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HABIT 2.2 Description of Models and Methods

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Protecting People and the Environment

HABIT 2.2 Description of Models and Methods

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ABSTRACT

To ensure the safe operation of commercial nuclear power plants, control room (CR) operators must be protected from dangers arising from possible exposure to hazardous chemicals that may be discharged as a result of equipment failure, operator errors, or events external to plant operation. General Design Criterion (GDC) 4, "Environmental and dynamic effects design bases," of Appendix A, "General Design Criteria for Nuclear Power Plants," to Title 10 of the *Code of Federal Regulations* Part 50, "Domestic licensing of production and utilization facilities," requires, in part, that structures, systems, and components important to safety be designed to accommodate the effects of and to be compatible with the environmental conditions associated with normal operation, maintenance, testing, and postulated accidents. GDC 19, "Control room," requires that a CR be provided from which actions can be taken to operate the nuclear power unit safely under normal conditions and to maintain it in a safe environment under accident conditions. Additionally, Regulatory Guide 1.78, "Evaluating the Habitability of a Nuclear Power Plant Control Room During a Postulated Hazardous Chemical Release," provides guidance and endorses the use of the HABIT computer code for examining CR habitability following a postulated release of toxic chemicals. The original version of HABIT was a package of computer codes designed to be used for the evaluation of CR habitability in the event of an accidental release of toxic chemicals and radioactive materials. Given information about the design of a nuclear power plant, a scenario for the release of toxic chemicals, and information about the air flows and protection systems of the CR, HABIT could be used to quick estimate the chemical exposure or radiological dose to CR personnel. This report describes current code updates and changes to the technical basis of HABIT.

HABIT is based on the external transport (EXTRAN) computer code for estimating transient concentrations at a specific downwind location (i.e., CR air intake) for four release scenarios: liquid burst, liquid leak, gas burst, and gas leak. EXTRAN combines procedures for estimating the amount of airborne material, a Gaussian puff dispersion model, and building-wake diffusion algorithms. This report describes the latest version, HABIT 2.2, which is an update to HABIT 2.0. It works in Microsoft© (MS) 64-bit operating systems such as MS Windows 10. HABIT 2.2 has fully integrated both the DEGADIS and SLAB codes and incorporated the Britter-McQuaid Workbook criteria for automatic screening the importance of denser-than-air effects. Finally, unlike previous versions, HABIT 2.2 has removed all the radiological dose calculation computer applications.

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ABBREVIATIONS AND SYMBOLS

atm	atmospheres or atmospheric
BMW	Britter-McQuaid Workbook
CFR	*Code of Federal Regulations*
CR	control room
CHEM	CR chemical computer code
CONHAB	CONtrol room HABitability code
DEGADIS	EPA DEnse GAas DISpersion Model computer code
EPA	U.S. Environmental Protection Agency
EXTRAN	external transport computer code
EOF	Emergency Operations Facility
FPFP_2	Fission Product Flow Path code
GB	gigabyte(s)
GDC	General Design Criterion
GUI	graphical user interface
HABIT	Computer Codes for Evaluation of Control Room Habitability
MS	Microsoft©
NRC	U.S. Nuclear Regulatory Commission
NUREG	U.S. Nuclear Regulatory Commission technical report designation
OS	operating system (computer)
RAMP	Radiation Protection Computer Code Analysis and Maintenance Program
RG	regulatory guide
SLAB	U.S. Department of Energy denser-than-air releases computer code
SNAP/RADTRAD	Symbolic Nuclear Analysis Package/RADionuclide, Transport, Removal And Dose Estimation code
SQAP	software quality assurance plan
SQLite	C-language library that implements an SQL database engine
TACT5	Transport of ACTivity code
TDI	tabbed document interface
TLV-STEL	threshold limit value–short-term exposure limit
TSC	Technical Support Center
XML	extensible markup language
cm^2/s	square centimeters per second
°C & K	temperature: degree Celsius and Kelvin, respectively
ft^3	cubic feet
ft^3/min	cubic feet per minute
ft^3/s	cubic feet per second
g/m^3	grams per cubic meter
g/ml	grams per milliliter
g/mol	grams per mole
J/g	joules per gram
J/g/°C	joules per gram per degree Celsius
J/gmol/K	joules per gram-molecule per Kelvin
J/kg	joules per kilogram
J/kg/K	joules per kilogram per Kelvin
J/kmol/K	joules per kilomole Kelvin
kg	kilogram
kg/kmol	kilograms per kilomole
kg/m^2s	kilograms per square meter second

kg/m^3	kilograms per cubic meter
kg/mol	kilograms per mole
kg/s	kilograms per second
m	meter
m/s	speed: meters per second
m/s^2	meters per second squared
m^2	square meter
m^3	cubic meter
m^3/min	cubic meters per minute
m^3/s	flow rate: cubic meters per second
mmHg	pressure: millimeters of mercury
N/m^2	newtons per square meter
ppm	parts per million
s	time: second
W/m^2	watts per square meter
W/m^2K	watts per square meter Kelvin

1 INTRODUCTION

To ensure the safe operation of commercial nuclear power plants, control room (CR) operators must be protected from harms and dangers arising from possible exposure to hazardous chemicals that may be discharged as a result of equipment failure, operator errors, or events external to plant operation. The U.S. Nuclear Regulatory Commission (NRC) has developed licensing regulations and guidance to ensure that CR operators are protected from dangers arising from possible exposure to hazardous chemicals. General Design Criterion (GDC) 4, "Environmental and dynamic effects design bases," of Appendix A, "General Design Criteria for Nuclear Power Plants," to Title 10 of the *Code of Federal Regulations* (10 CFR) Part 50, "Domestic licensing of production and utilization facilities" [1], requires, in part, that structures, systems, and components important to safety be designed to accommodate the effects of and to be compatible with the environmental conditions associated with normal operation, maintenance, testing, and postulated accidents. GDC 19, "Control room," of Appendix A to 10 CFR Part 50 [2] requires that a CR be provided from which actions can be taken to operate the nuclear power unit safely under normal conditions and to maintain it in a safe condition under accident conditions. Additionally, Regulatory Guide (RG) 1.78, "Evaluating the Habitability of a Nuclear Power Plant Control Room During a Postulated Hazardous Chemical Release" [3], provides guidance and endorses use of the Control Room Habitability Package (HABIT) computer code for examining CR habitability, includes Technical Support Center and Emergency Operations Facility, following a postulated release of toxic chemicals.

1.1   HABIT Code Background

HABIT is a package of computer codes designed to assist in the evaluation of CR habitability in the event of accidental spills of toxic chemicals.

1.1.1   HABIT Version 1.1

The early version of HABIT, i.e., version 1.1 (HABIT 1.1), was a package of computer codes designed to be used for the evaluation of CR habitability in the event of an accidental release of toxic chemicals or radioactive materials. Before the creation of HABIT 1.1, several computer codes could perform parts of the computations needed to estimate chemical exposures or radiological doses in CRs. Pacific Northwest National Laboratory combined these computer codes as modules in a unified package that could be used with a maximum of ease and a minimum of user preparation, as described in NUREG/CR-6210, "Computer Codes for Evaluation of Control Room Habitability (HABIT)," issued June 1996 [4], and NUREG/CR-6210, Supplement 1, "Computer Codes for Evaluation of Control Room Habitability (HABIT V1.1)," issued October 1998 [5]. The original HABIT 1.1 code was designed to run on a personal computer operating with either DOS 5.0 or in Microsoft© (MS) Windows XP operating system (OS)/32-bit environments.

HABIT 1.1 used two main computer codes (modules) for estimating CR habitability in the event of accidental release of toxic chemicals:

(1)   The external transport computer code (EXTRAN) determines the release rate of a chemical in the event of release due to leaks or ruptures of liquid or gas tanks and computes atmospheric dilution arriving at the intake to the CR [4] [5] [6] [7] [8].

(2)   The CR chemical computer code (CHEM) models the dilution of the chemical
        concentrations estimated by EXTRAN by air flows in the CR and determines the
        chemical exposure to CR personnel.

HABIT 1.1 also had three additional code modules to estimate radiological doses in the CR
associated with the intake of radionuclides: (1) the Transport of ACTivity code (TACT5), (2) the
Fission Product Flow Path code (FPFP_2), and (3) the CONtrol room HABitability code
(CONHAB). TACT5 is used to model situations in which contamination is released to the
atmosphere and subsequently enters the CR as described in NUREG/CR-6210 [4],
NUREG/CR-6210, Supplement 1 [5], and NUREG/CR-5106, "User's Guide for the TACT5
Computer Code," issued June 1998 [9]. FPFP_2 is used to model radioactive flow through the
plant. This code treats the flow paths as a linear sequence of flow elements called "spaces" and
"nodes," as described in NUREG/CR-6210 [4] and NUREG/CR-5658, "FPFP_2: A Code for
Following Airborne Fission Products in Generic Nuclear Plant Flow Paths," issued March 1991
[10]. CONHAB can accept contaminant inflow from up to two sources of outside air (i.e., two
TACT5 runs) and up to two sources of air from within the plant (i.e., two FPFP_2 runs), as
described in NUREG/CR-6210 [4], NUREG/CR-6210, Supplement 1 [5], and NUREG/CR-5659,
"Control Room Habitability System Review Models," issued December 1990 [11].

1.1.2   HABIT Version 1.2

In late 2014, the NRC computer system upgraded to MS Windows 7 OS/64-bit environments.
The "re-hosting" of HABIT 1.2 from its 1.1 platform was quickly and successfully completed in
February 2015. HABIT 1.2 could run on personal computers using the MS Windows 7
OS/64-bit environment and also complied with Section 508 of the United States Rehabilitation
Act of 1973, ensuring its accessibility to people with disabilities. The NRC added HABIT 1.2 to
the computer code packages in the Radiation Protection Computer Code Analysis and
Maintenance Program (RAMP) and made it available for download by the RAMP user
community.

HABIT 1.2 also included heavily debugged and streamlined Fortran codes and a new graphical
user interface (GUI) to allow the Fortran modules' output to be displayed and run from tabs
within a single window as described in the HABIT 1.2 user's guide [12]. The new GUI also
coordinated data management. Finally, the NRC performed a rigorous series of verifications
and validations to ensure the HABIT 1.2 output values were consistent with the documented
values in NUREG/CR-6210, Supplement 1 [5].

1.1.3   HABIT Version 2.0

Upon completion of HABIT 1.2, the NRC staff continually pursued the Advisory Committee on
Reactor Safeguards recommendations about HABIT's capability for assessing transport
phenomena of heavy-gas dispersion (i.e., denser-than-air transport models), resulting in the
release of HABIT 2.0. HABIT 2.0 added the U.S. Environmental Protection Agency's (EPA's)
DEnse GAs DISpersion Model (DEGADIS) code, described in the user's guide for DEGADIS 2.1
[13], and the U.S. Department of Energy's atmospheric dispersion model for denser-than-air
releases (SLAB) computer code, described in the user's manual for SLAB [14]. HABIT 2.0
expended the GUI and unified the input screen of the EXTRAN code as described in the
HABIT 2.2 user's guide [15]. Finally, HABIT 2.0 incorporated the Britter-McQuaid Workbook
(BMW) criteria [16] [17] to determine when the DEGADIS and/or SLAB models need to run.

1.1.4   HABIT Version 2.2

This report describes the latest enhancements to HABIT in release version HABIT 2.2. HABIT 2.1 was disapproved, redirected, and rebuilt into HABIT 2.2 with many GUI enhancements and features. The most significant enhancements, functions, and features are as follows:

(1)   As part of the effort to remove duplicative and overlapping functions of the codes in RAMP, the three computer codes (TACT5, FPFP_2, and CONHAB) used to estimate doses in the CR associated with the accidental releases of radionuclides were removed. HABIT 2.2 no longer allows the user to calculate radiation doses for CR habitability and only calculates chemical toxicity for CR habitability.

Note to Users: The Symbolic Nuclear Analysis Package/RADionuclide, Transport, Removal And Dose Estimation (SNAP/RADTRAD) code, another RAMP element, calculates the occupational radiation doses in the CR during accidental releases of radionuclides.

(2)   If an impacted receptor or CR is further than 99 meters (m) from the chemical release point, HABIT 2.2 allows 24 hours as the maximum time for environmental transport calculations.

(3)   HABIT 2.2 automatically calculates the importance of denser-than-air effects using the BMW criteria. The user can then select which denser-than-air code (i.e., DEGADIS or SLAB) to run.

(4)   The GUI screen for HABIT 2.2 was updated with easy-to-read fonts, improved waring and notification messaging, and a redesign of the graphing and plotting utilities for all the Fortran codes (i.e., EXTRAN, DEGADIS, and SLAB).

(5)   HABIT 2.2 has full backward compatibility to re-run the release "DeSiGn" files (i.e., "DSG", from HABIT 1.1).

(6)   HABIT 2.2 can be loaded onto and coexist in computers with earlier versions of HABIT (e.g., Versions 1.1, 1.2, or 2.0).

(7)   Habit 2.2 now uses zero-configuration SQLite database technology, which is a relational database management system contained in a C programming library. Using the SQLite embedded database to store data eliminated the use of extensible markup language (i.e., XML) files to store configuration files. The code will use "filename.s3db" as the default file extension. Additionally, the SQLite database will read embedded system during file retrieval and updates at the end of file closing. All result from the each of designs will recorded and can be retrieved individually.

