be used for generating the weights. This data is then followed by the mixture definitions, input in standard SCALE materials input format. This data is followed by a series of double records. The first record of each series is used to define whether or not this is the last pair in the series, the second record contains the cross section library name for which a set of weights is to be generated. The input/output (I/O) files utilized by GWAS are given below.

I/O File Number	Filename	Function
6	_prt*nnnn*[a]	Messages
94	input	Program Control Input
5	infile	Scratch File where input sequences are constructed
92	savefile	Scratch File where data is saved between passes
95	ingenwgt	Input File for GENWGTS
96	ft96f0001	Input File for BONAMI
97	ft97f001	Input File for NITAWL
98	ft98f001	Input File for XSDRNPM
7	_pun*nnnn*[a]	Output File containing the new Weights
11	ft11f001	File containing the Short Cross Section Library
8	ft08f001	Scratch random access unit
16	ft16f001	Scratch Unit
17	ft17f001	Scratch Unit used in Collapsing the Cross Sections
18	ft18f001	Scratch Unit
19	ft19f001	Scratch Unit used in Collapsing the Cross Sections
89	ft89f001	Standard Composition Library

[a]"*nnnn*" is numbered sequentially beginning with 0000.

The input to GWAS consists of two types of data blocks. The first data block is read only once, and defines everything about the problem except the cross section library. The second data block is repeated as often as the user needs, and defines the cross section library to be used for a particular set of weights. The data for the first data block is given below.

TITLE — an 80 character title to identify the problem output

CALTYPE — up to 12 characters identifying the type of geometry to be used in doing the adjoint calculation. This is read in freeform, and must be enclosed in single quotes.

IDWGT — the identification number to be assigned to the weights. This is the number used by KENO to select a set of weights. This number is an integer read in free form.

THICK — the interval thickness of reflector material for a set of weights. One weight for each group will be generated for an interval.

NUMINC — number of intervals for which a set of weights will be generated. The total reflector thickness will be NUMINC*THICK. One extra interval will be added to the outside of the reflector to reduce effect of leakage on the weights.

HALFFUEL — the radius or half thickness of the fuel zone that will be used as a source for generating the weights. XSDRNPM will use this as a first guess, and search for a radius or half thickness that yields a user specified k_{eff} (the default is 1.0).

WTTITL — up to 12 characters used as identification for the weights.

Standard Composition Data - data defining the mixtures in the problem in standard SCALE material information format, ending with the keywords END COMP. Mixture 1 will be used for the fuel, and mixture 2 will be used as the reflector material. This completes data block 1, which is then terminated with a record containing the keyword END.

The second data block has a record flagging whether or not there will be more data blocks after this one. If more data blocks will follow, then the record should be blank. If it is the last data block, then the first 8 characters of the record must contain the keyword LAST. The next record then contains the cross section library name to be used to generate the next set of weights.

M17.2.3 SAMPLE CASE

```
#shell
ln -fs $DATA/scale.rev04.xn218 ft70f001
end
#gwas
generate weights for a concrete slab
'slab' 301 5. 20 0.25 'concrete'
uranium 1 1 300 92235 100   end
mgconcrete 2 end
end comp
end

hansen-roach
end

27group
end

44group
end

last
218group
end
#clec_out
end
#gwas
generate weights for a graphite slab
'slab' 6100 20. 10 0.001 'graphite'
uranium 1 1 300 92235 100 end
c-12 2 den=2.2 end
end comp
end

hansen-roach
end

27group
end

44group
end

218group
end
last
238group
end
```

M17.3 KMART - KENO V.a POSTPROCESSOR

M17.3.1 INTRODUCTION

KMART (Keno Module for Activity-Reaction Rate Tabulation) is a new module whose primary purpose is to postprocess a KENO V.a restart file with the corresponding working cross section library to generate nuclide activity tables. It also allows collapsing and printing fluxes calculated by KENO V.a. The KENO V.a problem must have a mixing table, must calculate the fluxes, and must write a restart file containing the calculated data.

M17.3.2 KMART INPUT DATA

Input data for KMART is read into the program using free form blocked input similar to KENO V.a. The data blocks are started with a READ *BLOCK NAME* and ended with an END *BLOCK NAME*. There are three data blocks that KMART can read. The first data block is named INITIAL, and the input starts with the keywords READ INITIAL. There are three possible keyworded entries in this block that may be entered in any order.

Keyword	Variable	Description
PRTVOLS	PRINT_VOLUMES	a flag to cause the volumes calculated by KENO V.a to be printed by KMART.
KUNIT=	KUNIT	The logical unit number of the KENO V.a restart file.
XUNIT=	XUNIT	The logical unit number of the cross section library.

A sample data block is given below.

```
READ INITIAL   KUNIT=35 XUNIT=4   END INITIAL
```

One of the next two blocks is required, but it could be either one, or both can be specified if desired. If both are entered, they can be either one first. The next data block specified is named ACTIVITY, and the input starts with the keywords READ ACTIVITY. It contains the data specifying which activities are to be calculated. The activities are specified by pairs of numbers giving the nuclide identifier and the reaction type identifier desired. A list of reaction types, also known as MT numbers, can be found in Sect. F3.B. These pairs are repeated until all the desired activities have been specified. If the nuclides are identified by the SCALE scheme, then the nuclide can be specified most explicitly by using the mixture prefix defined by CSAS, or, by omitting the mixture prefix, the activity will be calculated for each region in which the nuclide occurs. If the nuclide specifies a natural element identifier (1000*Z) and individual isotopes occur on the cross section library, the isotope activities will be summed to produce the total activity for the element. The data pair is described below.

Variable	Description
NUCLIDE	The nuclide identification number on the cross section library for this activity request.
REACTION	The reaction type identifier for this activity request.

If no activities are desired, then the block can be omitted. A sample block is given below.

```
READ ACTIVITY 92235 18 92235 27 92235 1452  END ACTIVITY
```

The other input block is named COLLAPSE, and starts with the keywords READ COLLAPSE. There are two keyworded entries that may be input in this block. A flux factor to normalize the fluxes by can be specified. It defaults to 1. The last fine group in the current broad group is the other entry. The broad groups are specified sequentially starting with group one. If the flux factor is specified more than once, the last value given is used. The data is specified as below.

Keyword	Variable	Description
FACTOR	FACTOR	A flux multiplier used to scale the fluxes before printing (default 1.0)
LASTG=	LAST_GROUP	The last fine group to be included in the current broad group. The broad groups are input sequentially starting with group one.

If no collapsed fluxes are desired, then the block can be omitted. A sample block is given below.

```
READ COLLAPSE  FACTOR 1.0 LASTG=10 LASTG=20 LASTG=30 LASTG=44  END COLLAPSE
```

M17.3.3 KMART I/O SPECIFICATIONS

KMART requires the following I/O devices.

Logical Unit	Purpose
5	Standard definition input
6	Output
KUNIT	KENO V.a restart file
XUNIT	AMPX working cross section library
16	scratch file

The following is a sample input data stream for KMART:

```
#kmart
read initial   kunit=64 xunit=4 prtvols   end initial
read activity
    1001 27
    6012 27
    8016 27
   92235 18 92235 27 92235 1452
   92238 18 92238 27 92238 1452
   94238 18 94238 27 94238 1452
   94239 18 94239 27 94239 1452
   94240 18 94240 27 94240 1452
   94241 18 94241 27 94241 1452
   94242 18 94242 27 94242 1452
   92000 18 92000 27 92000 1452
   94000 18 94000 27 94000 1452
 end activity
read collapse    lastg=10 lastg=20 lastg=30 lastg=44
 end collapse
end
```

M17.4 K5TOK6 AND C5TOC6: INPUT FILE CONVERSION PROGRAMS FOR KENO AND CSAS

M17.4.1 INTRODUCTION

Program K5TOK6 can be used to automatically convert a KENO V.a input file to a KENO-VI input file. Program C5TOC6 can be used to automatically convert a CSAS input file to a CSAS6 input file. This functionality can be useful when converting a KENO V.a validation sequence to a KENO-VI validation sequence. It removes the problem of introducing a mistake or inadvertently changing the data when remodeling a geometry to the KENO-VI format. For some cases, however, the converted model may be a very inefficient KENO-VI model.

M17.4.2 DESCRIPTION AND INPUT GUIDE

Program K5TOK6 is a utility program that can be used to automatically convert a KENO V.a input file to a KENO-VI input file. Program C5TOC6 is a utility program that can be used to automatically convert a CSAS input file to a CSAS6 input file. For program K5TOK6, the "=KENOVA" record in the input stream is replaced by "=K5TOK6". The output file is then named _geom*nnn* where *nnn* is a unique 3-digit number. This allows a string of KENO V.a problems to be converted in one job. For program C5TOC6 the "=CSAS*BB*" record in the input stream (where the *BB* is 25 or 2x) is replaced by "=C5TOC6 PARM=CSAS*BB*", where PARM begins in column 11 or later, with optionally a SIZE field. The output file is named _geom*nnn* where *nnn* is a unique 3-digit number.

For large problems, the output file may need to be edited to specify an increased value for parameter *NB8* in KENO-VI and also an increased value for parameter *DAB* in CSAS6. **The conversion makes no attempt to optimize the output file, so it almost surely will be inefficient in its use of storage, and in its use of bodies. This can lead to models that are very inefficient in their running time also.**

The input/output (I/O) files for K6TOK6 and C5TOC6 are given below. Note that K5TOK6 requires the cross-section library designated by the "LIB=" parameter in the KENO V.a input file.

