AUG 2 5 1976

MEMORANDUM TO: Benard C. Rusche, Director
Office of Nuclear Reactor Regulation

FROM: Saul Levine, Acting Director
Office of Nuclear Regulatory Research

SUBJECT: SRI 7: THE SIMMER CODE FOR ANALYSIS OF HYPOTHETICAL CORE DISRUPTIVE ACCIDENTS IN LMFBR'S

A code called SIMMER-I (for Sa, Implicit Multifield, Multicomponent, Eulerian, Recriticality Trials) to follow the motion and neutronics of LMFBR cores during hypothetical core disruptive accidents (HCDA's) has been developed as part of our research program at Los Alamos Scientific Laboratory. The trial version of this code SIMMER-I is now available. We have transmitted copies of the draft users manual, listings of the code, sample problems and a magnetic tape containing the code to Mr. T. M. Speis of your staff. Work is in progress to make the code operational at the Brookhaven National Laboratory computer where it will be available for evaluation and possible technical assistance support for your staff on the Clinch River Breeder Reactor review.

We are preparing to have a workshop at LASL the week of September 13, 1976 where members of your staff and consultants from BNL will have an opportunity to run sample problems and have discussions with the code developers. A brief technical description of the SIMMER program is attached.

Original Signed by
Saul Levine

Saul Levine, Acting Director
Office of Nuclear Regulatory Research

Attachment:
As stated

cc: R. F. Fraley, ACRS
T. S. McCreless, ACRS

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Form AEC-318 (Rev. 9-53) AECM 0240

☆ U. S. GOVERNMENT PRINTING OFFICE: 1974-526-166

THE SIMMER CODE

Analyses of hypothetical core disruptive accidents (HCDA's) for liquid-metal cooled fast breeder reactors (LMFBR's) have predicted the evolution of highly distorted molten core geometries, and this has led to concern about recriticality during such accidents. In mid-1974 the Los Alamos Scientific Laboratory (LASL) began development of a code called SIMMER (for Sn, Implicit, Multifield, Multicomponent, Eulerian, Recriticality) to follow the motion and neutronics of LMFBR cores during HCDA's. This manual describes SIMMER-I, which is the first in a series of SIMMER computer codes designed to examine the dynamics of disrupted cores in LMFBR's.

Overview of SIMMER-I Models

SIMMER-I couples space-dependent neutronics with multifield, multicomponent fluid dynamics in an (r,z) representation of an LMFBR core. The code includes different neutronics models for accuracy and efficiency comparisons. A time-dependent neutron transport option is included to accurately calculate the neutron leakage and streaming if large voided regions develop during an accident calculation. The diffusion approximation breaks down in situations where material densities approach zero, but when such situations are not expected, a diffusion option is provided for including space-dependent effects. Either the quasistatic method or the extrapolation method is available for calculating the time-dependent behavior of the flux in both the transport and diffusion options. Cross sections used in the space-dependent neutronics calculation are determined at each neutronic time step using the Bondarenko formalism. The code includes additional options for performing point kinetics neutronics or using input values of power vs. time for scoping studies of whole core accidents or small scale studies of single subassembly phenomena.

The SIMMER-I fluid dynamics model is based on that developed in KACHINA program in which the relative motion of two fields, liquid and vapor, is calculated using the Implicit Multifield (IMF) method. The KACHINA model has been extended by the addition of a third component to each field to

follow the motion of the three LMFBR materials: fuel, steel, and sodium. In addition, a structure field has been added to model solid fuel, cladding, and subassembly can walls. Within each field, the materials, or components, move with the velocity of the field. This means, for example, that liquid fuel and liquid steel in the liquid field have the same velocity at a point in space. On the other hand, separate energy equations are solved for each component except for those in the vapor field where the mixture of vapors is treated with a single energy equation.

The structure field is fixed in space and acts as an infinite momentum sink for drag forces and mass transfer. Separate continuity and energy equations for the three structure components predict the thermal state of the structure field. If a can wall is in a mesh cell, radial motion in that cell is inhibited until the can wall is predicted to fail. Failure of structure in the present model depends only on melting. Melted materials enter the liquid field, while freezing materials leave the liquid field and enter the structure field.

Within the structure and fluid dynamics equations, terms are included to account for coupling between the fields and the components. Monentum coupling is accounted for by drag force terms; energy coupling is accounted for by heat transfer terms, and mass coupling is accounted for by phase transition terms. The drag correlations are simple in form. The heat transfer coefficients are simple constants multiplying the temperature differences between fields and components to determine heat transfer rates. Phase transitions are modeled with greater complexity. Melting and freezing are calculated by comparison of material energies with solidus and liquidus energies, and vaporization and condensation are calculated using nonequilibrium conduction-limited phase transition models in which the phase transition rates are proportional to the difference between saturation and component temperatures.

SIMMER-T and the SIMMER Program

In SIMMER-T development has concentrated on the numerical methods of two-phase fluid dynamics and time-dependent neutronics. The physics of exchange

coefficients for the two-phase fluid dynamics equations has received much less attention. These exchange coefficients model the interaction phenomena of heat transfer, momentum exchange, and phase transition and are primarily based on flow of dispersed droplets in a vapor field, although flow of bubbles in a liquid field is treated in some cases. Other two-phase flow regimes are not modeled, and it is likely that the user will find situations in which the SIMMER-I exchange coefficients are not valid. An important effort prior to the release of SIMMER-II will be the development of better models for these exchange coefficients.

The tabular equations of state that are part of the SIMMER program are not included in SIMMER-I. The equations of state for sodium, iron, and uranium dioxide have undergone extensive investigation using techniques which consistently describe the material equation of state for the density and energy range from normal atmospheric conditions to low densities and/or high energies. In place of these more sophisticated equations of state, which require tabular data and interpolation routines for use in SIMMER, analytic representations of the equations of state have been included in SIMMER-I. A later modification of SIMMER-I will include tabular equations of state.

The original scope of the SIMMER code was to examine the possibility of secondary criticality following disassembly of an LMFBR core. This included tracking the large scale motion of materials prior to, during, and after disassembly. Despite the elementary nature of the physics modeling, it has become apparent during the development of SIMMER-I that the eventual capabilities of SIMMER will allow the examination of other LMFBR accident situations such as gradual core meltdown, fluidization, and development of a disrupted core, i.e., the transition phase. The techniques also appear to be useful in the analysis of single subassembly phenomena involving fuel meltdown, extended material motion, freezing, plugging, clad relocation, and fluidization.