1.2   HABIT Code Quality Assurance Plan

In addition to the updates described in Section 1.1, the NRC developed HABIT under a software quality assurance plan (SQAP) [18]. The scope of the SQAP is to ensure the proper development of the HABIT software throughout its lifecycle. This plan details the structure and responsibilities of the development team and requires the proper documentation of all activities.

Development is based on the specific requirements to be fulfilled by the computer code, using accepted coding practices and rigorous validation and verification of the end-user software.

The NRC has defined the following three levels of software, per NUREG/BR-0167, "Software Quality Assurance Program and Guidelines," issued February 1993 [19]:

(1) Level 1: Technical application software used in a safety decision by the NRC

(2) Level 2: Technical or nontechnical application software not used in a safety decision by the NRC

(3) Level 3: Technical or nontechnical application software not used in a safety decision and having local or limited use by the NRC

The NRC has historically classified the HABIT software as Level 2, and the SQAP is written to conform to the Level 2 requirements.

2 INSTALLATION GUIDE

This section describes the computing system requirements, distribution, and installation process for HABIT 2.2. A dedicated user's guide [15] is available for the installation and for relevant technical explanations and figure illustrations.

2.1   Hardware and Software Requirements

HABIT 2.2 can be run on any computer with MS Windows OS versions Windows XP, Windows 7, and Windows 10. The following are the minimum computing requirements:

- Intel® Pentium® 4 or AMD Athlon® 64 processor (1.6 gigahertz or faster)

- Windows 7 with Service Pack 1, Windows 8, or Windows 10

- 2 gigabytes (GB) of RAM (8 GB recommended)

- 2 GB of available hard disk space for installation, with additional free space required during installation (cannot install on removable flash storage devices)

- 1024 x 768 pixel display (1280 x 800 recommended) with 16-bit color and 512 megabytes of VRAM (1 GB recommended)

2.2   Distribution

HABIT 2.2 can only be obtained from the NRC's RAMP website (https://ramp.nrc-gateway.gov/). HABIT 2.2 is only available for registered RAMP members with proper RAMP credentials (i.e., RAMP user ID and password). To become a RAMP member, interested individuals should refer to the membership requirements on the RAMP Web site.

The "HABIT22.zip" downloaded file package include following files:

- HABIT 2.2 installer file ("setup.exe")
- HABIT 2.2 SQLite embedded database files (".s3db" files)

2.3   Installing HABIT 2.2

HABIT 2.2 is installed via an installer executable file. The NRC recommends that users have administrative privileges for the computer on which HABIT 2.2 is to be installed. The executable installer will install the execution code, the HABIT 2.2 GUI, the available nuclide databases, and the associated parameter range files.

Once the "HABIT22.zip" file download is complete, double click on or open the "HABIT22.zip" file to unzip and extract the contents to your computer.

Once the HABIT 2.2 files been extracted, you will see the *HABIT22* folder in the directory selected during the extraction.

Double click the "setup.exe" file in the *HABIT22* folder and follow the onscreen prompts in the MS Installer Wizard window to install HABIT 2.2. For all HABIT 2.2 installation details, refer to the HABIT 2.2 user's guide [15].

Notes to Users: (1) Users with an earlier version of HABIT installed on their computer do not need to uninstall the previous version nor require administrative privileges to install HABIT 2.2. (2) The "setup.exe" file for HABIT 2.2 can be re-executed by the user at any time after the installation process to modify, repair, or remove the program.

Figure 2-1   HABIT Open Window

Figure 2-1 illustrates the unique design of the "HABIT open window," which displays the desktop icon for HABIT 2.2 in the upper left corner. In the window, **Please Load a Design before Proceeding** is an easy instruction for how to begin HABIT calculations. Users can also click **Exit** from this window if opening HABIT was a mistake. The open window in Figure 2-1 also displays the United States Government software disclaimer, which states the following:

> This computer program was created as work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor its contractors, nor any of their employees, makes any warranty, expressed or implied, or assumes any legal responsibility for any third party's use, or the results of such use, or of any information in or generated by this program, or represents that its use by such third party would not infringe privately-owned rights. In addition, you may not distribute this computer program or use this computer program without the permission of the U.S. Nuclear Regulatory Commission.

3 HABIT 2.2 GRAPHICAL USER INTERFACE DESIGN

This section gives an overview of the basic design features and options available to the user in the HABIT 2.2 GUI. The HABIT 2.2 **Main** GUI window can now be adjusted to fit the screen size of the monitor. It is designed for optimal display at 1024 x 768 pixels (1280 x 800 and better is recommended). As shown in Figure 3-1, the HABIT 2.2 **Main** GUI window has a main menu bar on the top and a file design information bar at the bottom. A tabbed document interface (TDI) in the center section allows all the major functions to be contained within a single GUI window.
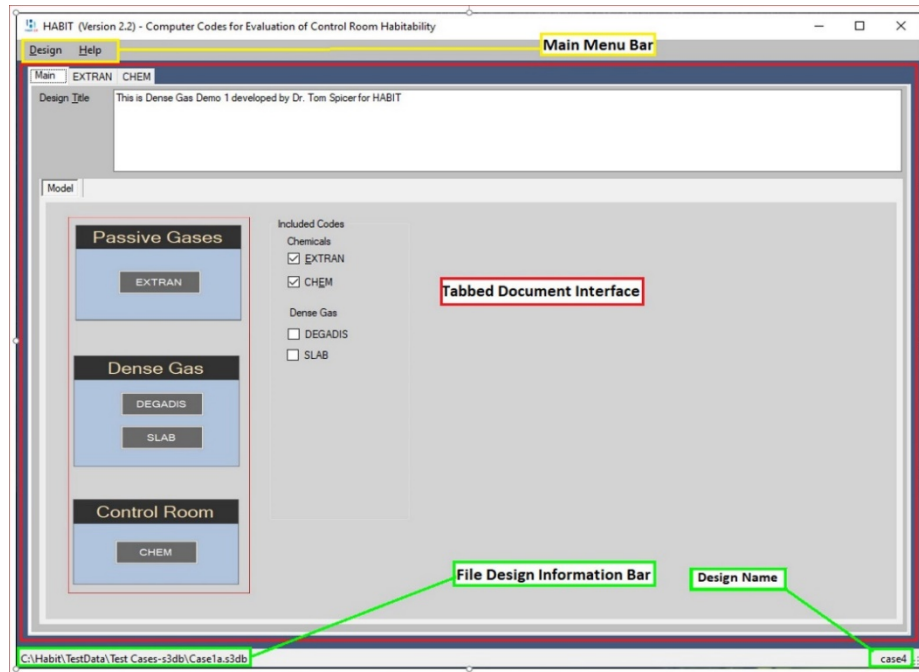
Figure 3-1   HABIT 2.2 Main GUI Window Features

Additionally, the color schemes and configurations chosen for the HABIT 2.2 **Main** GUI window comply with Section 508 of the Rehabilitation Act of 1973, ensuring the accessibility of HABIT 2.2 for people with disabilities. These color schemes are carried through all the models (EXTRAN, DEGADIS, SLAB, and CHEM) on the TDI. The CR flow diagrams use high-contrast colors and share the same color scheme as flow diagrams in other modules.

3.1   Main Menu Bar

As shown in Figure 3-1, the main menu bar provides drop-down menus for the **Design** and **Help** tools.

3.1.1   Design Tool Menu Options

The **Design** tool drop-down menu allows the user to select the following actions:

(1)   **Create New Design**
(2)   **Open Existing Design**

(3)   **Save Design**
(4)   **Save As New Design**
(5)   **Configuration**
(6)   **Exit**

3.1.1.1   Create New Design

To create a new design, select **Create New Design** from the **Design** tool drop-down menu. This will open a new display box like in the center of Figure 3-2 that prompts the user to enter the folder name for the design. Then click the **OK** button to create the new name for the design. Figure 3-2 shows this popup **Enter the name of your Design** box, with instructions and icon embraced by a full-display of HABIT 2.2 desktop.
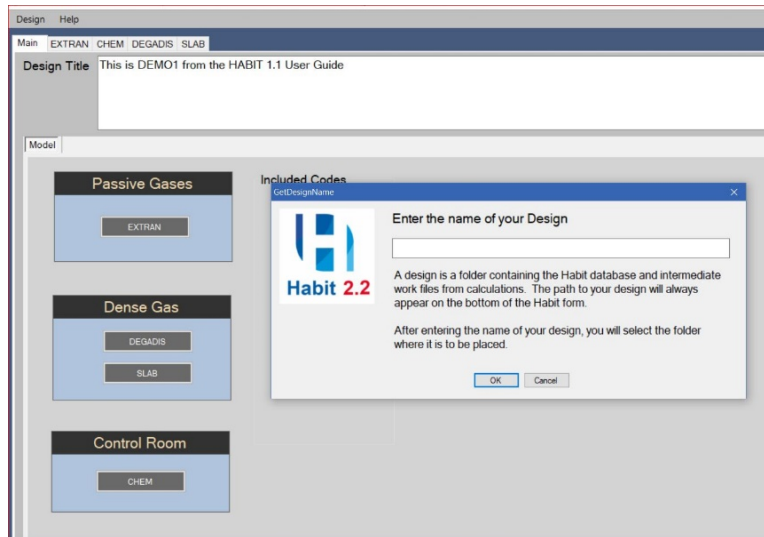
Figure 3-2   Enter the Name of Your Design Box

3.1.1.2   Open Existing Design

To load an existing design, select **Open Existing Design** from the **Design** tool drop-down menu. This will open an MS Windows OS File Explorer window. The user can then browse to the location of an existing folder and select the file to open in that folder. By default, design database files are stored in the user's *My Documents* folder, under the file extension ".s3db." Select the **OK** button to open the existing design. The loaded design will display on the file design information bar as shown in Figure 3-1. The modules included in the design will be loaded. The tabs for the included modules will be available for editing with previously saved values already loaded.

3.1.1.3   Save Design

Select the **Save Design** option from the **Design** tool menu to save in the default database all output files and input files for each module included in the design (".inp" files, etc.). Then select the **OK** button to continue.

3.1.1.4   Save As New Design

Like **Create New Design**, the **Save As New Design** menu option will open an input widow similar to the one shown in Figure 3-2 for creating a new design. Again, the user can enter a file name for the design and click the **OK** button to continue.

3.1.1.5   Configuration

Selecting **Configuration** from the **Design** tool drop-down menu will open the **Configuration** window shown in Figure 3-3. The left side of this window displays each of the computer codes (modules) and overall HABIT design.
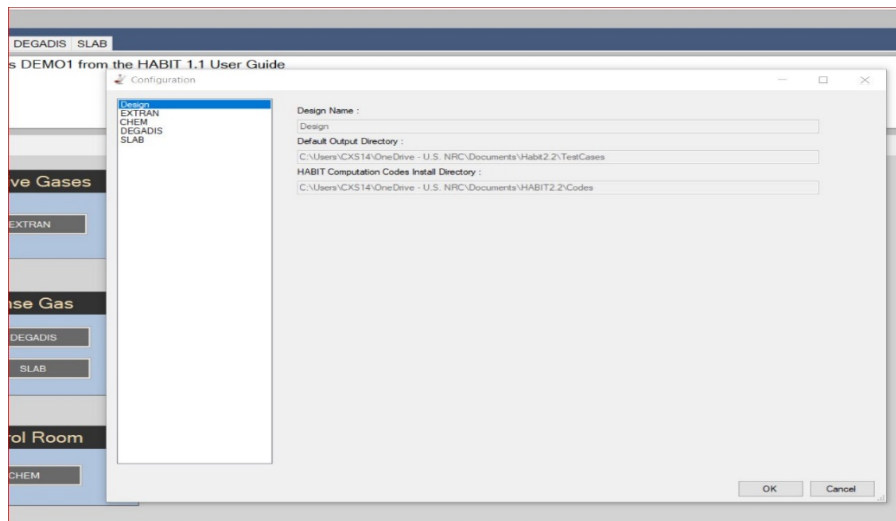
Figure 3-3   Configuration Window Design

The right side of the **Configuration** window displays information about each of the computer codes (modules) and overall HABIT design, such as the location of module executable files and input and output directory locations for each module. Select either the **OK** or **Cancel** button to continue.

3.1.1.6   Exit

The last option under the **Design** tool drop-down menu is **Exit**. Select **Exit** to end the current computation. This may open the **Save Design** window asking the user to save the design. Using the red **X** button method is not preferred for exiting HABIT 2.2 because it could end the program without saving the data.

3.1.2   Help Tool Menu Options

The **Help** tool drop-down menu allows the user to select the following items:

(1)   **User Guide**
(2)   **NUREG/CR-6210**
(3)   **About**

3.1.2.1 User Guide

Select this option to open a PDF file of the HABIT 2.2 user's guide [15].

3.1.2.2 NUREG/CR-6210

Select this option to open a PDF file of NUREG/CR-6210 [4].