I/O File	Function
5	KENO V.a (or CSAS) input file
6	Output
7	Input file generated for KENO-VI (or CSAS6)

Sample K5TOK6 Problem

```
#k5tok6
93.2% uo2f2 h/u-235=337
read param    npg=600 fdn=yes nub=yes  lib=4  end param
read geom
cuboid      1 1 2p3.81 2p60.325 25.50 0
reflector   2 1 4r.318 0 .318 1
cuboid      0 1 2p4.128 2p65. 150. -1.
core 0  1 -12.384 -65. -29.
cylinder  0 1 142.8 212. -60.
cylinder  3 1 144.8 212. -62.
```

```
cuboid    0 1 275.5 -638.9 475. -744.2 588. -62.
reflector 4 1 5r0 .32 1
reflector 5 1 5r0 1.27 1
reflector 3 1 5r0 .64 1
reflector 0 1 5r0 365 1
reflector 6 2 6r5 6
reflector 6 8 0 5 4r0 6
end geom
read bias id=301 2 13 end bias
read array nux=3 nuy=1 nuz=1 end array
end data
end
#shell
cp _geom000 $RTNDIR/k6.inp
end
```

Sample Converted KENO-VI Input File

```
#kenovi
93.2% uo2f2 h/u-235=337
read param    npg=600 fdn=yes nub=yes  lib=41  end param
read geometry
unit          1
cuboid     1
              3.810000E+00 -3.810000E+00  6.032500E+01
             -6.032500E+01  2.550000E+01  0.000000E+00
media      1    1       1
cuboid     2
              4.128000E+00 -4.128000E+00  6.064300E+01
             -6.064300E+01  2.550000E+01 -3.180000E-01
media      2    1       2  -1
cuboid     3
              4.128000E+00 -4.128000E+00  6.500000E+01
             -6.500000E+01  1.500000E+02 -1.000000E+00
media      0    1       3  -2  -1
boundary     3
global
unit          2
cuboid     1
              1.238399E+01 -1.238399E+01  6.499993E+01
             -6.499993E+01  1.219999E+02 -2.899997E+01
array      1       1
               place 1 1 1  -8.256000E+00  0.000000E+00 -2.800000E+01
cylinder   2
              1.428000E+02  2.120000E+02 -6.000000E+01
            origin   x=  0.000000E+00   y=  0.000000E+00
media      0    1       2  -1
cylinder   3
              1.448000E+02  2.120000E+02 -6.200000E+01
            origin   x=  0.000000E+00   y=  0.000000E+00
media      3    1       3  -2  -1
cuboid     4
              2.755000E+02 -6.389000E+02  4.750000E+02
             -7.442000E+02  5.880000E+02 -6.200000E+01
media      0    1       4  -3  -2  -1
cuboid     5
              2.755000E+02 -6.389000E+02  4.750000E+02
             -7.442000E+02  5.880000E+02 -6.232000E+01
media      4    1       5  -4  -3  -2  -1
cuboid     6
              2.755000E+02 -6.389000E+02  4.750000E+02
             -7.442000E+02  5.880000E+02 -6.359000E+01
```

```
media      5    1       6  -5  -4  -3  -2  -1
cuboid     7
              2.755000E+02 -6.389000E+02  4.750000E+02
             -7.442000E+02  5.880000E+02 -6.423000E+01
media      3    1       7  -6  -5  -4  -3  -2  -1
cuboid     8
              2.755000E+02 -6.389000E+02  4.750000E+02
             -7.442000E+02  5.880000E+02 -4.292300E+02
media      0    1       8  -7  -6  -5  -4  -3  -2  -1
cuboid     9
              2.805000E+02 -6.439000E+02  4.800000E+02
             -7.492000E+02  5.930000E+02 -4.342300E+02
media      6    2       9  -8  -7  -6  -5  -4  -3  -2  -1
cuboid    10
              2.855000E+02 -6.489000E+02  4.850000E+02
             -7.542000E+02  5.980000E+02 -4.392300E+02
media      6    3      10  -9  -8  -7  -6  -5  -4  -3  -2  -1
cuboid    11
              2.905000E+02 -6.539000E+02  4.900000E+02
             -7.592000E+02  6.030000E+02 -4.442300E+02
media      6    4      11 -10  -9  -8  -7  -6  -5  -4  -3  -2  -1
cuboid    12
              2.955000E+02 -6.589000E+02  4.950000E+02
             -7.642000E+02  6.080000E+02 -4.492300E+02
media      6    5      12 -11 -10  -9  -8  -7  -6  -5  -4  -3  -2  -1
cuboid    13
              3.005000E+02 -6.639000E+02  5.000000E+02
             -7.692000E+02  6.130000E+02 -4.542300E+02
media      6    6      13 -12 -11 -10  -9  -8  -7  -6  -5  -4  -3  -2  -1

cuboid    14
              3.055000E+02 -6.689000E+02  5.050000E+02
             -7.742000E+02  6.180000E+02 -4.592300E+02
media      6    7      14 -13 -12 -11 -10  -9  -8  -7  -6  -5  -4  -3  -2
             -1
cuboid    15
              3.055000E+02 -6.739000E+02  5.050000E+02
             -7.742000E+02  6.180000E+02 -4.592300E+02
media      6    8      15 -14 -13 -12 -11 -10  -9  -8  -7  -6  -5  -4  -3
             -2  -1
cuboid    16
              3.055000E+02 -6.789000E+02  5.050000E+02
             -7.742000E+02  6.180000E+02 -4.592300E+02
media      6    9      16 -15 -14 -13 -12 -11 -10  -9  -8  -7  -6  -5  -4
             -3  -2  -1
cuboid    17
              3.055000E+02 -6.839000E+02  5.050000E+02
             -7.742000E+02  6.180000E+02 -4.592300E+02
media      6   10      17 -16 -15 -14 -13 -12 -11 -10  -9  -8  -7  -6  -5
             -4  -3  -2  -1
cuboid    18
              3.055000E+02 -6.889000E+02  5.050000E+02
             -7.742000E+02  6.180000E+02 -4.592300E+02
media      6   11      18 -17 -16 -15 -14 -13 -12 -11 -10  -9  -8  -7  -6
             -5  -4  -3  -2  -1
cuboid    19
              3.055000E+02 -6.939000E+02  5.050000E+02
             -7.742000E+02  6.180000E+02 -4.592300E+02
media      6   12      19 -18 -17 -16 -15 -14 -13 -12 -11 -10  -9  -8  -7
             -6  -5  -4  -3  -2  -1
cuboid    20
              3.055000E+02 -6.989000E+02  5.050000E+02
             -7.742000E+02  6.180000E+02 -4.592300E+02
```

```
media     6   13      20 -19 -18 -17 -16 -15 -14 -13 -12 -11 -10  -9  -8
                      -7  -6  -5  -4  -3  -2  -1
boundary    20
end geometry

read bias id=301 2 13 end bias
read array nux=3 nuy=1 nuz=1 end array
end data
end
```