3.1.2.3 About

Select **About** to open the window shown in Figure 3-4, which displays the HABIT 2.2 desktop icon and the NRC Technical Reference Model certificate number. Select the **OK** button to return the user to the HABIT 2.2 **Main** GUI (Figure 3-1).
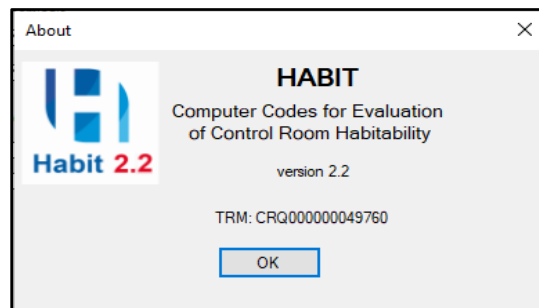
Figure 3-4   About Window

3.2   Tabbed Document Interface

The middle section of the HABIT 2.2 **Main** GUI contains the TDI, which allows all the major functions associated with each tab to be displayed in a single window. Figure 3-5 shows the HABIT 2.2 TDI with the **Main** tab selected and all the available computer code (module) tabs (i.e., EXTRAN, CHEM, DEGADIS, and SLAB).
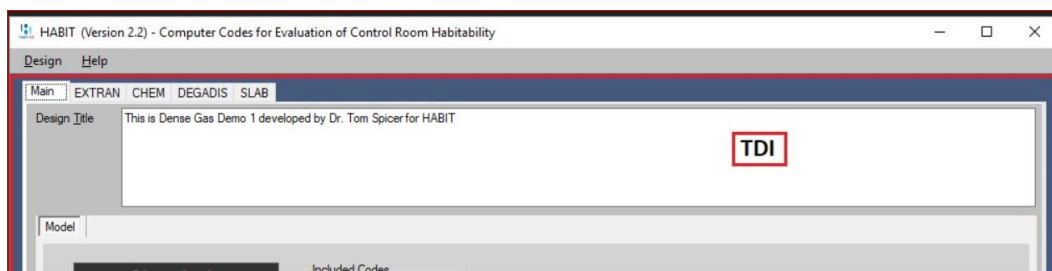
Figure 3-5   TDI Main Tab

All the tabs in the TDI contain GUI widgets that help the user select options on the various tabs. The GUI widget types used in HABIT 2.2 include the following:

- Radio button: This widget is used when the user must select from a list of two or more options that are mutually exclusive. The default selections are the items listed first.

- Check box: This widget is used when the user may select any number of choices (including zero, one, or several) from a list of options. An All Stand Alone check box is used for a single option that the user can either check or un-check.

Finally, the HABIT 2.2 GUI displays field validation warning, field validation error, and module-specific validation error messages when the user-provided input data are in question:

- Field validation warning message: These warning messages alert the user that the required value in the field is wrong or uses a bad syntax, as shown in Figure 3-6. The NRC recommends that these validation warnings be fixed before the codes are run, as the application does allow attempts to run the Fortran code despite the warnings.

- Field validation error message: These validation errors occur when the user attempts to enter alphabetical characters into a numeric field (e.g., Figure 3-7). The user must fix these errors before data entry can continue.

- Module-specific validation error message: This type of validation error message is specific to the EXTRAN module and is produced by the **Check Inputs** button, which checks for all parameters required by the EXTRAN Fortran code. Figure 3-8 shows an example of the validation error message a user could get if inappropriate input is detected.
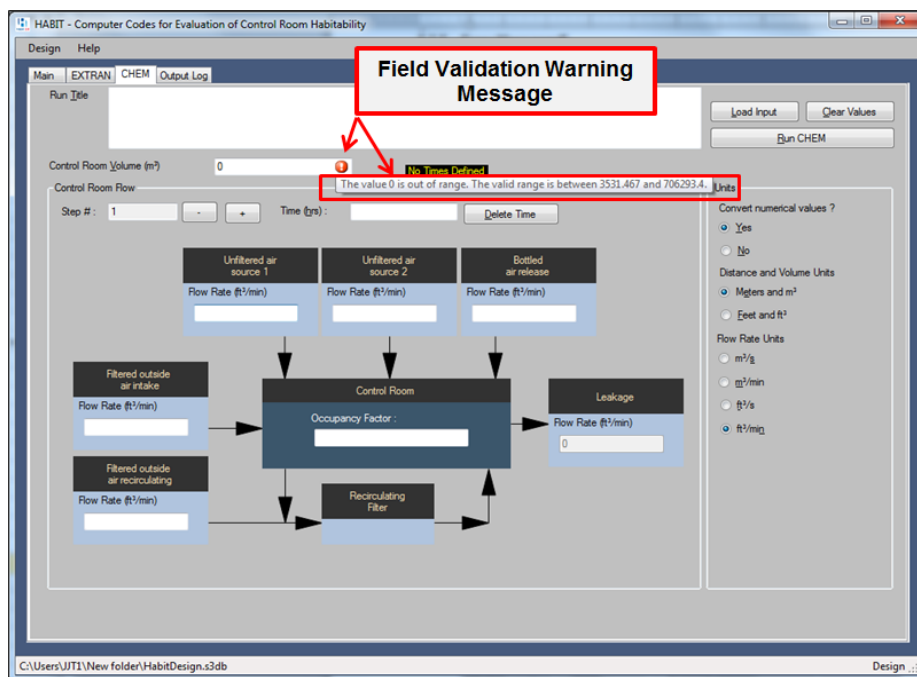
Figure 3-6   Validation Warning Message: Field Input Out of Range
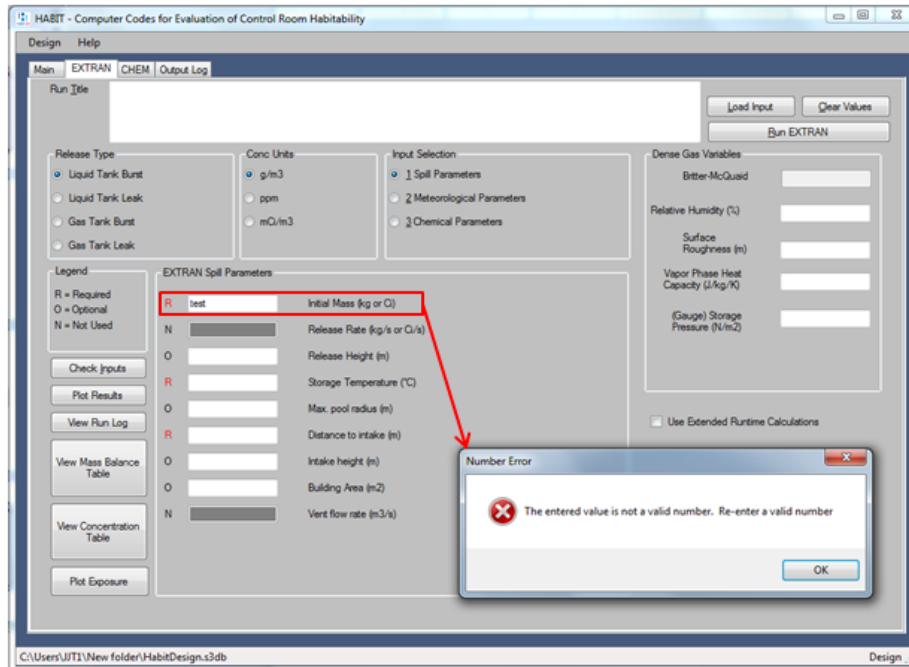
Figure 3-7   Validation Error Message: Number Error
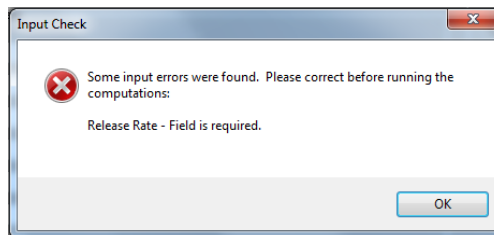
Figure 3-8   A Module-Specific Validation Error Message

3.2.1   Main Tab

The **Main** tab provides a visualization of the HABIT design package. Figure 3-1 and Figure 3-5 show TDI options and the associated modules that were selected. The user can use the **Main** tab to manage the design package. Users have the option to change the modules included in the design and to show only the included modules in the flow diagram.

3.2.2   EXTRAN Tab

HABIT 2.2 uses the EXTRAN module to determine the release rate of a chemical in the event of a release caused by leaks or ruptures of liquid or gas tanks. Figure 3-9 displays the **EXTRAN** tab; Section 4.1 discusses the use and function of each button and field on the tab. The values for the parameters will be pre-populated when imported from a previous design; otherwise, the user can enter the appropriate values. When the mouse pointer is hovered over an input field, the GUI will display the valid range for that field.
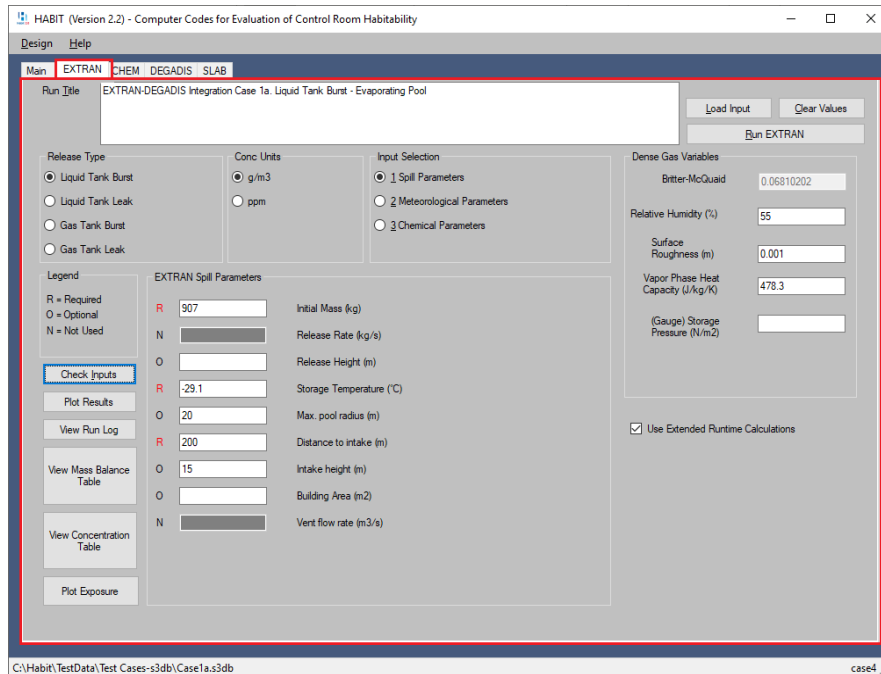
Figure 3-9   TDI EXTRAN Tab

3.2.3   CHEM Tab

The CHEM module estimates the dilution of the chemical that flowed to the CR. Figure 3-10 displays the **CHEM** tab; Section 4.2 discusses the use and function of each button and field on the tab. The **CHEM** tab displays the design of the CHEM module. The values for the parameters will be pre-populated when imported from a previous design; otherwise, the user can enter the appropriate values.
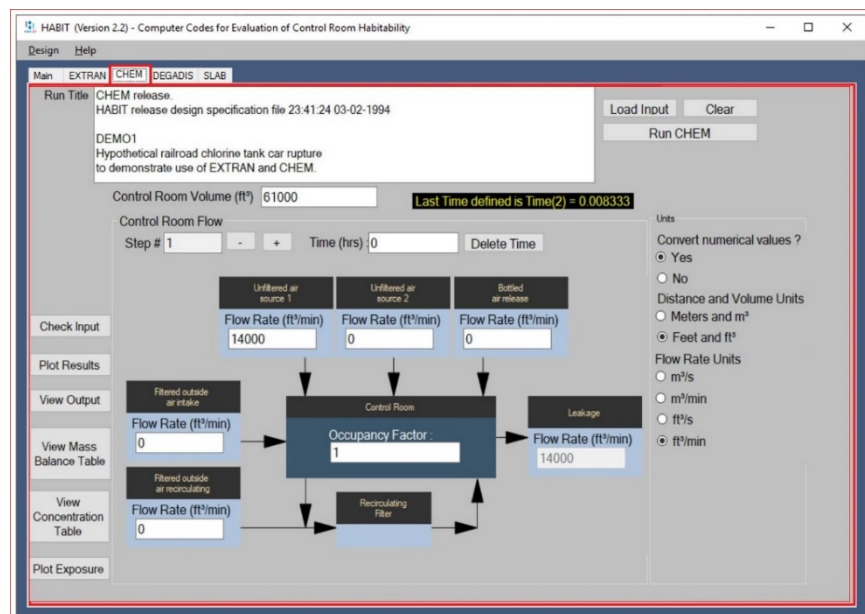
Figure 3-10   TDI CHEM Tab