Sample C5TOC6 Problem

```
#c5toc6     parm='csas25,size=500000'
tmi 1500 ppm boron
27groupndf4  latticecell
uo2         1 .925    583 92235 1.98 92238 98.02 end
uo2         2 .925    583 92235 2.64 92238 97.36 end
uo2         3 .925    583 92235 2.96 92238 97.04 end
zircalloy   4 1.0     583 end
arbmcrod        10.17 5 0 0 1
47107 41.088 47109 38.912 49113 0.632 49115 14.368 48000 5.0
            5 1.0     583 end
ss304       6 1.0     583 end
arbmpois1         3.70 2 0 1 0 13027 2 8016 3
            7 0.97952 583 end
b4c         7 2.048-2 583 end
arbmpois2         3.70 2 0 1 0 13027 2 8016 3
            8 0.98150 583 end
b4c         8 1.85-2  583 end
arbmpois3         3.70 2 0 1 0 13027 2 8016 3
            9 0.98444 583 end
b4c         9 1.556-2 583 end
arbmbacid     8.5788-3 3 1 1 0 5000 1 1001 3 8016 3
           10 .7707   583 5010 18.32 5011 81.68 end
h2o        10 .7707   583 end
end comp
squarepitch  1.44272 .9398 3 10 1.0922 4 .97536 0 end
more data
res=1 cylinder   .4699   dan(1)=0.2858256
res=2 cylinder   .4699   dan(2)=0.2858256
res=5 cylinder   .5588
end more
tmi critical core  1500wppm-11/83 (fn=critical)--ti-2   583 deg kelvin   homog.
read param  plt=yes  gen=203 npg=500 tme=120 end param
read geom
unit 20
com='layer 2 oriface rod unit'
cylinder     6 1   .60906  210.34 -210.34
cuboid      10 1 4p0.72136 210.34 -210.34
unit 21
com='layer 2 2.96% enr. fuel rod'
cylinder     3 1 .4699   2p182.88
cylinder     0 1 .48768  2p182.88
cylinder     0 1 .48768    199.84 -206.24
cylinder     4 1 .5461     199.84 -206.24
cylinder     6 1 .5461     210.34 -210.34
cuboid      10 1 4p0.72136 210.34 -210.34
unit 22
com='layer 2 2.64% enr. fuel rod'
cylinder     2 1 .4699   2p182.88
cylinder     0 1 .48768  2p182.88
cylinder     0 1 .48768    199.84 -206.24
cylinder     4 1 .5461     199.84 -206.24
```

```
cylinder     6 1 .5461     210.34 -210.34
cuboid      10 1 4p0.72136 210.34 -210.34
unit 23
com='layer 2 1.98% enr. fuel rod'
cylinder     1 1 .4699   2p182.88
cylinder     0 1 .48768  2p182.88
cylinder     0 1 .48768    199.84 -206.24
cylinder     4 1 .5461     199.84 -206.24
cylinder     6 1 .5461     210.34 -210.34
cuboid      10 1 4p0.72136 210.34 -210.34
unit 25
cylinder     5 1 .5588    2p45.72
cylinder     6 1 .6121     210.34  -49.82
cylinder     0 1 .6121     210.34 -210.34
cuboid      10 1 4p.72136 2p210.34
unit 26
com='layer 2 1.395% lumped burnable poison rod (lbp1)'
cylinder     7 1 .5461   2p160.02
cylinder     0 1 .5461     260.4875 -160.02
cylinder     4 1 .635      260.58   -160.10
cuboid      10 1 4p0.72136 260.58   -160.10
unit 27
com='layer 2 1.260% lumped burnable poison rod (lbp2)'
cylinder     8 1 .5461   2p160.02
cylinder     0 1 .5461     260.4875 -160.02
cylinder     4 1 .635      260.58   -160.10
cuboid      10 1 4p0.72136 260.58   -160.10
unit 28
com='layer 2 1.060% lumped burnable poison rod (lbp3)'
cylinder     9 1 .5461   2p160.02
cylinder     0 1 .5461     260.4875 -160.02
cylinder     4 1 .635      260.58   -160.10
cuboid      10 1 4p0.72136 260.58   -160.10
unit 29
com='layer 2 central water unit in each assembly (instrumentation)'
cuboid      10 1 4p0.72136 260.58   -160.10
'.....................................................................
com='z-layer 2--intact pins--no rubble'
unit 231
com='layer 2 2.96% enr. fuel and orfice rod assembly'
array       20   -10.824   -10.824  -210.34
cuboid      10 1 4p10.90549        2p210.34
unit 232
com='layer 2 2.96% enr. fuel and control rod assembly--out'
array       21   -10.824   -10.824  -210.34
cuboid      10 1 4p10.90549        2p210.34
unit 233
com='layer 2 2.64% enr. fuel and 1.395% lbp1 rod assembly'
array       22   -10.824   -10.824  -210.34
cuboid      10 1 4p10.90549        2p210.34
unit 234
com='layer 2 2.96% enr. fuel and 1.260% lbp2 rod assembly'
array       23   -10.824   -10.824  -210.34
cuboid      10 1 4p10.90549        2p210.34
unit 235
com='layer 2 1.98% enr. fuel and control rod assembly--out'
array       24   -10.824   -10.824  -210.34
cuboid      10 1 4p10.90549        2p210.34
unit 236
com='layer 2 2.64% enr. fuel and 1.260% lbp2 rod assembly'
array       25   -10.824   -10.824  -210.34
cuboid      10 1 4p10.90549        2p210.34
unit 237
com='layer 2 2.64% enr. fuel and 1.060% lbp3 rod assembly'
```

```
array       26   -10.824   -10.824  -210.34
cuboid      10 1 4p10.90549        2p210.34
unit 238
com='layer 2 1.98% enr. fuel and axial power shaping rod assembly--out'
array       27   -10.824   -10.824  -210.34
cuboid      10 1 4p10.90549        2p210.34
unit 239
com='layer 2 2.64% enr. fuel and control rod assembly--out'
array       28   -10.824   -10.824  -210.34
cuboid      10 1 4p10.90549        2p210.34
'.....................................................................
'.....................................................................
unit 300
array       30  -54.52745  -21.81098 -210.34375
cuboid       6 1 2p54.528    21.811    -23.716   2p210.3438
unit 310
array       31  -54.52745  -21.81098 -210.34375
cuboid       6 1 2p54.528    23.716    -21.811   2p210.3438
unit 320
array       32  -21.81098  -10.90549 -210.34375
unit 330
array       33  -21.81098  -54.52745 -210.34375
cuboid       6 1 21.811     -23.716   2p54.528   2p210.3438
unit 340
array       34  -21.81098  -54.52745 -210.34375
cuboid       6 1 23.716     -21.811   2p54.528   2p210.3438
unit 350
array       35 -10.90549   -21.81098 -210.34375
com='units for ss core form'
unit 400
cuboid       6 1 2p11.85     2p.9525 2p210.34
unit 410
cuboid       6 1 2p.9525   2p20.85   2p210.34
unit 420
cuboid       6 1 2p.9525    2p9.94   2p210.34
unit 430
cuboid       6 1 2p22.76     2p.9525 2p210.34
unit  440
cuboid       6 1 2p.9525   2p10.91   2p210.34
unit 500
array      100  -119.961  -119.961   -210.34
cylinder    10 1   179.07 2p220.34
hole 300     0.0    -141.78    0.0
hole 310     0.0     141.78    0.0
hole 320   -76.34   -130.87    0.0
hole 320    76.34   -130.87    0.0
hole 320   -76.34    130.87    0.0
hole 320    76.34    130.87    0.0
hole 330  -141.78      0.0     0.0
hole 340   141.78      0.0     0.0
hole 350  -130.87     76.34    0.0
hole 350   130.87     76.34    0.0
hole 350  -130.87    -76.34    0.0
hole 350   130.87    -76.34    0.0
hole 400 -153.65     -55.50    0.0
hole 400  153.65     -55.50    0.0
hole 400 -153.65      55.50    0.0
hole 400  153.65      55.50    0.0
hole 400  131.84     -99.13    0.0
hole 400 -131.84     -99.13    0.0
hole 400  131.84      99.13    0.0
hole 400 -131.84      99.13    0.0
hole 400 -110.03     120.93    0.0
hole 400  110.03     120.93    0.0
```

```
hole 400 -110.03    -120.93    0.0
hole 400  110.03    -120.93    0.0
hole 410  142.74     -77.31    0.0
hole 410 -142.74     -77.31    0.0
hole 410  142.74      77.31    0.0
hole 410 -142.74      77.31    0.0
hole 420  120.92    -110.03    0.0
hole 420 -120.92    -110.03    0.0
hole 420  120.92     110.03    0.0
hole 420 -120.92     110.03    0.0
hole 420   99.11    -131.83    0.0
hole 420  -99.11    -131.83    0.0
hole 420   99.11     131.83    0.0
hole 420  -99.11     131.83    0.0
hole 430   77.29    -142.74    0.0
hole 430  -77.29    -142.74    0.0
hole 430   77.29     142.74    0.0
hole 430  -77.29     142.74    0.0
hole 440   55.49    -154.61    0.0
hole 440  -55.49    -154.61    0.0
hole 440   55.49     154.61    0.0
hole 440  -55.49     154.61    0.0
cylinder     6 1  184.15  2p220.34
cylinder    10 1  186.69  2p220.34
cylinder     6 1  191.77  2p220.34
cylinder    10 1  217.77  250.82  -220.34
cylinder     6 1  239.17  250.82  -220.34
cuboid       0 1  4p239.17 250.82 -220.34
unit 600
hemisphe-z  10 1  217.17
hemisphe-z   6 1   239.17
cuboid       0 1  6p239.17
global  unit 700
array       200  -239.17 -239.17 -478.34
end geometry
read array
ara=20 nux=15 nuy=15 nuz=1
com='level 2 array describing 2.96% enriched fuel oriface rod assembly'
fill 30r21  5r21 20 2r21 1b7  3r21 20 4r21 1b7  15r21
2r21 20 2r21 20 2r21 1b7  15r21  7r21 29 1b112 end fill
'.....................................................................
ara=21 nux=15 nuy=15 nuz=1
com='level 2 array describing 2.96% enriched fuel control rod assembly'
fill 30r21  5r21 29 2r21 1b7  3r21 29 4r21 1b7  15r21
2r21 29 2r21 29 2r21 1b7  15r21  7r21 29 1b112 end fill
'.....................................................................
ara=22 nux=15 nuy=15 nuz=1
com='level 2 array describing 2.64% enriched fuel lbp1(1.395%) rod assembly'
fill 30r22  5r22 26 2r22 1b7  3r22 26 4r22 1b7  15r22
2r22 26 2r22 26 2r22 1b7  15r22  7r22 29 1b112 end fill
'.....................................................................
ara=23 nux=15 nuy=15 nuz=1
com='level 2 array describing 2.96% enriched fuel lbp2(1.26%) rod assembly'
fill 30r21  5r21 27 2r21 1b7  3r21 27 4r21 1b7  15r21
2r21 27 2r21 27 2r21 1b7  15r21  7r21 29 1b112 end fill
'.....................................................................
ara=24 nux=15 nuy=15 nuz=1
com='level 2 array describing 1.98% enriched fuel control rod assm with rubble'
fill 30r23  5r23 29 2r23 1b7  3r23 29 4r23 1b7  15r23
2r23 29 2r23 29 2r23 1b7  15r23  7r23 29 1b112 end fill
'.....................................................................
ara=25 nux=15 nuy=15 nuz=1
com='level 2 array describing 2.64% enriched fuel lbp2(1.26%) rod assembly'
fill 30r22  5r22 27 2r22 1b7  3r22 27 4r22 1b7  15r22
```

```
2r22 27 2r22 27 2r22 1b7  15r22  7r22 29 1b112 end fill
'.....
ara=26 nux=15 nuy=15 nuz=1
com='level 2 array describing 2.64% enriched fuel 1bp3(1.06%) rod assembly'
fill 30r22  5r22 28 2r22 1b7  3r22 28 4r22 1b7  15r22
2r22 28 2r22 28 2r22 1b7  15r22  7r22 29 1b112 end fill
'.....
ara=27 nux=15 nuy=15 nuz=1
com='level 2 array describing 1.98% enr. fuel axial power shaping rod assembly'
fill 30r23  5r23 25 2r23 1b7  3r23 25 4r23 1b7  15r23
2r23 25 2r23 25 2r23 1b7  15r23  7r23 29 1b112 end fill
'.....
ara=28 nux=15 nuy=15 nuz=1
com='level 2 array describing 2.64% enriched fuel control rod assembly'
fill 30r22  5r22 29 2r22 1b7  3r22 29 4r22 1b7  15r22
2r22 29 2r22 29 2r22 1b7  15r22  7r22 29 1b112 end fill
'.....
ara=30 nux=5 nuy=2 nuz=1
fill  5*231 232 233 232 1b2  end fill
'.....'
ara=31 nux=5 nuy=2 nuz=1
fill 232 233 232 233 232 5*231 end fill
'.....'
ara=32 nux=2 nuy=1 nuz=1
fill 2*231   end fill
'.....'
ara=33 nux=2 nuy=5 nuz=1
fill 231 232 231 233 231 232 1b4   end fill
'.....'
ara=34 nux=2 nuy=5 nuz=1
fill 232 231 233 231 232 231 233 231 232 231  end fill
'.....'
ara=35 nux=1 nuy=2 nuz=1

fill 231 231 end fill
'.....
'.....
ara=100 nux=11 nuy=11 nuz=1
com='tmi critical core 1500wppm '
fill  231 234 235 236 235 236 1b5
234 235 237 238 236 235 1b5
235 237 235 237 235 236 1b5
236 238 239 235 233 235 1b5
235 236 235 233 235 233 1b5
236 235 236 235 233 234 1b60
end fill
ara=200  nux=1 nuy=1 nuz=2  gbl=200
fill  600 500  end fill
end array
read plot ttl='x-y slice through z=50.0'
scr=yes  lpi=10
xul=-180.0     yul=180.00 zul=50.0    xlr=180.00 ylr=-180.0   zlr=50.0
uax=1.0  vdn=-1.0 nax=1024  nch=' 123456789*'
end plot
end data
end
#shell
cp _geom* $RTNDIR
end
```

Sample Converted CSAS6 Output File

```
#csas26     parm='size=00500000'
tmi 1500 ppm boron
27groupndf4  latticecell
uo2         1 .925     583 92235 1.98 92238 98.02 end
uo2         2 .925     583 92235 2.64 92238 97.36 end
uo2         3 .925     583 92235 2.96 92238 97.04 end
zircalloy   4 1.0      583 end
arbmcrod          10.17 5 0 0 1
47107 41.088 47109 38.912 49113 0.632 49115 14.368 48000 5.0
            5 1.0      583 end
ss304       6 1.0      583 end
arbmpois1           3.70 2 0 1 0 13027 2 8016 3
            7 0.97952 583 end
b4c         7 2.048-2 583 end
arbmpois2           3.70 2 0 1 0 13027 2 8016 3
            8 0.98150 583 end
b4c         8 1.85-2  583 end
arbmpois3           3.70 2 0 1 0 13027 2 8016 3
            9 0.98444 583 end
b4c         9 1.556-2 583 end
arbmbacid     8.5788-3 3 1 1 0 5000 1 1001 3 8016 3
           10 .7707    583 5010 18.32 5011 81.68 end
h2o        10 .7707    583 end
end comp
squarepitch  1.44272 .9398 3 10 1.0922 4 .97536 0 end
more data
res=1 cylinder    .4699    dan(1)=0.2858256
res=2 cylinder    .4699    dan(2)=0.2858256
res=5 cylinder    .5588
end more
read param  plt=yes  gen=203 npg=500 tme=120 end param
read geometry
unit          20
com=^layer 2 oriface rod unit^
cylinder    1
               6.090600E-01  2.103400E+02 -2.103400E+02
             origin   x=  0.000000E+00   y=  0.000000E+00
media      6    1       1
cuboid      2
               7.213600E-01 -7.213600E-01  7.213600E-01
              -7.213600E-01  2.103400E+02 -2.103400E+02
media     10    1       2  -1
boundary      2
unit          21
com=^layer 2 2.96% enr. fuel rod^
cylinder    1
               4.699000E-01  1.828800E+02 -1.828800E+02
             origin   x=  0.000000E+00   y=  0.000000E+00
media      3    1       1
cylinder    2
               4.876800E-01  1.828800E+02 -1.828800E+02
             origin   x=  0.000000E+00   y=  0.000000E+00
media      0    1       2  -1
cylinder    3
               4.876800E-01  1.998400E+02 -2.062400E+02
             origin   x=  0.000000E+00   y=  0.000000E+00
media      0    1       3  -2  -1
cylinder    4
               5.461000E-01  1.998400E+02 -2.062400E+02
             origin   x=  0.000000E+00   y=  0.000000E+00
media      4    1       4  -3  -2  -1
```

```
cylinder   5
              5.461000E-01  2.103400E+02 -2.103400E+02
            origin   x=  0.000000E+00   y=  0.000000E+00
media     6    1       5  -4  -3  -2  -1
cuboid     6
              7.213600E-01 -7.213600E-01  7.213600E-01
             -7.213600E-01  2.103400E+02 -2.103400E+02
media    10    1       6  -5  -4  -3  -2  -1
boundary     6
unit         22
com=^layer 2 2.64% enr. fuel rod^
cylinder   1
              4.699000E-01  1.828800E+02 -1.828800E+02
            origin   x=  0.000000E+00   y=  0.000000E+00
media     2    1       1
cylinder   2
              4.876800E-01  1.828800E+02 -1.828800E+02
            origin   x=  0.000000E+00   y=  0.000000E+00
media     0    1       2  -1
cylinder   3
              4.876800E-01  1.998400E+02 -2.062400E+02
            origin   x=  0.000000E+00   y=  0.000000E+00
media     0    1       3  -2  -1

cylinder   4
              5.461000E-01  1.998400E+02 -2.062400E+02
            origin   x=  0.000000E+00   y=  0.000000E+00
media     4    1       4  -3  -2  -1
cylinder   5
              5.461000E-01  2.103400E+02 -2.103400E+02
            origin   x=  0.000000E+00   y=  0.000000E+00
media     6    1       5  -4  -3  -2  -1
cuboid     6
              7.213600E-01 -7.213600E-01  7.213600E-01
             -7.213600E-01  2.103400E+02 -2.103400E+02
media    10    1       6  -5  -4  -3  -2  -1
boundary     6
unit         23
com=^layer 2 1.98% enr. fuel rod^
cylinder   1
              4.699000E-01  1.828800E+02 -1.828800E+02
            origin   x=  0.000000E+00   y=  0.000000E+00
media     1    1       1
cylinder   2
              4.876800E-01  1.828800E+02 -1.828800E+02
            origin   x=  0.000000E+00   y=  0.000000E+00
media     0    1       2  -1
cylinder   3
              4.876800E-01  1.998400E+02 -2.062400E+02
            origin   x=  0.000000E+00   y=  0.000000E+00
media     0    1       3  -2  -1


cylinder   4
              5.461000E-01  1.998400E+02 -2.062400E+02
            origin   x=  0.000000E+00   y=  0.000000E+00
media     4    1       4  -3  -2  -1
cylinder   5
              5.461000E-01  2.103400E+02 -2.103400E+02
            origin   x=  0.000000E+00   y=  0.000000E+00
media     6    1       5  -4  -3  -2  -1
cuboid     6
              7.213600E-01 -7.213600E-01  7.213600E-01
             -7.213600E-01  2.103400E+02 -2.103400E+02
```

```
media    10    1       6  -5  -4  -3  -2  -1
boundary     6
unit         25
cylinder   1
             5.588000E-01  4.572000E+01 -4.572000E+01
           origin   x=  0.000000E+00   y=  0.000000E+00
media     5    1       1
cylinder   2
             6.121000E-01  2.103400E+02 -4.982000E+01
           origin   x=  0.000000E+00   y=  0.000000E+00
media     6    1       2  -1
cylinder   3
             6.121000E-01  2.103400E+02 -2.103400E+02
           origin   x=  0.000000E+00   y=  0.000000E+00
media     0    1       3  -2  -1
cuboid     4
             7.213600E-01 -7.213600E-01  7.213600E-01
            -7.213600E-01  2.103400E+02 -2.103400E+02
media    10    1       4  -3  -2  -1
boundary     4
unit         26
com=^layer 2 1.395% lumped burnable poison rod (lbp1)^
cylinder   1
             5.461000E-01  1.600200E+02 -1.600200E+02
           origin   x=  0.000000E+00   y=  0.000000E+00
media     7    1       1
cylinder   2
             5.461000E-01  2.604875E+02 -1.600200E+02
           origin   x=  0.000000E+00   y=  0.000000E+00
media     0    1       2  -1
cylinder   3
             6.350000E-01  2.605800E+02 -1.601000E+02
           origin   x=  0.000000E+00   y=  0.000000E+00
media     4    1       3  -2  -1
cuboid     4
             7.213600E-01 -7.213600E-01  7.213600E-01
            -7.213600E-01  2.605800E+02 -1.601000E+02
media    10    1       4  -3  -2  -1
boundary     4
unit         27
com=^layer 2 1.260% lumped burnable poison rod (lbp2)^
cylinder   1
             5.461000E-01  1.600200E+02 -1.600200E+02
           origin   x=  0.000000E+00   y=  0.000000E+00
media     8    1       1
cylinder   2
             5.461000E-01  2.604875E+02 -1.600200E+02
           origin   x=  0.000000E+00   y=  0.000000E+00
media     0    1       2  -1
cylinder   3
             6.350000E-01  2.605800E+02 -1.601000E+02
           origin   x=  0.000000E+00   y=  0.000000E+00
media     4    1       3  -2  -1
cuboid     4
             7.213600E-01 -7.213600E-01  7.213600E-01
            -7.213600E-01  2.605800E+02 -1.601000E+02
media    10    1       4  -3  -2  -1
boundary     4
unit         28
com=^layer 2 1.060% lumped burnable poison rod (lbp3)^
cylinder   1
             5.461000E-01  1.600200E+02 -1.600200E+02
           origin   x=  0.000000E+00   y=  0.000000E+00
media     9    1       1
```

```
cylinder   2
              5.461000E-01  2.604875E+02 -1.600200E+02
            origin   x=  0.000000E+00   y=  0.000000E+00
media     0    1       2  -1
cylinder   3
              6.350000E-01  2.605800E+02 -1.601000E+02
            origin   x=  0.000000E+00   y=  0.000000E+00
media     4    1       3  -2  -1
cuboid     4
              7.213600E-01 -7.213600E-01  7.213600E-01
             -7.213600E-01  2.605800E+02 -1.601000E+02
media    10    1       4  -3  -2  -1
boundary     4
unit         29
com=^z-layer 2--intact pins--no rubble^
cuboid     1
              7.213600E-01 -7.213600E-01  7.213600E-01
             -7.213600E-01  2.605800E+02 -1.601000E+02
media    10    1       1
boundary     1
unit        231
com=^layer 2 2.96% enr. fuel and orfice rod assembly^
cuboid     1
              1.081679E+01 -1.082399E+01  1.081679E+01
             -1.082399E+01  2.103398E+02 -2.103398E+02
array    20       1
               place 1 1 1  -1.010264E+01 -1.010264E+01  0.000000E+00
cuboid     2
              1.090549E+01 -1.090549E+01  1.090549E+01
             -1.090549E+01  2.103400E+02 -2.103400E+02
media    10    1       2  -1
boundary     2
unit        232
com=^layer 2 2.96% enr. fuel and control rod assembly--out^
cuboid     1
              1.081679E+01 -1.082399E+01  1.081679E+01
             -1.082399E+01  2.103398E+02 -2.103398E+02
array    21       1
               place 1 1 1  -1.010264E+01 -1.010264E+01  0.000000E+00
cuboid     2
              1.090549E+01 -1.090549E+01  1.090549E+01
             -1.090549E+01  2.103400E+02 -2.103400E+02
media    10    1       2  -1
boundary     2
unit        233
com=^layer 2 2.64% enr. fuel and 1.395% lbp1 rod assembly^
cuboid     1
              1.081679E+01 -1.082399E+01  1.081679E+01
             -1.082399E+01  2.103398E+02 -2.103398E+02
array    22       1
               place 1 1 1  -1.010264E+01 -1.010264E+01  0.000000E+00
cuboid     2
              1.090549E+01 -1.090549E+01  1.090549E+01
             -1.090549E+01  2.103400E+02 -2.103400E+02
media    10    1       2  -1
boundary     2
unit        234
com=^layer 2 2.96% enr. fuel and 1.260% lbp2 rod assembly^
cuboid     1
              1.081679E+01 -1.082399E+01  1.081679E+01
             -1.082399E+01  2.103398E+02 -2.103398E+02
array    23       1
               place 1 1 1  -1.010264E+01 -1.010264E+01  0.000000E+00
```

```
cuboid     2
             1.090549E+01 -1.090549E+01  1.090549E+01
            -1.090549E+01  2.103400E+02 -2.103400E+02
media     10    1       2  -1
boundary     2
unit       235
com=^layer 2 1.98% enr. fuel and control rod assembly--out^
cuboid     1
             1.081679E+01 -1.082399E+01  1.081679E+01
            -1.082399E+01  2.103398E+02 -2.103398E+02
array     24       1
              place 1 1 1  -1.010264E+01 -1.010264E+01  0.000000E+00
cuboid     2
             1.090549E+01 -1.090549E+01  1.090549E+01
            -1.090549E+01  2.103400E+02 -2.103400E+02
media     10    1       2  -1
boundary     2
unit       236
com=^layer 2 2.64% enr. fuel and 1.260% lbp2 rod assembly^
cuboid     1
             1.081679E+01 -1.082399E+01  1.081679E+01
            -1.082399E+01  2.103398E+02 -2.103398E+02

array     25       1
              place 1 1 1  -1.010264E+01 -1.010264E+01  0.000000E+00
cuboid     2
             1.090549E+01 -1.090549E+01  1.090549E+01
            -1.090549E+01  2.103400E+02 -2.103400E+02
media     10    1       2  -1