3.2.4   DEGADIS Tab

The DEGADIS module estimates the releases of chemicals that are dense or slightly heavier than air. As shown in Figure 3-11, the **DEGADIS** tab contains four input tabs: **Atmospheric Parameters**, **Release Specifics**, **Graph**, and **Material Specifics**. Section 4.3 discusses the use and function of each button and field on the four DEGADIS tabs. The values for the parameters will be pre-populated when imported from a previous design or when available from running the EXTRAN module; otherwise, the user can enter the appropriate values.
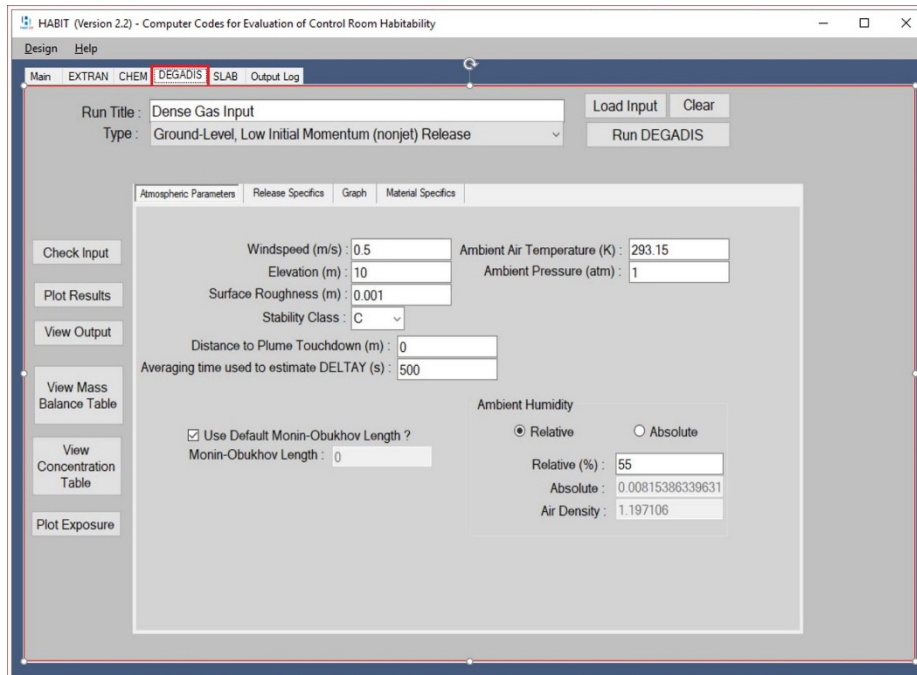
Figure 3-11   TDI DEGADIS Tab

3.2.5   SLAB Tab

HABIT 2.2 uses the SLAB module, like the DEGADIS module, to run releases of chemicals that are dense or slightly heavier than air. SLAB has only one input page, as shown in Figure 3-12. Section 4.4 discusses the use and function of each button and field on the **SLAB** tab. The values for the parameters will be pre-populated when imported from a previous design or when available from running the EXTRAN module; otherwise, the user can enter the appropriate values.
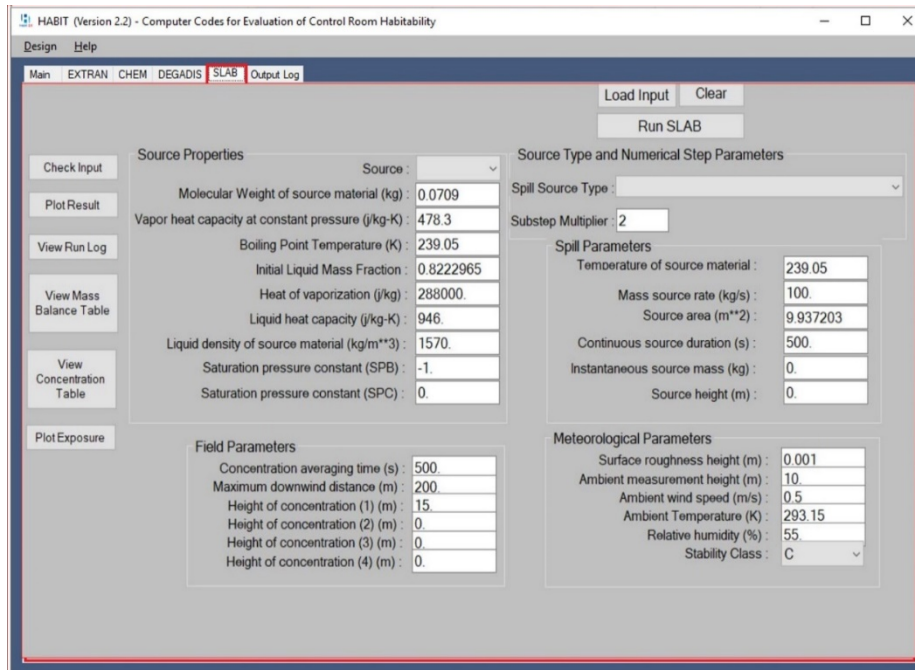
Figure 3-12   TDI SLAB Tab

3.2.6   Output Log Tab

The **Output Log** will be empty at zero activity. However, the user can use it to manage the design package and to direct MS-DOS output from the Fortran formulations and computations so they are visible from within the application, as shown in Figure 3-13. The **Output Log** tab also contains three buttons on the bottom of the window that provide the following additional features:

- Cancel Running Computations button: This button allows the user to cancel any running HABIT 2.2 computations. It is normally only used while running longer executing codes such as DEGADIS and SLAB.

- Clear Log button: This button allows the user to clear the output log screen, as shown in Figure 3-13.

- View Output Directory button: This button opens an MS Windows OS File Explorer window, as shown in Figure 3-14, allowing the user to view the output directory and the files created from the Fortran code. All output file extensions can be found on page 16 of NUREG/CR-6210 [4].
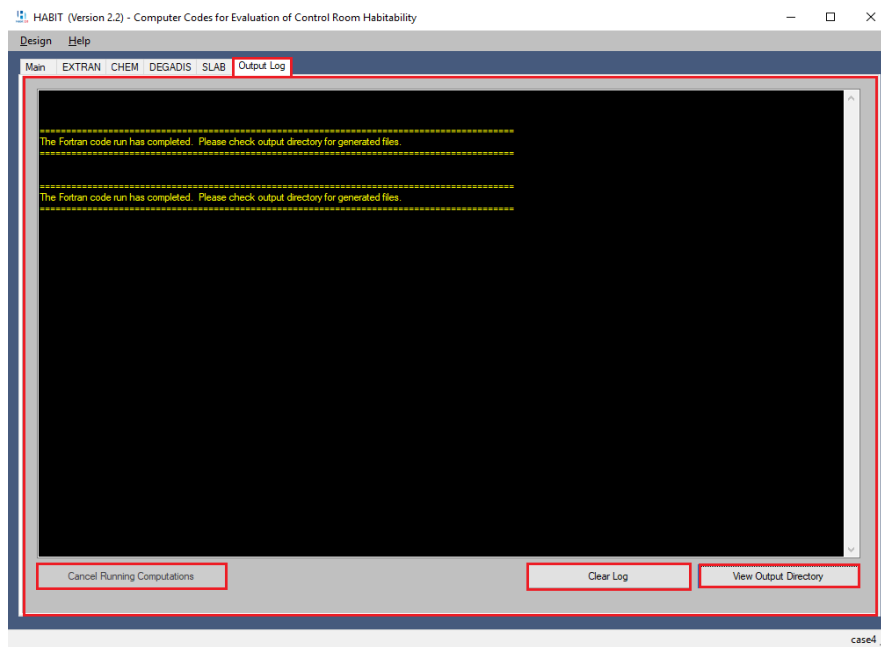
Figure 3-13   TDI Output Log Tab
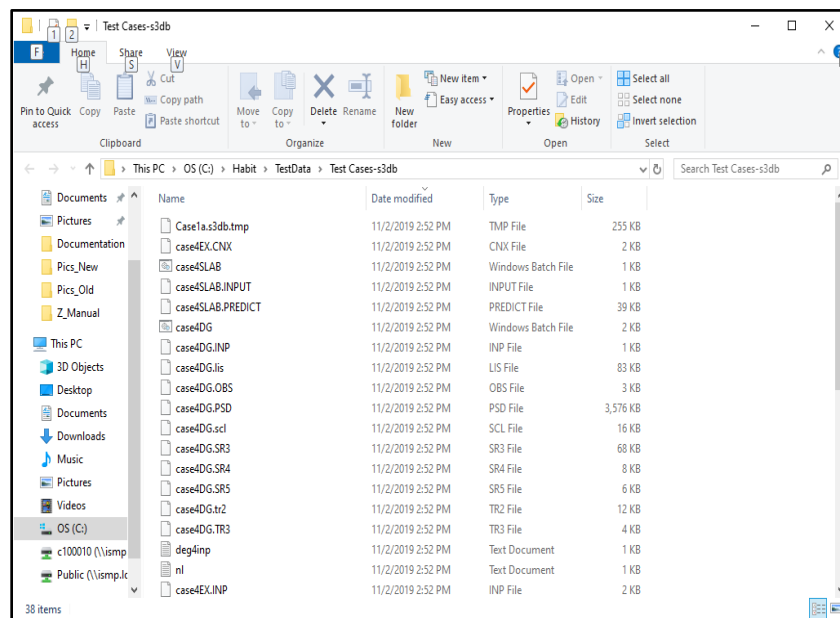
Figure 3-14   HABIT 2.2 Output File Directory

3.3   File Design Information Bar

The file design information bar at the bottom of the GUI window displays information about the currently loaded HABIT design. As shown in Figure 3-1, the bottom right corner shows the name of the loaded design, while the bottom left corner displays the loaded file name (design file name or input file). All file extensions can be found on page 16 of NUREG/CR-6210 [4].

4 HABIT 2.2 MODULES

This section discusses in greater detail the methods used to by each computer code (module) in HABIT 2.2 to assess the potential effects of accidental releases of toxic substances on the habitability of a nuclear power plant CR. Section 4.1 discusses the technical basis of EXTRAN and the features of the **EXTRAN** tab on the TDI of the HABIT 2.2 **Main** GUI. Section 4.2 discusses the technical basis of CHEM and the features of the **CHEM** tab on the TDI. Section 4.3 discusses the technical basis of DEGADIS and the features of the **DEGADIS** tab on the TDI. Section 4.4 discusses the technical basis of SLAB and the features of the **SLAB** tab on the TDI.

Figure 4-1 shows the workflow path performed by HABIT 2.2 as the user evaluates the effects of accidental releases of toxic substances on CR habitability.
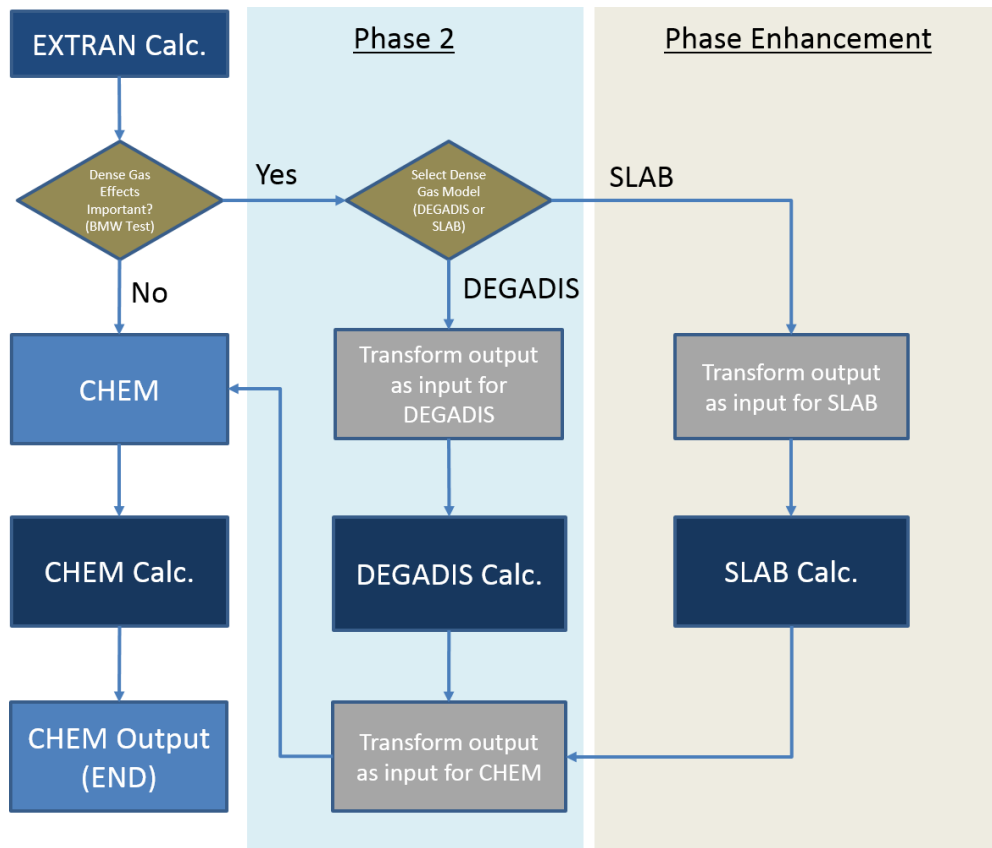
Figure 4-1   HABIT 2.2 Flowchart