boundary     2
unit       237
com=^layer 2 2.64% enr. fuel and 1.060% lbp3 rod assembly^
cuboid     1
             1.081679E+01 -1.082399E+01  1.081679E+01
            -1.082399E+01  2.103398E+02 -2.103398E+02
array     26       1
              place 1 1 1  -1.010264E+01 -1.010264E+01  0.000000E+00
cuboid     2
             1.090549E+01 -1.090549E+01  1.090549E+01
            -1.090549E+01  2.103400E+02 -2.103400E+02
media     10    1       2  -1
boundary     2
unit       238
com=^layer 2 1.98% enr. fuel and axial power shaping rod assembly--out^
cuboid     1
             1.081679E+01 -1.082399E+01  1.081679E+01
            -1.082399E+01  2.103398E+02 -2.103398E+02
array     27       1
              place 1 1 1  -1.010264E+01 -1.010264E+01  0.000000E+00

cuboid     2
             1.090549E+01 -1.090549E+01  1.090549E+01
            -1.090549E+01  2.103400E+02 -2.103400E+02
media     10    1       2  -1
boundary     2
unit       239
com=^layer 2 2.64% enr. fuel and control rod assembly--out^
cuboid     1
             1.081679E+01 -1.082399E+01  1.081679E+01
            -1.082399E+01  2.103398E+02 -2.103398E+02
array     28       1
              place 1 1 1  -1.010264E+01 -1.010264E+01  0.000000E+00
```

```
cuboid     2
             1.090549E+01 -1.090549E+01  1.090549E+01
            -1.090549E+01  2.103400E+02 -2.103400E+02
media     10    1       2  -1
boundary     2
unit       300
cuboid     1
             5.452740E+01 -5.452740E+01  2.181096E+01
            -2.181096E+01  2.103360E+02 -2.103435E+02
array     30       1
              place 1 1 1  -4.362196E+01 -1.090549E+01 -3.753662E-03
cuboid     2
             5.452800E+01 -5.452800E+01  2.181100E+01
            -2.371600E+01  2.103438E+02 -2.103438E+02
media      6    1       2  -1
boundary     2
unit       310
cuboid     1
             5.452740E+01 -5.452740E+01  2.181096E+01
            -2.181096E+01  2.103360E+02 -2.103435E+02
array     31       1
              place 1 1 1  -4.362196E+01 -1.090549E+01 -3.753662E-03
cuboid     2
             5.452800E+01 -5.452800E+01  2.371600E+01
            -2.181100E+01  2.103438E+02 -2.103438E+02
media      6    1       2  -1
boundary     2
unit       320
cuboid     1
             2.181096E+01 -2.181096E+01  1.090548E+01
            -1.090548E+01  2.103360E+02 -2.103435E+02
array     32       1
              place 1 1 1  -1.090549E+01  0.000000E+00 -3.753662E-03
boundary     1
unit       330
cuboid     1
             2.181096E+01 -2.181096E+01  5.452740E+01
            -5.452740E+01  2.103360E+02 -2.103435E+02
array     33       1
              place 1 1 1  -1.090549E+01 -4.362196E+01 -3.753662E-03
cuboid     2
             2.181100E+01 -2.371600E+01  5.452800E+01
            -5.452800E+01  2.103438E+02 -2.103438E+02
media      6    1       2  -1
boundary     2
unit       340
cuboid     1
             2.181096E+01 -2.181096E+01  5.452740E+01
            -5.452740E+01  2.103360E+02 -2.103435E+02
array     34       1
              place 1 1 1  -1.090549E+01 -4.362196E+01 -3.753662E-03
cuboid     2
             2.371600E+01 -2.181100E+01  5.452800E+01
            -5.452800E+01  2.103438E+02 -2.103438E+02
media      6    1       2  -1
boundary     2
unit       350
com=^units for ss core form^
cuboid     1
             1.090548E+01 -1.090548E+01  2.181096E+01
            -2.181096E+01  2.103360E+02 -2.103435E+02
array     35       1
              place 1 1 1   0.000000E+00 -1.090549E+01 -3.753662E-03
boundary     1
```

```
unit         400


cuboid      1
               1.185000E+01 -1.185000E+01  9.525000E-01
              -9.525000E-01  2.103400E+02 -2.103400E+02
media      6    1        1
boundary     1
unit         410
cuboid      1
               9.525000E-01 -9.525000E-01  2.085000E+01
              -2.085000E+01  2.103400E+02 -2.103400E+02
media      6    1        1
boundary     1
unit         420
cuboid      1
               9.525000E-01 -9.525000E-01  9.940000E+00
              -9.940000E+00  2.103400E+02 -2.103400E+02
media      6    1        1
boundary     1
unit         430
cuboid      1
               2.276000E+01 -2.276000E+01  9.525000E-01
              -9.525000E-01  2.103400E+02 -2.103400E+02
media      6    1        1
boundary     1
unit         440

cuboid      1
               9.525000E-01 -9.525000E-01  1.091000E+01
              -1.091000E+01  2.103400E+02 -2.103400E+02
media      6    1        1
boundary     1
unit         500
cuboid      1
               1.199597E+02 -1.199609E+02  1.199597E+02
              -1.199609E+02  2.103398E+02 -2.103398E+02
array    100        1
                place 1 1 1  -1.090555E+02 -1.090555E+02  0.000000E+00
cylinder    2
               1.790700E+02  2.203400E+02 -2.203400E+02
             origin   x=  0.000000E+00   y=  0.000000E+00
media     10    1        2  -1
                        -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19 -20 -21
                       -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32 -33 -34
                       -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46 -47
                       -48 -49 -50 -51 -52
cuboid      9
               5.452800E+01 -5.452800E+01  2.181100E+01
              -2.371600E+01  2.103438E+02 -2.103438E+02
             origin x=  0.000000E+00  y= -1.417800E+02  z=  0.000000E+00
hole    300   9  -1 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19 -20
            -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32 -33
            -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
            -47 -48 -49 -50 -51 -52
             origin x=  0.000000E+00  y= -1.417800E+02  z=  0.000000E+00
cuboid     10
               5.452800E+01 -5.452800E+01  2.371600E+01
              -2.181100E+01  2.103438E+02 -2.103438E+02
             origin x=  0.000000E+00  y=  1.417800E+02  z=  0.000000E+00
hole    310  10  -1  -9 -11 -12 -13 -14 -15 -16 -17 -18 -19 -20
            -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32 -33
            -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
            -47 -48 -49 -50 -51 -52
```

```
          origin x=  0.000000E+00  y=  1.417800E+02  z=  0.000000E+00

cuboid    11
             2.181096E+01 -2.181096E+01  1.090548E+01
            -1.090548E+01  2.103360E+02 -2.103435E+02
           origin x= -7.634000E+01  y= -1.308700E+02  z=  0.000000E+00
hole   320  11  -1  -9 -10 -12 -13 -14 -15 -16 -17 -18 -19 -20
           -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32 -33
           -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
           -47 -48 -49 -50 -51 -52
           origin x= -7.634000E+01  y= -1.308700E+02  z=  0.000000E+00
cuboid    12
             2.181096E+01 -2.181096E+01  1.090548E+01
            -1.090548E+01  2.103360E+02 -2.103435E+02
           origin x=  7.634000E+01  y= -1.308700E+02  z=  0.000000E+00
hole   320  12  -1  -9 -10 -11 -13 -14 -15 -16 -17 -18 -19 -20
           -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32 -33
           -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
           -47 -48 -49 -50 -51 -52
           origin x=  7.634000E+01  y= -1.308700E+02  z=  0.000000E+00
cuboid    13
             2.181096E+01 -2.181096E+01  1.090548E+01
            -1.090548E+01  2.103360E+02 -2.103435E+02
           origin x= -7.634000E+01  y=  1.308700E+02  z=  0.000000E+00
hole   320  13  -1  -9 -10 -11 -12 -14 -15 -16 -17 -18 -19 -20
           -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32 -33
           -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
           -47 -48 -49 -50 -51 -52
           origin x= -7.634000E+01  y=  1.308700E+02  z=  0.000000E+00
cuboid    14
             2.181096E+01 -2.181096E+01  1.090548E+01
            -1.090548E+01  2.103360E+02 -2.103435E+02
           origin x=  7.634000E+01  y=  1.308700E+02  z=  0.000000E+00
hole   320  14  -1  -9 -10 -11 -12 -13 -15 -16 -17 -18 -19 -20
           -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32 -33
           -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
           -47 -48 -49 -50 -51 -52
           origin x=  7.634000E+01  y=  1.308700E+02  z=  0.000000E+00
cuboid    15
             2.181100E+01 -2.371600E+01  5.452800E+01
            -5.452800E+01  2.103438E+02 -2.103438E+02
           origin x= -1.417800E+02  y=  0.000000E+00  z=  0.000000E+00
hole   330  15  -1  -9 -10 -11 -12 -13 -14 -16 -17 -18 -19 -20
           -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32 -33
           -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
           -47 -48 -49 -50 -51 -52
           origin x= -1.417800E+02  y=  0.000000E+00  z=  0.000000E+00

cuboid    16
             2.371600E+01 -2.181100E+01  5.452800E+01
            -5.452800E+01  2.103438E+02 -2.103438E+02
           origin x=  1.417800E+02  y=  0.000000E+00  z=  0.000000E+00
hole   340  16  -1  -9 -10 -11 -12 -13 -14 -15 -17 -18 -19 -20
           -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32 -33
           -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
           -47 -48 -49 -50 -51 -52
           origin x=  1.417800E+02  y=  0.000000E+00  z=  0.000000E+00
cuboid    17
             1.090548E+01 -1.090548E+01  2.181096E+01
            -2.181096E+01  2.103360E+02 -2.103435E+02
           origin x= -1.308700E+02  y=  7.634000E+01  z=  0.000000E+00
hole   350  17  -1  -9 -10 -11 -12 -13 -14 -15 -16 -18 -19 -20
           -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32 -33
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          -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x= -1.308700E+02  y=  7.634000E+01  z=  0.000000E+00
cuboid    18
             1.090548E+01 -1.090548E+01  2.181096E+01
            -2.181096E+01  2.103360E+02 -2.103435E+02
           origin x=  1.308700E+02  y=  7.634000E+01  z=  0.000000E+00
hole   350  18  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -19 -20
          -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32 -33
          -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x=  1.308700E+02  y=  7.634000E+01  z=  0.000000E+00
cuboid    19
             1.090548E+01 -1.090548E+01  2.181096E+01
            -2.181096E+01  2.103360E+02 -2.103435E+02
           origin x= -1.308700E+02  y= -7.634000E+01  z=  0.000000E+00
hole   350  19  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -20
          -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32 -33
          -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x= -1.308700E+02  y= -7.634000E+01  z=  0.000000E+00
cuboid    20
             1.090548E+01 -1.090548E+01  2.181096E+01
            -2.181096E+01  2.103360E+02 -2.103435E+02
           origin x=  1.308700E+02  y= -7.634000E+01  z=  0.000000E+00
hole   350  20  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32 -33
          -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x=  1.308700E+02  y= -7.634000E+01  z=  0.000000E+00
cuboid    21
             1.185000E+01 -1.185000E+01  9.525000E-01
            -9.525000E-01  2.103400E+02 -2.103400E+02
           origin x= -1.536500E+02  y= -5.550000E+01  z=  0.000000E+00
hole   400  21  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32 -33
          -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x= -1.536500E+02  y= -5.550000E+01  z=  0.000000E+00
cuboid    22
             1.185000E+01 -1.185000E+01  9.525000E-01
            -9.525000E-01  2.103400E+02 -2.103400E+02
           origin x=  1.536500E+02  y= -5.550000E+01  z=  0.000000E+00
hole   400  22  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32 -33
          -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x=  1.536500E+02  y= -5.550000E+01  z=  0.000000E+00
cuboid    23
             1.185000E+01 -1.185000E+01  9.525000E-01
            -9.525000E-01  2.103400E+02 -2.103400E+02
           origin x= -1.536500E+02  y=  5.550000E+01  z=  0.000000E+00
hole   400  23  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -24 -25 -26 -27 -28 -29 -30 -31 -32 -33
          -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x= -1.536500E+02  y=  5.550000E+01  z=  0.000000E+00
cuboid    24
             1.185000E+01 -1.185000E+01  9.525000E-01
            -9.525000E-01  2.103400E+02 -2.103400E+02
           origin x=  1.536500E+02  y=  5.550000E+01  z=  0.000000E+00
hole   400  24  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -25 -26 -27 -28 -29 -30 -31 -32 -33
          -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
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          -47 -48 -49 -50 -51 -52
           origin x=  1.536500E+02  y=  5.550000E+01  z=  0.000000E+00

cuboid    25
              1.185000E+01 -1.185000E+01  9.525000E-01
             -9.525000E-01  2.103400E+02 -2.103400E+02
           origin x=  1.318400E+02  y= -9.913000E+01  z=  0.000000E+00
hole   400  25  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -24 -26 -27 -28 -29 -30 -31 -32 -33
          -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x=  1.318400E+02  y= -9.913000E+01  z=  0.000000E+00
cuboid    26
              1.185000E+01 -1.185000E+01  9.525000E-01
             -9.525000E-01  2.103400E+02 -2.103400E+02
           origin x= -1.318400E+02  y= -9.913000E+01  z=  0.000000E+00
hole   400  26  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -24 -25 -27 -28 -29 -30 -31 -32 -33
          -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x= -1.318400E+02  y= -9.913000E+01  z=  0.000000E+00
cuboid    27
              1.185000E+01 -1.185000E+01  9.525000E-01
             -9.525000E-01  2.103400E+02 -2.103400E+02
           origin x=  1.318400E+02  y=  9.913000E+01  z=  0.000000E+00
hole   400  27  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -24 -25 -26 -28 -29 -30 -31 -32 -33
          -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x=  1.318400E+02  y=  9.913000E+01  z=  0.000000E+00
cuboid    28
              1.185000E+01 -1.185000E+01  9.525000E-01
             -9.525000E-01  2.103400E+02 -2.103400E+02
           origin x= -1.318400E+02  y=  9.913000E+01  z=  0.000000E+00
hole   400  28  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -24 -25 -26 -27 -29 -30 -31 -32 -33
          -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x= -1.318400E+02  y=  9.913000E+01  z=  0.000000E+00
cuboid    29
              1.185000E+01 -1.185000E+01  9.525000E-01
             -9.525000E-01  2.103400E+02 -2.103400E+02
           origin x= -1.100300E+02  y=  1.209300E+02  z=  0.000000E+00
hole   400  29  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -24 -25 -26 -27 -28 -30 -31 -32 -33
          -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x= -1.100300E+02  y=  1.209300E+02  z=  0.000000E+00
cuboid    30
              1.185000E+01 -1.185000E+01  9.525000E-01
             -9.525000E-01  2.103400E+02 -2.103400E+02
           origin x=  1.100300E+02  y=  1.209300E+02  z=  0.000000E+00
hole   400  30  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -31 -32 -33
          -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x=  1.100300E+02  y=  1.209300E+02  z=  0.000000E+00
cuboid    31
              1.185000E+01 -1.185000E+01  9.525000E-01
             -9.525000E-01  2.103400E+02 -2.103400E+02
           origin x= -1.100300E+02  y= -1.209300E+02  z=  0.000000E+00
hole   400  31  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -32 -33
          -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
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          -47 -48 -49 -50 -51 -52
           origin x= -1.100300E+02  y= -1.209300E+02  z=  0.000000E+00

cuboid    32
              1.185000E+01 -1.185000E+01  9.525000E-01
             -9.525000E-01  2.103400E+02 -2.103400E+02
           origin x=  1.100300E+02  y= -1.209300E+02  z=  0.000000E+00
hole   400  32  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -33
          -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x=  1.100300E+02  y= -1.209300E+02  z=  0.000000E+00
cuboid    33
              9.525000E-01 -9.525000E-01  2.085000E+01
             -2.085000E+01  2.103400E+02 -2.103400E+02
           origin x=  1.427400E+02  y= -7.731000E+01  z=  0.000000E+00
hole   410  33  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32
          -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x=  1.427400E+02  y= -7.731000E+01  z=  0.000000E+00
cuboid    34
              9.525000E-01 -9.525000E-01  2.085000E+01
             -2.085000E+01  2.103400E+02 -2.103400E+02
           origin x= -1.427400E+02  y= -7.731000E+01  z=  0.000000E+00
hole   410  34  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32
          -33 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x= -1.427400E+02  y= -7.731000E+01  z=  0.000000E+00
cuboid    35
              9.525000E-01 -9.525000E-01  2.085000E+01
             -2.085000E+01  2.103400E+02 -2.103400E+02
           origin x=  1.427400E+02  y=  7.731000E+01  z=  0.000000E+00
hole   410  35  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32
          -33 -34 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x=  1.427400E+02  y=  7.731000E+01  z=  0.000000E+00
cuboid    36
              9.525000E-01 -9.525000E-01  2.085000E+01
             -2.085000E+01  2.103400E+02 -2.103400E+02
           origin x= -1.427400E+02  y=  7.731000E+01  z=  0.000000E+00
hole   410  36  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32
          -33 -34 -35 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x= -1.427400E+02  y=  7.731000E+01  z=  0.000000E+00
cuboid    37
              9.525000E-01 -9.525000E-01  9.940000E+00
             -9.940000E+00  2.103400E+02 -2.103400E+02
           origin x=  1.209200E+02  y= -1.100300E+02  z=  0.000000E+00
hole   420  37  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32
          -33 -34 -35 -36 -38 -39 -40 -41 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x=  1.209200E+02  y= -1.100300E+02  z=  0.000000E+00
cuboid    38
              9.525000E-01 -9.525000E-01  9.940000E+00
             -9.940000E+00  2.103400E+02 -2.103400E+02
           origin x= -1.209200E+02  y= -1.100300E+02  z=  0.000000E+00
hole   420  38  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32
          -33 -34 -35 -36 -37 -39 -40 -41 -42 -43 -44 -45 -46
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          -47 -48 -49 -50 -51 -52
           origin x= -1.209200E+02  y= -1.100300E+02  z=  0.000000E+00
cuboid    39
             9.525000E-01 -9.525000E-01  9.940000E+00
            -9.940000E+00  2.103400E+02 -2.103400E+02
           origin x=  1.209200E+02  y=  1.100300E+02  z=  0.000000E+00
hole   420  39  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32
          -33 -34 -35 -36 -37 -38 -40 -41 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x=  1.209200E+02  y=  1.100300E+02  z=  0.000000E+00
cuboid    40
             9.525000E-01 -9.525000E-01  9.940000E+00
            -9.940000E+00  2.103400E+02 -2.103400E+02
           origin x= -1.209200E+02  y=  1.100300E+02  z=  0.000000E+00
hole   420  40  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32
          -33 -34 -35 -36 -37 -38 -39 -41 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x= -1.209200E+02  y=  1.100300E+02  z=  0.000000E+00
cuboid    41
             9.525000E-01 -9.525000E-01  9.940000E+00
            -9.940000E+00  2.103400E+02 -2.103400E+02
           origin x=  9.911000E+01  y= -1.318300E+02  z=  0.000000E+00
hole   420  41  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32
          -33 -34 -35 -36 -37 -38 -39 -40 -42 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x=  9.911000E+01  y= -1.318300E+02  z=  0.000000E+00
cuboid    42
             9.525000E-01 -9.525000E-01  9.940000E+00
            -9.940000E+00  2.103400E+02 -2.103400E+02
           origin x= -9.911000E+01  y= -1.318300E+02  z=  0.000000E+00
hole   420  42  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32
          -33 -34 -35 -36 -37 -38 -39 -40 -41 -43 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x= -9.911000E+01  y= -1.318300E+02  z=  0.000000E+00
cuboid    43
             9.525000E-01 -9.525000E-01  9.940000E+00
            -9.940000E+00  2.103400E+02 -2.103400E+02
           origin x=  9.911000E+01  y=  1.318300E+02  z=  0.000000E+00
hole   420  43  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32
          -33 -34 -35 -36 -37 -38 -39 -40 -41 -42 -44 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x=  9.911000E+01  y=  1.318300E+02  z=  0.000000E+00
cuboid    44
             9.525000E-01 -9.525000E-01  9.940000E+00
            -9.940000E+00  2.103400E+02 -2.103400E+02