EXTRAN estimates the rate at which material becomes airborne so DEGADIS and SLAB can then calculate atmospheric dispersion calculations to determine the impact. The output of EXTRAN often uses in some cases to provide the rate the released material becomes airborne, particularly for evaporating liquid pools. After EXTRAN performs its calculation, HABIT 2.2 will use the BMW criteria [16] [17] to evaluate the release to determine the importance of denser-than-air effects. The BMW criteria propose correlations for modeling the dispersion of

denser-than-air contaminants from area sources for plumes and puffs based on field test data. Both DEGADIS and SLAB are strictly atmospheric dispersion models in the sense that they require the airborne rate of the dispersing material, which must be provided by the user. The analysis of the field test data identified the dominant independent variables as (1) density of released contaminant after depressurization to atmospheric pressure, (2) volumetric release rate or total volume released, (3) characteristic wind speed, and (4) characteristic source dimension. The correlations proposed by the BMW criteria are also limited by the lowest concentrations that could be predicted (1,000 to 2,000 parts per million (ppm)), but they also propose criteria by which the importance of denser-than-air effects can be assessed. The BMW criteria indicate that for steady-state or continuous (plume) releases, denser-than-air effects are important based on Equation (4-1).

$$\frac{g\left(dm/\rho_s\right)}{D_s\, U_r^3} \left(\frac{\rho_s - \rho_a}{\rho_a}\right) > 0.0034 \qquad (4\text{-}1)$$

where g = is the gravitational acceleration constant (m/s^2)
       dm = is the release rate (kg/s)
       ρ_s = is the density of the chemical substance (kg/m^3)
       D_s = is the is the (low-momentum) horizontal dimension of the source (m)
       U_r = is the wind speed at 10 m (m/s)
       ρ_a = is the ambient air density (kg/m^3)

The BMW criteria for instantaneous (puff) gas releases, denser-than-air effects are important based on Equation (4-2).

$$\frac{g\left(m/\rho_s\right)^{1/3}}{U_r^2} \left(\frac{\rho_s - \rho_a}{\rho_a}\right) > 0.04 \qquad (4\text{-}2)$$

where g = is the gravitational acceleration constant (m/s^2)
       m = is the total mass of released material (kg)
       ρ_s = is the density of the chemical substance (kg/m^3)
       U_r = is the wind speed at 10 m (m/s)
       ρ_a = is the ambient air density (kg/m^3)

For examples, the choice of values to be used in the BMW criteria depends on the release type and ambient wind speed, and how they are modeled in EXTRAN.

HABIT 2.2 will not automatically run the denser-than-air models of DEGADIS and SLAB but will inform the user that "**The Britter-McQuaid Workbook method has determined that the dense-gas effects are important to this run**," as shown in Figure 4-2. The selection buttons on the window shown in Figure 4-2 allow the user to select the model to be used to perform the dense gas calculations. It is important to note that these selection buttons do not actually perform the dense gas calculations of DEGADIS and SLAB but rather allow EXTRAN to create DEGADIS and SLAB input files based upon common input parameters used in all three codes. For example, the **DEGADIS** button and the **SLAB** button allow user to run the system separately using the system creates input files (i.e., "DesignDG.inp" and "DesignSLAB.inp" files), respectively. Additionally, the user can either choose to simultaneously create both the DEGADIS and SLAB code input files by selecting the **All Models** button or choose to not create the dense gas code input files by selecting the **Skip Dense Gas** button.
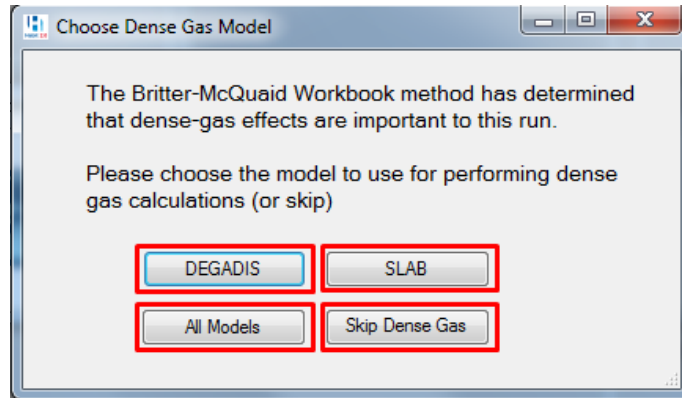
Figure 4-2 Choose Dense Gas Model Window

4.1 EXTRAN Module

4.1.1 EXTRAN Code Description

As used in HABIT 2.2, the EXTRAN module is a tool to estimate short-term concentrations at a single location downwind (CR intake) of a release of toxic substance. The code estimates the amount of toxic material entering the atmosphere and then models the movement of the material downwind as it diffuses. The **EXTRAN** tab provides a user-friendly method to calculate the concentrations from accidental releases of toxic substances at nuclear power plant CR air intakes.

4.1.1.1 General Description

As noted in NUREG/CR-6210 [4], EXTRAN was originally developed by Pacific Northwest National Laboratory after reviewing procedures used by the NRC for estimating atmospheric transport and diffusion for CR habitability assessments [20]. EXTRAN combines procedures for estimating the amount of airborne material, a Gaussian puff model, and building-wake diffusion coefficient algorithms [8].

This document uses the phrase "toxic substance" in its discussion of EXTRAN; however, it should be noted that many other liquids and gases satisfy the physical assumptions stated below and can, therefore, be modeled by EXTRAN. One notable case is that many explosive gases and liquids that produce explosive gases can be modeled by EXTRAN.

Using EXTRAN, the user postulates a release scenario for a toxic substance, including the environmental conditions and the physical and chemical characteristics of the substance. EXTRAN will calculate a concentration time history at the CR room air intake from the time the substance first arrives at the air intake until actions can be taken to protect CR occupants.

4.1.1.2 EXTRAN Source Term

EXTRAN will compute the concentrations of toxic substances for both gases and liquid accidental releases as described in Section 6.2 of NUREG/CR-6210 [4]. When modeling the source from a gas tank burst or leak, the user inputs the specifications for the source term by entering the mass of material in the tank and the leak rate. As described in NUREG/CR-6210 [4], the mass balance associated with gaseous releases is simply all the material leaving the

tank that directly enters the atmosphere. EXTRAN does not maintain an energy balance for gaseous releases. If the scenario involves a catastrophic failure of a tank containing a gas, it assumed all the gas enters the atmosphere at the time of the failure.

EXTRAN assumes that when a tank containing liquefied gases or volatile liquids fails, the material is distributed between the tank, a pool in the vicinity of the tank, and in a plume in the atmosphere downwind of the tank. EXTRAN computes the atmospheric source term from user-supplied information about the liquid's material properties, its storage conditions, and the environment. The concentrations at the CR intake can only be made if material can be realistically distributed between these locations as a function of time following the release. Mass must not be gained or lost between the release point and the receptor. The factors and equations used by EXTRAN to calculate the mass balance for liquefied gases and volatile liquids are described in Section 6.2.1.B.a of NUREG/CR-6210 [4]. The factors and equations used by EXTRAN to calculate the energy balance for liquefied gases and volatile liquids are described in Section 6.2.1.B.b of NUREG/CR-6210 [4].

4.1.1.3   EXTRAN Transport and Diffusion

As noted in Section 6.2.2 of NUREG/CR-6210 [4], EXTRAN includes a Gaussian puff dispersion model. The Gaussian puff model permits a more realistic treatment of temporal variations in release source terms and concentrations. Section 6.2.2.A of NUREG/CR-6210 [4] provides the parameters and equations used by the Gaussian puff model in EXTRAN to disperse the toxic substances downwind. Concentrations of the toxic substances in the puffs are directly proportional to the mass that is included in the puff. If the toxic substance is a liquefied gas and both flashing and evaporation are occurring, two puffs will be released simultaneously. One of these puffs will have the mass of the liquid that has flashed from Equation (6.1) of NUREG/CR-6210, and the other will have the mass that has evaporated from Equation (6.3) of NUREG/CR-6210 [4]. Otherwise, only one puff will be released, and the mass in the puff will be determined using Equation (6.3) of NUREG/CR-6210 [4].

Section 6.2.2 of NUREG/CR-6210 [4] also discusses the factors and equations affecting the diffusion coefficients and transportation of the puffs of the toxic substance downwind from the release point. In general, the diffusion coefficients increase with increasing distance from the source and generally decrease as the atmosphere becomes more stable. Equation (6.23) of NUREG/CR-6210 [4] shows that the decrease in concentrations in puffs as they move downwind is due only to increases in the magnitudes of the diffusion coefficients. Finally, puffs are assumed to move with the wind directly from the release point to the CR air intake. The time required for material to arrive at the CR the intake is determined by the wind speed and the growth of the puffs.

4.1.2   EXTRAN TDI Features

4.1.2.1   General Features of the EXTRAN TDI Tab

The user should be aware of some of the basic features associated with the **EXTRAN** tab in the HABIT 2.2 TDI as shown in Figure 4-3. The values for the parameters will be pre-populated when imported from a previous design; otherwise, the user can enter the appropriate values. When the mouse pointer is hovered above an input field, the code will display bubble help with the valid range for that field. Additionally, as shown in Figure 4-3, the **EXTRAN** tab contains a **Legend** section that provides the user with general guidelines about the input of various parameters. There are three types of parameters:

(1)   required input parameters, indicated by a red "**R**" label next to the parameter input field
(2)   optional input parameters, indicated by an "**O**" label next to the input field
(3)   not used input parameters, indicated by an "**N**" label next to the input field
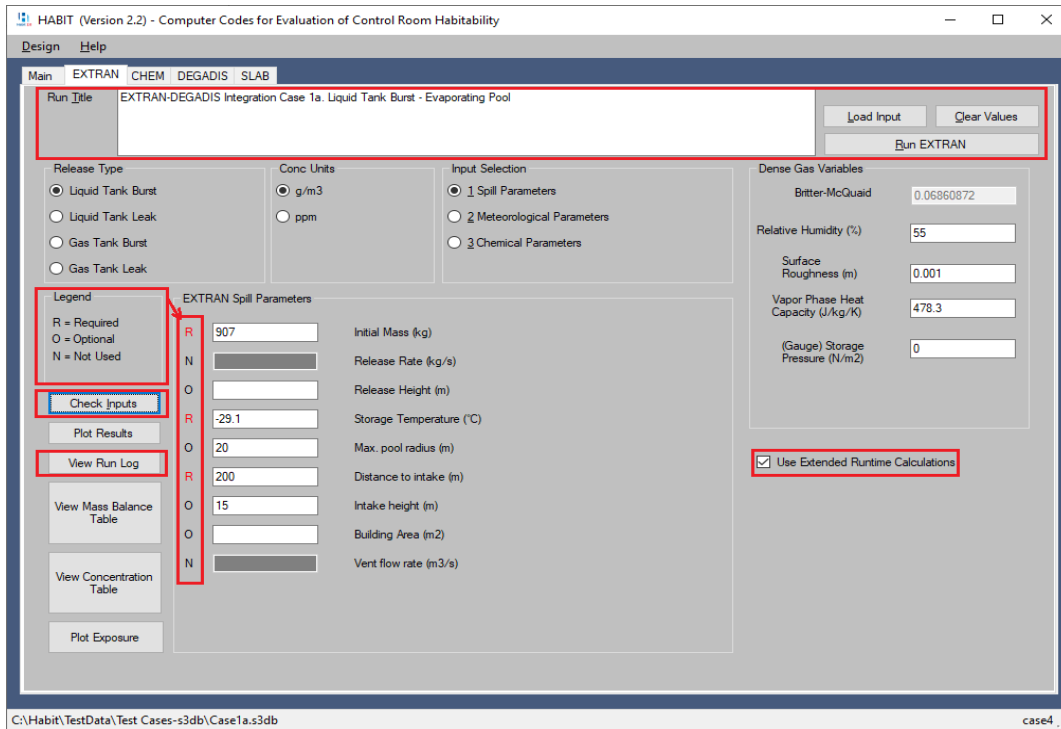
Figure 4-3   EXTRAN Tab General Features

The other general features on the **EXTRAN** tab include the following:

- The **Run Title** input text box is where the user can input a title and a brief description of the EXTRAN run. This input text box has an 80-character limit.