           origin x= -9.911000E+01  y=  1.318300E+02  z=  0.000000E+00
hole   420  44  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32
          -33 -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -45 -46
          -47 -48 -49 -50 -51 -52
           origin x= -9.911000E+01  y=  1.318300E+02  z=  0.000000E+00
cuboid    45
             2.276000E+01 -2.276000E+01  9.525000E-01
            -9.525000E-01  2.103400E+02 -2.103400E+02
           origin x=  7.729000E+01  y= -1.427400E+02  z=  0.000000E+00
hole   430  45  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
          -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32
          -33 -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -46
          -47 -48 -49 -50 -51 -52
```

```
            origin x=  7.729000E+01  y= -1.427400E+02  z=  0.000000E+00
cuboid    46
               2.276000E+01 -2.276000E+01  9.525000E-01
              -9.525000E-01  2.103400E+02 -2.103400E+02
            origin x= -7.729000E+01  y= -1.427400E+02  z=  0.000000E+00
hole   430  46  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
           -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32
           -33 -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45
           -47 -48 -49 -50 -51 -52
            origin x= -7.729000E+01  y= -1.427400E+02  z=  0.000000E+00
cuboid    47
               2.276000E+01 -2.276000E+01  9.525000E-01
              -9.525000E-01  2.103400E+02 -2.103400E+02
            origin x=  7.729000E+01  y=  1.427400E+02  z=  0.000000E+00
hole   430  47  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
           -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32
           -33 -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45
           -46 -48 -49 -50 -51 -52
            origin x=  7.729000E+01  y=  1.427400E+02  z=  0.000000E+00
cuboid    48
               2.276000E+01 -2.276000E+01  9.525000E-01
              -9.525000E-01  2.103400E+02 -2.103400E+02
            origin x= -7.729000E+01  y=  1.427400E+02  z=  0.000000E+00
hole   430  48  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
           -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32
           -33 -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45
           -46 -47 -49 -50 -51 -52
            origin x= -7.729000E+01  y=  1.427400E+02  z=  0.000000E+00
cuboid    49
               9.525000E-01 -9.525000E-01  1.091000E+01
              -1.091000E+01  2.103400E+02 -2.103400E+02
            origin x=  5.549000E+01  y= -1.546100E+02  z=  0.000000E+00
hole   440  49  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
           -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32
           -33 -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45
           -46 -47 -48 -50 -51 -52
            origin x=  5.549000E+01  y= -1.546100E+02  z=  0.000000E+00
cuboid    50
               9.525000E-01 -9.525000E-01  1.091000E+01
              -1.091000E+01  2.103400E+02 -2.103400E+02
            origin x= -5.549000E+01  y= -1.546100E+02  z=  0.000000E+00
hole   440  50  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
           -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32
           -33 -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45
           -46 -47 -48 -49 -51 -52
            origin x= -5.549000E+01  y= -1.546100E+02  z=  0.000000E+00
cuboid    51
               9.525000E-01 -9.525000E-01  1.091000E+01
              -1.091000E+01  2.103400E+02 -2.103400E+02
            origin x=  5.549000E+01  y=  1.546100E+02  z=  0.000000E+00
hole   440  51  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
           -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32
           -33 -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45
           -46 -47 -48 -49 -50 -52
            origin x=  5.549000E+01  y=  1.546100E+02  z=  0.000000E+00
cuboid    52
               9.525000E-01 -9.525000E-01  1.091000E+01
              -1.091000E+01  2.103400E+02 -2.103400E+02
            origin x= -5.549000E+01  y=  1.546100E+02  z=  0.000000E+00
hole   440  52  -1  -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19
           -20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32
           -33 -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45
           -46 -47 -48 -49 -50 -51
            origin x= -5.549000E+01  y=  1.546100E+02  z=  0.000000E+00
```

```
cylinder   3
              1.841500E+02  2.203400E+02 -2.203400E+02
            origin   x=  0.000000E+00   y=  0.000000E+00
media      6    1       3  -2  -1
cylinder   4
              1.866900E+02  2.203400E+02 -2.203400E+02
            origin   x=  0.000000E+00   y=  0.000000E+00
media     10    1       4  -3  -2  -1
cylinder   5
              1.917700E+02  2.203400E+02 -2.203400E+02
            origin   x=  0.000000E+00   y=  0.000000E+00
media      6    1       5  -4  -3  -2  -1
cylinder   6
              2.177700E+02  2.508200E+02 -2.203400E+02
            origin   x=  0.000000E+00   y=  0.000000E+00
media     10    1       6  -5  -4  -3  -2  -1
cylinder   7
              2.391700E+02  2.508200E+02 -2.203400E+02
            origin   x=  0.000000E+00   y=  0.000000E+00
media      6    1       7  -6  -5  -4  -3  -2  -1
cuboid     8
              2.391700E+02 -2.391700E+02  2.391700E+02
             -2.391700E+02  2.508200E+02 -2.203400E+02
media      0    1       8  -7  -6  -5  -4  -3  -2  -1
boundary     8
unit       600
sphere     1
              2.171700E+02
            origin
                    x=  0.000000E+00
                    y=  0.000000E+00
                    z=  0.000000E+00
            chord -z=  0.000000E+00
media     10    1       1
sphere     2
              2.391700E+02
            origin
                    x=  0.000000E+00
                    y=  0.000000E+00
                    z=  0.000000E+00
            chord -z=  0.000000E+00
media      6    1       2  -1

cuboid     3
              2.391700E+02 -2.391700E+02  2.391700E+02
             -2.391700E+02  2.391700E+02 -2.391700E+02
media      0    1       3  -2  -1
boundary     3
global
unit       700
cuboid     1
              2.391698E+02 -2.391698E+02  2.391698E+02
             -2.391698E+02  4.711595E+02 -4.783395E+02
array   200       1
              place 1 1 1   0.000000E+00  0.000000E+00 -2.391700E+02
boundary     1
end geometry

read array
ara=20 nux=15 nuy=15 nuz=1
com='level 2 array describing 2.96% enriched fuel oriface rod assembly'
fill 30r21  5r21 20 2r21 1b7  3r21 20 4r21 1b7  15r21
2r21 20 2r21 20 2r21 1b7  15r21  7r21 29 1b112 end fill
'.....................................................................
```

```
ara=21 nux=15 nuy=15 nuz=1
com='level 2 array describing 2.96% enriched fuel control rod assembly'
fill 30r21  5r21 29 2r21 1b7  3r21 29 4r21 1b7  15r21
2r21 29 2r21 29 2r21 1b7  15r21  7r21 29 1b112 end fill
'.....................................................................
ara=22 nux=15 nuy=15 nuz=1
com='level 2 array describing 2.64% enriched fuel 1bp1(1.395%) rod assembly'
fill 30r22  5r22 26 2r22 1b7  3r22 26 4r22 1b7  15r22
2r22 26 2r22 26 2r22 1b7  15r22  7r22 29 1b112 end fill
'.....................................................................
ara=23 nux=15 nuy=15 nuz=1
com='level 2 array describing 2.96% enriched fuel 1bp2(1.26%) rod assembly'
fill 30r21  5r21 27 2r21 1b7  3r21 27 4r21 1b7  15r21
2r21 27 2r21 27 2r21 1b7  15r21  7r21 29 1b112 end fill
'.....................................................................
ara=24 nux=15 nuy=15 nuz=1
com='level 2 array describing 1.98% enriched fuel control rod assm with rubble'
fill 30r23  5r23 29 2r23 1b7  3r23 29 4r23 1b7  15r23
2r23 29 2r23 29 2r23 1b7  15r23  7r23 29 1b112 end fill
'.....................................................................
ara=25 nux=15 nuy=15 nuz=1
com='level 2 array describing 2.64% enriched fuel 1bp2(1.26%) rod assembly'
fill 30r22  5r22 27 2r22 1b7  3r22 27 4r22 1b7  15r22
2r22 27 2r22 27 2r22 1b7  15r22  7r22 29 1b112 end fill
'.....................................................................
ara=26 nux=15 nuy=15 nuz=1
com='level 2 array describing 2.64% enriched fuel 1bp3(1.06%) rod assembly'
fill 30r22  5r22 28 2r22 1b7  3r22 28 4r22 1b7  15r22
2r22 28 2r22 28 2r22 1b7  15r22  7r22 29 1b112 end fill
'.....................................................................
ara=27 nux=15 nuy=15 nuz=1
com='level 2 array describing 1.98% enr. fuel axial power shaping rod assembly'
fill 30r23  5r23 25 2r23 1b7  3r23 25 4r23 1b7  15r23
2r23 25 2r23 25 2r23 1b7  15r23  7r23 29 1b112 end fill
'.....................................................................
ara=28 nux=15 nuy=15 nuz=1
com='level 2 array describing 2.64% enriched fuel control rod assembly'
fill 30r22  5r22 29 2r22 1b7  3r22 29 4r22 1b7  15r22
2r22 29 2r22 29 2r22 1b7  15r22  7r22 29 1b112 end fill
'.....................................................................
ara=30 nux=5 nuy=2 nuz=1
fill  5*231 232 233 232 1b2  end fill
'.....................................................................'
ara=31 nux=5 nuy=2 nuz=1
fill 232 233 232 233 232 5*231 end fill
'.....................................................................'
ara=32 nux=2 nuy=1 nuz=1
fill 2*231   end fill
'.....................................................................'
ara=33 nux=2 nuy=5 nuz=1
fill 231 232 231 233 231 232 1b4   end fill
'.....................................................................'
ara=34 nux=2 nuy=5 nuz=1
fill 232 231 233 231 232 231 233 231 232 231  end fill
'.....................................................................'
ara=35 nux=1 nuy=2 nuz=1
fill 231 231 end fill
'.....................................................................
'.....................................................................
ara=100 nux=11 nuy=11 nuz=1
com='tmi critical core 1500wppm '
fill  231 234 235 236 235 236 1b5
234 235 237 238 236 235 1b5
235 237 235 237 235 236 1b5
```

```
236 238 239 235 233 235 1b5
235 236 235 233 235 233 1b5
236 235 236 235 233 234 1b60
end fill
ara=200  nux=1 nuy=1 nuz=2  gbl=200
fill  600 500  end fill
end array
read plot ttl='x-y slice through z=50.0'
scr=yes  lpi=10
xul=-180.0     yul=180.00 zul=50.0    xlr=180.00 ylr=-180.0   zlr=50.0
uax=1.0  vdn=-1.0 nax=1024  nch=' 123456789*'
end plot
end data
end
```