- The **Load Input** button opens an MS Windows OS File Explorer window, as shown in Figure 4-4. The user can then browse to the location of an existing folder and select the EXTRAN input file (i.e., "DesignEX.inp") to open in that folder. Select the **Open** button to open the existing design.
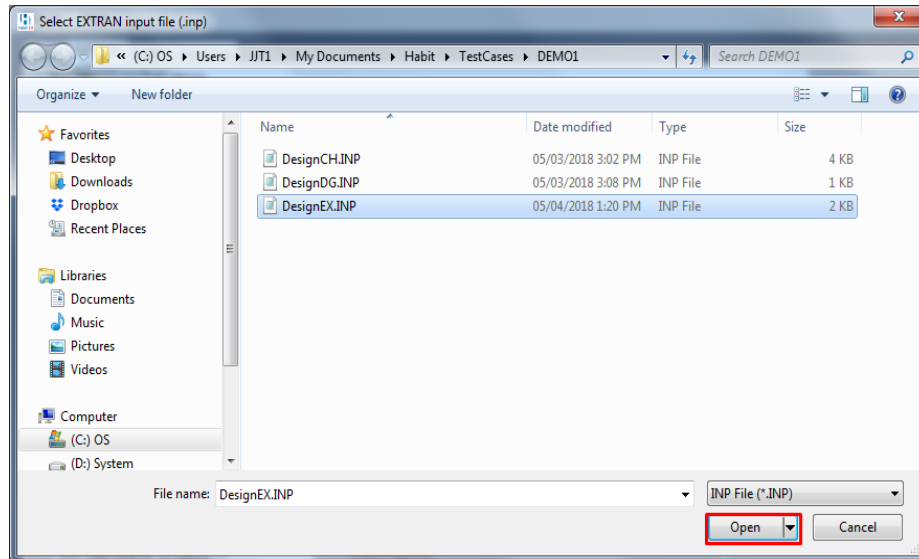
Figure 4-4   Select EXTRAN Input File (.inp) Window

- The **Clear Values** button clears all values of EXTRAN input parameters from the tab and starts over with blank parameter input fields. Selecting this button will open the **Clear Form** confirmation window shown in Figure 4-5. Selecting the **Yes** button shown in Figure 4-5 will clear all the current values from the tab and return the user to a blank **EXTRAN** tab. Selecting the **No** button will retain the current values and return the user to the **EXTRAN** tab.
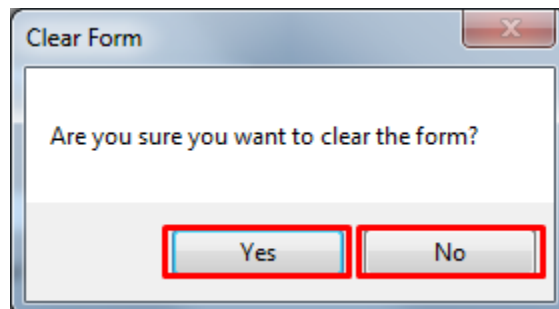
Figure 4-5   Clear Form Window

- The **Run EXTRAN** button will execute the program against the user-provided input parameters in the **EXTRAN** tab. If there are any errors not corrected prior to selecting this button, the code will display a warning message as shown in Figure 4-6. To close this message window, select the **OK** button; a red exclamation point icon will appear to the right of the missing required input parameters field as shown in Figure 4-7.
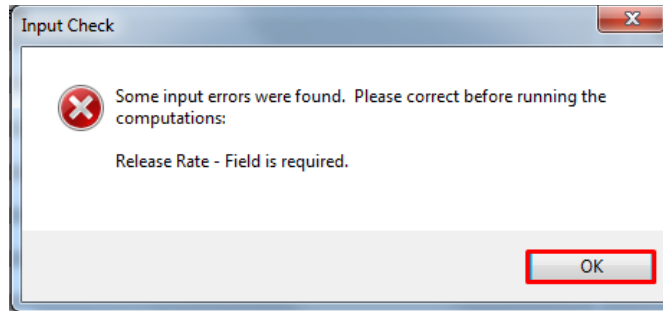
Figure 4-6   Warning Message in Input Check Window
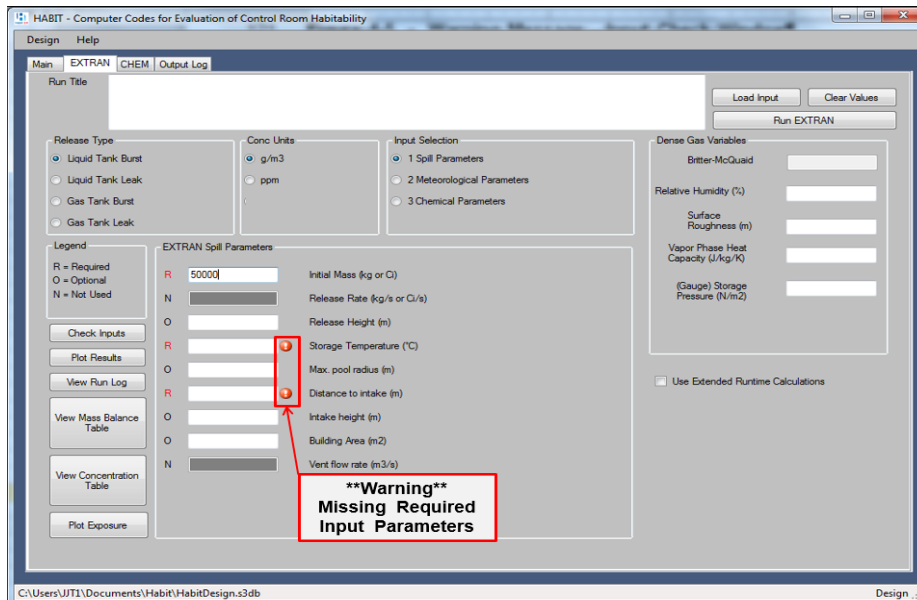
Figure 4-7   EXTRAN Tab Indication of Missing Required Input Fields

- The **Check Inputs** button will perform required field validation on all required input parameters and provide a report to the user on the status of all required input parameter fields. If required input parameters are missing from the EXTRAN model, the warning window shown in Figure 4-6 will appear. If all required EXTRAN input parameters are entered, the validation message shown in Figure 4-8 will appear. Selecting the **OK** button will close this window.
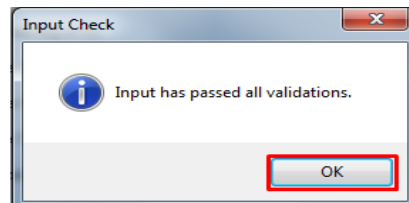
Figure 4-8   Validation Message in Input Check Window

- The **View Run Log** button will open the **EXTRAN Output Log** window as shown in Figure 4-9. Similar to the HABIT 2.2 TDI **Output Log** tab described in Section 3.2.6, this

4-7

window will allow the user to view the MS-DOS output from the EXTRAN Fortran formulations.
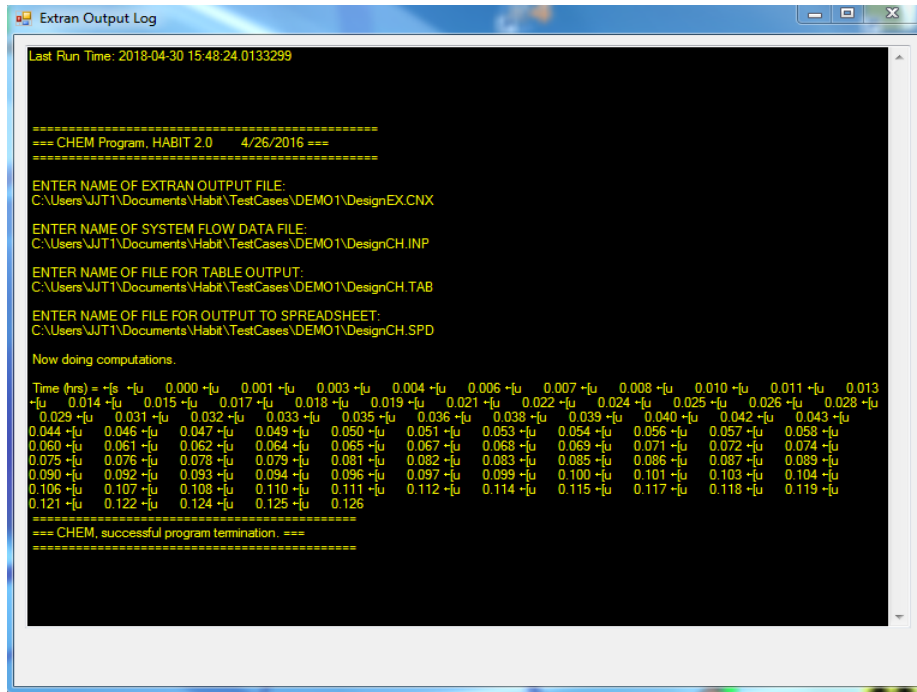
Figure 4-9   EXTRAN Output Log Window

- The **Use Extended Runtime Calculations** check box shows in Figure 4-3. If checked, it allows the code to predict extended operation for 24 hours. If **Use Extended Runtime Calculations** is unchecked, the default runtime is 2 hours only. If an impacted receptor (i.e., CR, TSC, EOF) is further than 99 m from the chemical release point, HABIT 2.2 allows 24 hours runtime automatically as the maximum for environmental transport calculations.

4.1.2.2   Release Type Section

The **EXTRAN** tab **Release Type** section has radio buttons for four options of the types of chemical releases, as shown in Figure 4-10: (1) **Liquid Tank Burst**, (2) **Liquid Tank Leak**, (3) **Gas Tank Burst**, and (4) **Gas Tank Leak**. The two liquid options deal with materials stored as liquids, and the two gas options deal with materials stored as gases. EXTRAN models flashing liquid releases assuming the liquid phase completely rains out on the ground. The **Liquid Tank Burst** and **Gas Tank Burst** options are used for cases in which the tank fails catastrophically and empties instantaneously. The **Liquid Tank Leak** and the **Gas Tank Leak** options are used for cases in which the release takes place over some time interval. Generally, the burst options result in a greater maximum concentration than the tank leak options. However, the tank leak options may be the more realistic failure modes. Finally, it is possible to approximate a tank burst with the tank leak option by increasing the magnitude of the leak rate.
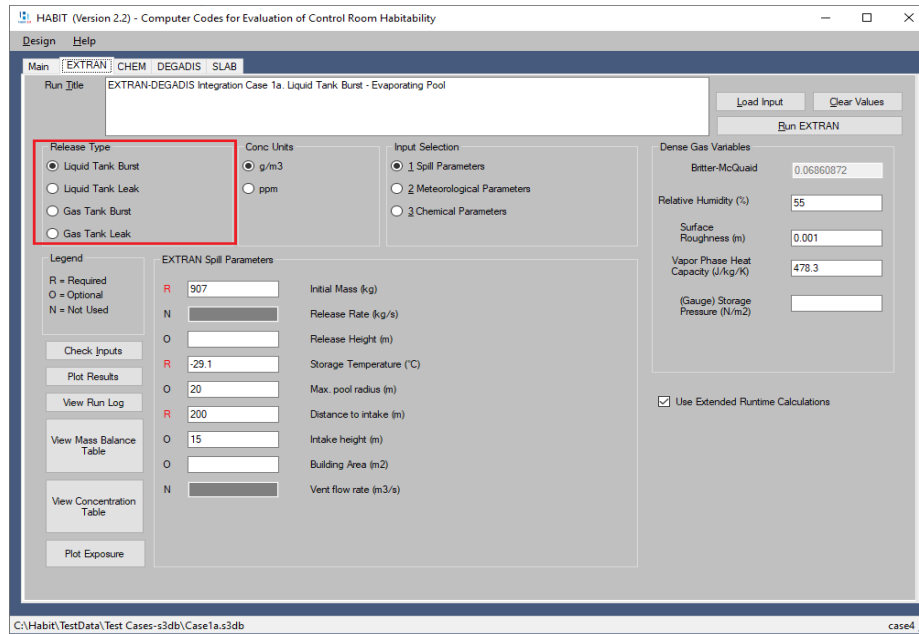
Figure 4-10   EXTRAN Tab Release Type Section

4.1.2.3   Concentration Units Section

The **EXTRAN** tab contains two options for the concentration units for chemicals under the **Conc Units** section, as shown in Figure 4-11. The two options for concentration units are grams per cubic meter (g/m^3) and parts per million (ppm). The units specified by the user in the **EXTRAN** tab will also be used in **CHEM** tab. The default set of units is g/m^3.
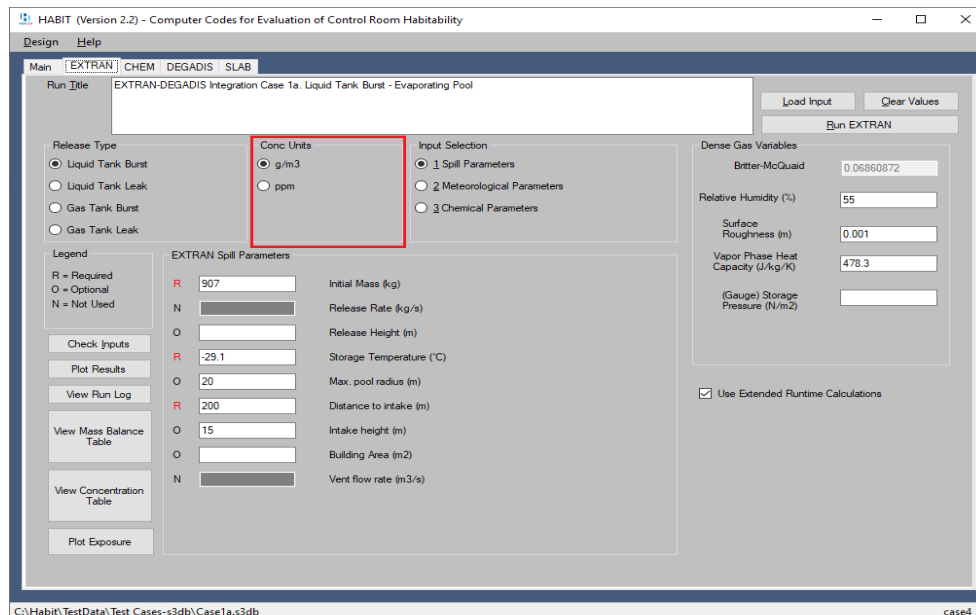
Figure 4-11   EXTRAN Tab Concentration Units Section

4.1.2.4   Input Selection Section

The **EXTRAN** tab **Input Selection** section contains three options for the input, as shown in Figure 4-12. Each of these options is linked to the **EXTRAN Input Parameters** section in the middle of the **EXTRAN** tab. The three input selections for the concentration units are (1) **Spill Parameters**, (2) **Meteorological Parameters**, and (3) **Chemical Parameters**. The rest of this section describes the input parameters for each of these options.

EXTRAN Spill Parameters: This set of parameters is used to define the physical scenario associated with a potential accident as shown in Figure 4-12. These input fields describe the type of accident, amount of material, where the release occurs in relation to the intake, and how the material enters the atmosphere. The input spill parameters are as follows:

- Initial Mass: This is the actual amount of material in the tank at the time of failure. The mass amount should be entered in kilograms (kg) at the time of the failure, not the amount of material that the tank could contain. This is a required field for all four EXTRAN release types. The valid range of values for this field is from 0 to $1x10^6$ kg.

- Release Rate: This parameter is only used for **Liquid Tank Leak** and **Gas Tank Leak** release types and is required in both cases. The release rate should be entered in kilograms per second (kg/s) and will remain constant at the entered value until the tank is empty. When the tank is empty, the release rate will be set to zero. The valid range of values for this field is from 0 to $5x10^5$ kg/s.
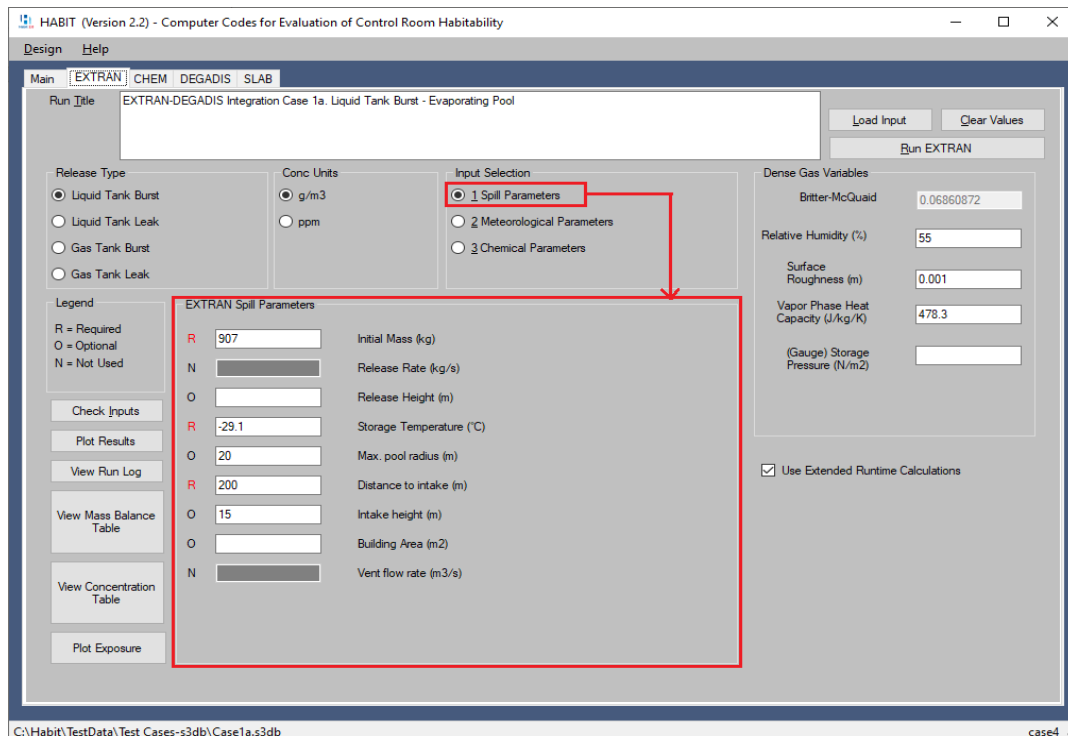
Figure 4-12   EXTRAN Tab Input Section for Spill Parameters

- Release Height: For a liquid, this is the height in m of the pool above the ground and not the height of the hole in the tank. For a gas, the release height may be the height of the

hole. Release heights greater than zero may result from failure of a tank on a flat roof or loss of the top of a large tank. In the first of these situations, the pool might be formed on the roof; in the second, the pool may be within the original tank. Use ground level near the CR air intake as the reference height. This is an optional field for all four EXTRAN release types. The valid range of values for this field is from 0 to 1.5×10^2 m.

- Storage Temperature: This is the temperature for the storage tank in degrees Celsius (°C). It is a required field for all four release types in EXTRAN. This temperature determines the expansion of gases upon release and the rate of evaporation of liquids. Typically, the tank temperature should be near the air temperature unless the tank is cooled or heated. The valid range of values for this field is between -40 and 50 °C. In estimating the tank temperature, users should also consider factors such as the size of the tank, the exposure of the tank to solar radiation, the insulation of tank, and perhaps the time of day and time of year. A temperature near the daytime high temperature for the season may be a reasonable choice for the tank temperature.

- Maximum Pool Radius: This is the maximum estimated radius of the spill pool in meters. Most large tanks are typically surrounded by berms for the purpose of containing spills from the tank. If the release type selected is a liquid tank burst or leak, then it may be appropriate to specify a maximum pool radius. This is an optional field for both the **Liquid Tank Leak** and the **Liquid Tank Burst** release types and is not used for the **Gas Tank Leak** and the **Gas Tank Burst** release types. If no value or a zero value is entered, the code will assume that a berm does not exist, and the code will spread the liquid without horizontal restriction until the pool depth decreases to 0.01 m. The valid range of values for this field is from 0 to 100 m.

- Distance to Intake: This is the distance from the release point to the CR intake in units of m. It is important to remember that concentrations in plumes decrease as the distance from the release point increases. If there are structures between the tank release point and the CR intake, enter a distance corresponding to the shortest possible path the material could take to the CR intake. This is a required field for all four EXTRAN release types. The valid range of values for this field is from 0 to 1×10^4 m.

- Intake Height: This is the intake height in m above the reference height level. The reference height for EXTRAN is ground level near the CR air intake. Concentration estimates are sensitive to the difference between the release height and the intake height when the distance between the tank and intake is small. As the distance increases, this sensitivity decreases. Maximum concentration estimates can be obtained by setting both the release height and intake height to zero. If the release and intake heights are the same but are not equal to zero, the concentration will be up to a factor of 2 lower than when the heights are equal to zero. This is an optional field for all four EXTRAN release types. The valid range of values for this field is from 0 to 100 m.

- Building Area: EXTRAN includes a model to estimate diffusion in the wakes of buildings and structures. This value is the estimate of the cross-sectional area in units of square meters (m^2) of the structure projected on a plane perpendicular to the wind direction. The user should note that the area requested is the area of the tank or a structure near the tank and that it is not necessarily the area of the reactor containment building or of the CR air intake structure. If the area is zero, the enhanced diffusion due to the wake of the structure will be neglected. This is an optional field for all four EXTRAN release types. The valid range of values for this field is from 0 to 100 m^2.

- Vent Flow Rate: This is the volume per unit in units of cubic meters per second (m^3/s) of air leaving the tank vent if the release is through a vent. This is an optional field for the **Gas Tank Leak** release type and is not used for the other three EXTRAN release types. Within EXTRAN, the vent flow rate prevents the concentration at the intake from becoming unreasonably large. When the vent flow is greater than zero, concentrations in the environment cannot become larger than the concentration in the vent. The vent flow is particularly important when the distance between the release point and air intake is small. The valid range of values for this field is from 0 to 50 m^3/s.

EXTRAN Meteorological Parameters: This set of parameters is used to define the meteorological (environmental) conditions at the time of the release, as shown in Figure 4-13. EXTRAN uses the meteorological parameters in calculations in various ways. As a result, no single set of meteorological parameters can be given the label "worst case." Worst case conditions must be determined by trial and error considering the physical scenario and the material. For example, sometimes worst case conditions involve low wind speeds. However, if the release is in a building wake and involves a volatile liquid, worst case conditions involve high wind speeds.

In selecting a set of meteorological conditions for EXTRAN, maintain consistency within the parameter set. For example, a combination of high temperature, high solar radiation, and strongly stable atmospheric conditions leads to larger concentrations than high temperature, high solar radiation, and unstable atmospheric conditions. But the latter combination is realistic, while the former is not. Thus, the former set ought not to be used in CR habitability assessments. The input meteorological parameters are as follows:

- Wind Speed: This is the wind speed at a height of 10 m above ground level in units of meters per second (m/s). It is used in computing evaporation rates, diffusion, and transport. Depending on the specific scenario, increasing the wind speed may increase or decrease the predicted maximum concentration. If the scenario involves evaporation or wake diffusion, increasing the wind speed is likely to result in an increase in the maximum concentration. Otherwise, an increase in wind speed will decrease the concentration. This is a required field for all four EXTRAN release types. The valid range of values for this field is from 0 to 30 m/s.

- Atmospheric Stability Class: Atmospheric stability classes are defined in Table 2-2 of RG 1.23, Revision 1, "Meteorological Monitoring Programs for Nuclear Power Plants," issued March 2007 [21]. This parameter field has a drop-down menu with options **A** through **G**, ranging from extremely unstable **A** to extremely stable **G**. The atmospheric stability is determining the dilution factor of the plume concentration from the release source to the CR air intake. If there is no building wake involved, the atmospheric stability has a significant effect on the maximum concentration. Otherwise, the effect of stability on concentration is small. **Atmospheric stability class** is a required field for all four EXTRAN release types.

- Air Temperature: This is the environmental ambient air temperature in units of °C. The ambient air temperature determines if a liquid will flash or not. It is also a factor in the energy balance that determines the rate of evaporation from pools, and it determines the volume occupied by gases. In general, increasing the air temperature increases the maximum concentration at the CR air intake following liquid releases and decreases the concentration following gas releases. EXTRAN converts the air temperature to Kelvin (K) as needed within the code to perform calculations. **Air temperature** is a required

field for all four EXTRAN release types. The valid range of values for this field is from negative 40 to 50 °C.
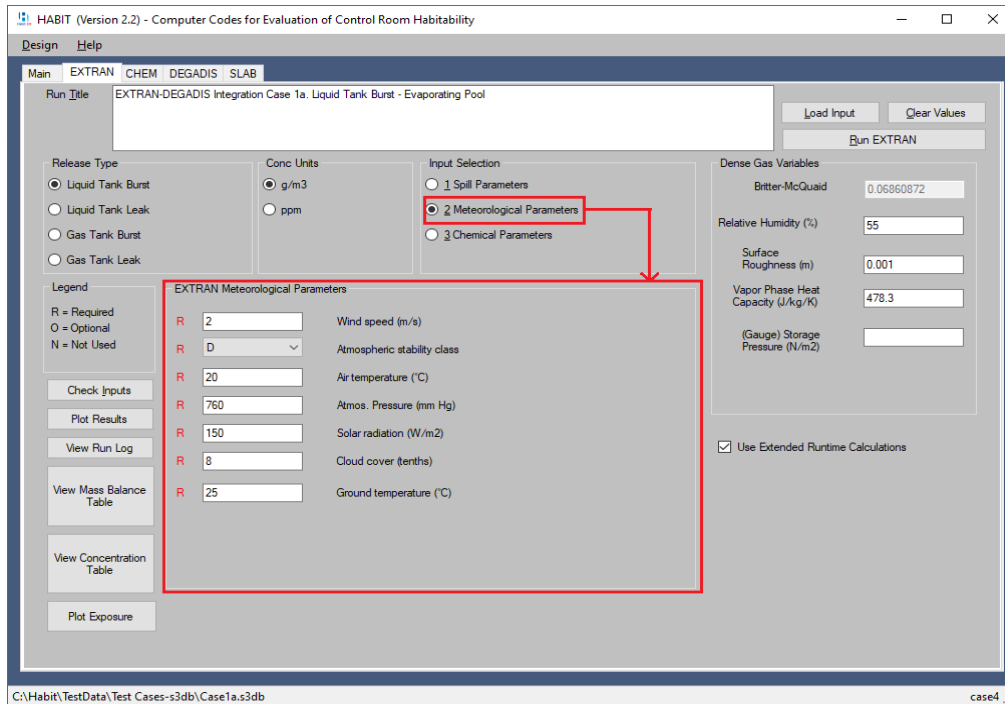
Figure 4-13   EXTRAN Tab Input Section for Meteorological Parameters

- Atmospheric Pressure: This is the environmental atmospheric pressure in units of millimeters of mercury (mmHg). Atmospheric pressure is used in adjusting the air density, the boiling point of liquids, and the saturation vapor pressure. Atmospheric pressures in other units (i.e., in inches, millibars, pounds per square inch, or other units) must be converted to mmHg. A range of typical atmospheric pressures is from 600 to 800 mmHg. This range is larger than would be reasonable for a single location because pressure is a function of elevation. The upper end of the range (720 to 800 mmHg) is appropriate for sea-level locations. The lower end of the range (600 to 670 mmHg) is appropriate for elevations of 5,000 to 6,000 feet above sea level. **Atmos. Pressure** is a required field for all four EXTRAN release types. The valid range of values overall for this field is from 600 to 800 mmHg.