M17.5 Q0RDPN: AN INPUT FILE CONVERSION PROGRAM

M17.5.1 INTRODUCTION

Program Q0RDPN can be used to convert a SCALE FIDO-type binary input file for a functional module to an ASCII format. This ASCII file can then be modified with a text editor, and the control sequence run with modified data.

M17.5.2 DESCRIPTION AND INPUT GUIDE

Q0RDPN is a utility program that can be used to convert a binary input file for a functional module to an ASCII file. This file can then be edited so that the functional module can be executed easily using slightly modified data. While a binary input file for any code using FIDO-type input can be converted, this program is primarily geared toward the functional modules in the neutronic modules of the SCALE system. A list of the modules for which default array definitions and unit numbers are built into the code is given in Table M17.2.1. If a name is given that is not in the table, then the user must specify the types of all arrays, the number of title records at the beginning of the binary file, and the logical unit number of the binary file.

Table M17.2.1 Q0RDPN module table

Module	Input Unit (NIN)	Maximum Array No.
BONAMI	96	12
NITAWL	97	6
XSDRN	98	52
COUPLE	93	83
ORIGEN	94	84
ICE	92	11

The input/output (I/O) files utilized by Q0RDPN are listed below.

I/O File	Function
5	Program control input
6	Messages
NIN	Input binary file
NOUT	Output ASCII file

The input consists of the following items (input in free-form).

MODULE	ASCII name of the module for which the binary file was created. If the name is in Table M17.2.1, then only this item and the next need to be specified. Otherwise all the input items must be specified.	
NOUT	The logical unit number to which the ASCII will be written.	
NIN	The logical unit number for the binary input file.	
NUMTTL	Number of title records beginning the binary input file.	

Repeat the following items until all the data are specified:

IAR	Array number for data on the binary file.	
ITYPE	Numeric data type for IAR.	0 - integer (default) 1 - real 2 - double precision 3 - both integer and real

Only non-integer arrays must be specified, as everything else is defaulted to integer.

Data reading is finished by specifying IAR = –10, or reaching the end-of-data.

NOTE: The 3** record for NITAWL as written by a SCALE control module will contain the nuclide ID numbers as integers. This will cause them to be converted to very small real numbers. The 3$$ record will follow the 3** record and will contain the nuclide ID numbers in integer format.

In the sample case in Fig. M17.2.1, the module specified in the Q0RDPN input is "O0O001," the control sequence alias for XSDRNPM. If "XSDRN" had been specified, none of the data following "32" (nout) would have been required. The input is presented here in this manner to illustrate the specification of all input items. The resulting ASCII file generated by Q0RDPN is shown in Fig. M17.2.2.

The CSAS1X sequence executes BONAMI, NITAWL, and XSDRNPM, whose aliases are O0O008, O0O002, and O0O001, respectively. When called in SCALE by its alias, the module reads its input from the binary input file created by the control module. To run the problem specified in Fig. M17.2.1 using a modified version of the XSDRNPM input file in Fig. M17.2.2, an input file such as that shown in Fig. M17.2.3 would be used.

```
#csas1x     parm=(check,size=600000)
'
' problem id --
' citation id --    exp. no.  --
'
' 2.35% u-235 enriched uo2 rods, 1.27cm od al clad, 1.1176 cm id,
' 1.1176 cm od uo2 91.44 cm long, rod 97.79 cm long.
' lead walls (10.2 x 164.0 x 123.4) on floor reflecting in h2o.
' 3-19x16 clusters, 2.032 cm square pitch. 13.72 cm separation
' between clusters.  0.66 cm from fuel clusters to wall
' reference: pnl-2827 pg.14
' scale module: csas25
'
0.8 in pitch lattice cell,2.35 wt% enriched fuel.
44g latticecell
uo2  1 0.84 293 92235 2.35 92238 97.65 end uo2
al  2 1.0  end al
h2o  3 1.0  end h2o
plexiglass  4 1.0  end plexiglass
h2o         5      end
pb        6 .97533 end
end comp
squarepitch  2.032 1.1176 1 3 1.27 2  end
end
#q0rdpn
 o0o001
 32 98 1
 5 1 15 1 31 1 32 1 33 2 34 2 35 1 38 1 41 1 42 1 43 1 47 1
 48 1
end
#shell
cp ft32f001 $RTNDIR/o0o001.input
end
```

Figure M17.2.1 Sample case

```
0.8 in pitch lattice cell,2.35 wt% enriched fuel.
  -1$$
600000
 e
   1$$
2 3 32 1 2r 3 12 8 3 1 20 25 3r 0
 e
   2$$
-2 -1 4r 0 -1 3r 0
 e
   3$$
1 11r 0
 e
   4$$
-1 44 0 -2 5r 0
 e
   5**
2r  1.00000-04  1.00000+00 2r  0.00000+00  1.42089+00 3r  0.00000+00
 e
 t
  13$$
3r 1 3 2r -3 2 3 4r -3
 e
  14$$
1092235 1092238 1008016 3008016 4008016 5008016 2013027 3001001 4001001
5001001 4006012 6082000
 e
  15**
 4.88650-04  2.00485-02  4.10743-02  3.33846-02 2r  1.00000-20
 6.03066-02  6.67692-02 4r  1.00000-20
 e
 t
  33##
1408r  7.81250-03
 e
 t
  35**
 0.00000+00  3.09291-02  7.25427-02  1.36380-01  2.79400-01  4.22420-01
 4.86257-01  5.27871-01  5.58800-01  5.68692-01  5.96900-01  6.25108-01
 6.35000-01  6.45474-01  6.57039-01  6.69951-01  6.84563-01  7.01394-01
 7.21238-01  7.45418-01  7.76371-01  8.19435-01  8.90717-01  9.61999-01
 1.00506+00  1.03602+00  1.06019+00  1.08004+00  1.09687+00  1.11148+00
 1.12439+00  1.13596+00  1.14643+00
 e
  36$$
8r 1 4r 2 20r 3
 e
  39$$
1 2 3
 e
  51$$
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27
28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
 e
 t
```

Figure M17.2.2 Converted ASCII input file for XSDRNPM

```
#o0o008
end
#o0o002
end
#xsdrnpm
.
.
.
modified ASCII input file
.
.
.
end
```

Figure M17.2.3 Sample input file for modified CSAS1X sequence

M17.6 AWL

M17.6.1 AWL INPUT GUIDE

AWL is a program to convert AMPX working libraries between ASCII format and binary format. It reads three numbers from logical unit 5 and prints output to logical unit 6.

M17.6.2 AWL INPUT

(1) NITP - logical unit number for the input working library.
(2) NOTP - logical unit number for the output working library.
(3) MODE - mode defining type of conversion: **1** - ASCII to Binary
2 - Binary to ASCII

M17.7 MAL

M17.7.1 MAL INPUT GUIDE

MAL is a program to convert a KENO albedo library between ASCII format and binary format. It reads three numbers from logical unit 5 and prints output to logical unit 6.

M17.7.2 MAL INPUT

(1) NITP - logical unit number for the input working library.
(2) NOTP - logical unit number for the output working library.
(3) MODE - mode defining type of conversion: **1** - ASCII to Binary
2 - Binary to ASCII

M17.8 WGT

M17.8.1 WGT INPUT GUIDE

WGT is a program to convert a KENO weights library between ASCII format and binary format. It reads three numbers from logical unit 5 and prints output to logical unit 6.

M17.8.2 MAL INPUT

(1) NITP - logical unit number for the input working library.
(2) NOTP - logical unit number for the output working library.
(3) MODE - mode defining type of conversion: **1** - ASCII to Binary
2 - Binary to ASCII

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11. ABSTRACT *(200 words or less)*

SCALE, a modular code system for Standardized Computer Analyses Licensing Evaluation, has been developed by Oak Ridge National Laboratory at the request of the U.S. Nuclear Regulatory Commission. The SCALE system utilizes well-established computer codes and methods within standard analysis sequences that (1) allow an input format designed for the occasional user and/or novice, (2) automate the data processing and coupling between modules, and (3) provide accurate and reliable results. System development has been directed at problem-dependent cross-section processing and analysis of criticality safety, shielding, heat transfer, and depletion/decay problems. Since the initial release of SCALE in 1980, the code system has been heavily used for evaluation of nuclear fuel facility and package designs. This revision documents Version 4.4 of the system.

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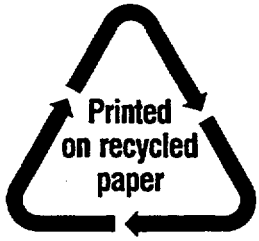

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