- Solar Radiation: During the day, solar radiation adds energy to the liquid pool, thereby increasing the evaporation rate. Therefore, this meteorological parameter is required for both the **Liquid Tank Leak** and the **Liquid Tank Burst** release types and is not used for the **Gas Tank Leak** and the **Gas Tank Burst** release types. The solar radiation parameter is in units of watts per square meter (W/m^2). For nighttime release, the user should enter a value of 0 W/m^2. During the day, solar radiation is a function of latitude, season, and time of day. The data in Tables 6.1 and 6.2 of NUREG/CR-6210 [4] provide some guidance for selection of reasonable solar radiation values. The valid range of values for this field is from 0 to 1.2x10^3 W/m^2.

- Cloud Cover: Cloud cover is the fraction of the sky covered by clouds. It is used in calculating the long-wave solar radiation from the atmosphere. During the daytime,

long-wave solar radiation will add energy to liquid pools, thereby increasing the evaporation rate. Therefore, this meteorological parameter is required for both the **Liquid Tank Leak** and the **Liquid Tank Burst** release types and is not used for the **Gas Tank Leak** and the **Gas Tank Burst** release types. Cloud cover is entered in units of tenths. For example, if clouds cover half the sky, the cloud cover would be entered as 5 and EXTRAN converts the 5 to 0.5. EXTRAN makes an initial estimate of the long-wave radiation from the air temperature and then refines this estimate using the cloud cover. Cloud cover increases the long-wave solar radiation flux to the liquid pool. This increase ranges from 0 to 60 W/m^2. Table 6.2 of NUREG/CR-6210 [4] provides some guidance in observed cloud cover values. However, users should model releases with both 0 and 10 tenths to understand the effects of cloud cover on the release scenario. The valid range of values for this field is from 0 to 10 tenths.

- Ground Temperature: Along with the pool temperature, ground temperature controls the energy flux from the ground to the pool. Therefore, this meteorological parameter is required for both the **Liquid Tank Leak** and the **Liquid Tank Burst** release types and is not used for the **Gas Tank Leak** and the **Gas Tank Burst** release types. Ground temperature is entered in units of °C and controls the energy flux from the ground to the pool. Increasing the ground temperature increases evaporation. During the day, the ground temperature in the shade is about the same as the air temperature, while the ground temperature in the open is several degrees warmer than the air temperature. At night, the ground temperature is generally lower than the air temperature. The valid range of values for this field is from -40 to 60 °C.

EXTRAN Chemical Parameters: This set of parameters is used to define the physical characteristics of the chemical effluent, as shown in Figure 4-14. These characteristics include the molecular weight, boiling point, heat capacity, heat of vaporization, and specific gravity (or density) of the liquid phase, and the molecular diffusion coefficient. The input chemical parameters are as follows:

- List of Chemicals: HABIT 2.2 comes with a data file, "CHEMICAL.DAT," that contains information about the physical characteristics of 21 chemicals.[1] The **List of Chemicals** field is a drop-down menu with the names of all 21 chemicals in the "CHEMICAL.DAT" file. The user can either select one of these chemicals or select **Other**. When a chemical from the drop-down menu is selected, the required chemical parameters will automatically appear in the **EXTRAN Chemical Parameters** fields. When the option **Other** is selected, the user will have to manually enter the values in the parameter fields. The "CHEMICAL.DAT" file is an ASCII-type file that can be readily edited to add chemicals and chemical compounds.

- Chemical Name: This is an optional input parameter that provides the chemical name and appears in the EXTRAN output.

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[1]   The 21 chemicals are chlorine; ammonia; sulfur dioxide; acetone; benzene; bromine; carbon disulfide; carbon tetrachloride; diethylamine; ethyl acetate; ethyl benzene; ethyl ether; hydrogen; hydrogen cyanide; isopropyl alcohol; methanol; phosgene; propane; toluene; carbon dioxide; and sulfuric acid.
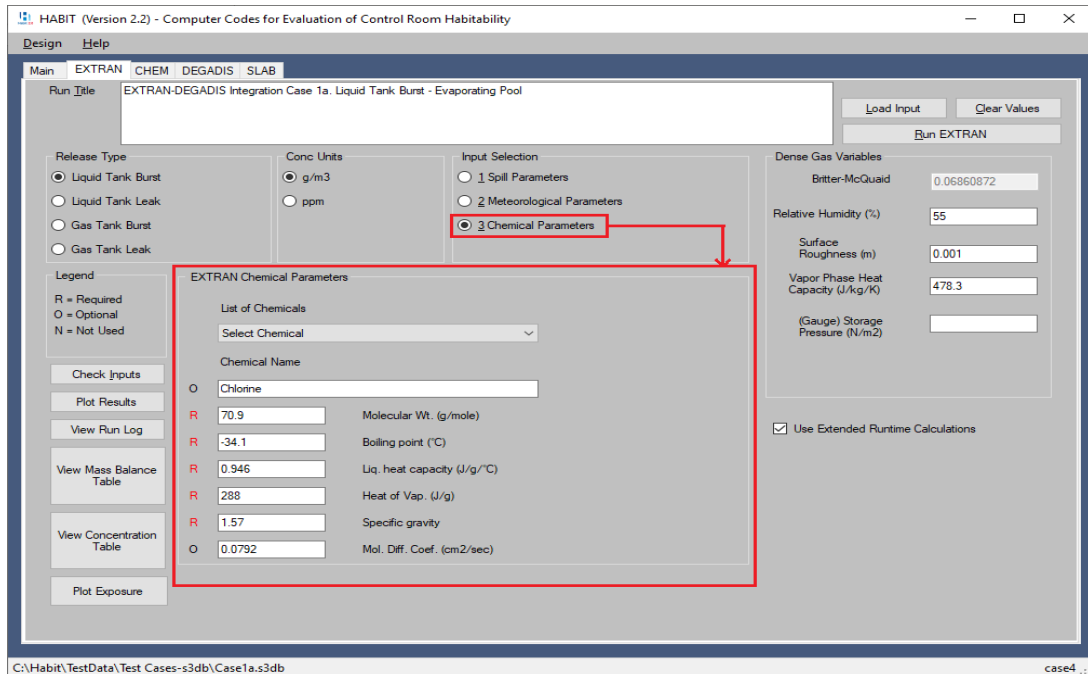
Figure 4-14 EXTRAN Tab Input Section for Chemical Parameters

- Molecular Weight: This parameter provides the molecular weight in units of grams per mole (g/mol) for the chemical or the chemical compound. EXTRAN uses the molecular weight in thermodynamic computations for volatile liquids and in estimating the initial volume of gasses. **Molecular Wt.** is a required field for all four EXTRAN release types. The valid range of values for this field is from 2 to 200 g/mol.

- Boiling Point: This parameter provides the boiling point for the chemical in units of °C. Absolute boiling point temperatures are computed within EXTRAN as needed. Boiling point temperatures are a function of pressure and should be the boiling point at 1 atmosphere of pressure (760 mmHg). EXTRAN will adjust the boiling point to the actual atmospheric pressure entered in the **EXTRAN Meteorological Parameters** input section. **Boiling point** is a required field for all four EXTRAN release types. The valid range of values for this field is from -255 to 500 °C.

- Liquid Heat Capacity: The liquid heat capacity determines the fraction of a liquefied gas that flashes upon release and temperature change in the spill pool. Liquid heat capacity is in units of joules per gram per degree Celsius (J/g/°C). Liquid heat capacities given in units of calories per gram per degree Celsius are converted to the required units by multiplying by 4.184. Within EXTRAN, the heat capacity is a constant, independent of temperature and pressure. Liquid heat capacity is required for the **Liquid Tank Leak**, **Liquid Tank Burst**, and **Gas Tank Burst** release types and is not used for the **Gas Tank Burst** release type. The valid range of values for this field is from -0.25 to 10 J/g/°C.

- Heat of Vaporization: The heat of vaporization is the energy used in calculating the evaporation of liquids. The heat of vaporization is in units of joules per gram (J/g). **Heat**

4-15

of Vap. is a required field for EXTRAN. The valid range of values for this field is from 100 to 2,000 J/g.

- Specific Gravity: EXTRAN uses density in calculating the volume and area of the pool formed by a release of liquids. The user can enter either the density, in units of grams per milliliter (g/ml), or the specific gravity of the liquid. EXTRAN assumes that the density of water is 1 g/ml; therefore, the density and specific gravity are numerically identical. This is a required field for both the **Liquid Tank Leak** and the **Liquid Tank Burst** release types and is not used for the **Gas Tank Leak** and the **Gas Tank Burst** release types. The valid range of values for this field is between 0.05 and 5 g/ml.

- Molecular Diffusion Coefficient: The rate of evaporation of the pool depends in part on diffusion of the vapor near the pool surface. This diffusion is characterized by a molecular diffusion coefficient. The molecular diffusion coefficient is in units of square centimeters per second (cm^2/s) and must be entered if the substance is a volatile liquid. Molecular diffusion coefficients typically have values near 0.1 cm^2/s. It is an optional field for both the **Liquid Tank Leak** and the **Liquid Tank Burst** release types and is not used for the **Gas Tank Leak** and the **Gas Tank Burst** release types. If no value or a zero is entered into this field, EXTRAN will estimate the molecular diffusion coefficient from kinetic theory. The valid range of values for this field is from 0 to 0.2 cm^2/s.

4.1.2.5   Dense Gas Variables Parameter Section

Figure 4-15 displays the **Dense Gas Variables** input section of the **EXTRAN** tab. As shown in Figure 4-1, after the EXTRAN calculations are completed, HABIT 2.2 will evaluate the release to determine the importance of denser-than-air effects using the BMW criteria [16] [17].

- Britter-McQuaid: This field on the **EXTRAN** tab is initially greyed out and blank for new HABIT designs and is not a user-supplied or editable input field. HABIT 2.2 will evaluate the release using BMW criteria Equations (4-1) and (4-2) for the importance of denser-than-air effects for continuous (plume) and instantaneous (puff) releases, respectively. HABIT 2.2 will then estimate the maximum concentration from the denser-than-air effects and provide the BMW value in this field, as shown in Figure 4-14. Additionally, as shown in Figure 4-2, HABIT 2.2 informs the user of the importance of the denser-than-air effects and makes the user select the dense gas model input files to be created.

- Relative Humidity: This parameter is the environmental relative humidity in units of percent humidity. This field is not required for EXTRAN but is an additional dense gas parameter required for DEGADIS and SLAB. This field is editable by the user. The valid range of values for this field is from 0 to unity (i.e., 100 %).
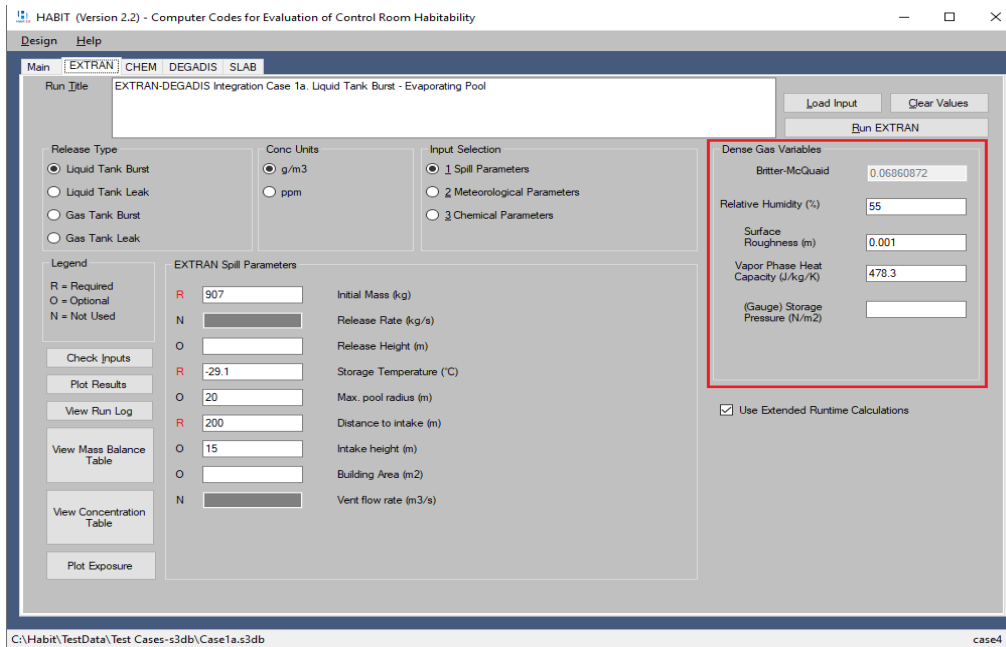
Figure 4-15   EXTRAN Tab Dense Gas Variables Section

- <u>Surface Roughness</u>: The overall effects of surface roughness will be to apply retardation to the horizontal, buoyancy-induced spreading of the plume or cloud and to enhance the mixing between plume and environment as a result of the ambient and plume turbulence [16]. The combination of these effects is likely to, but need not, reduce the downwind distance to a given concentration and reduce the cross-stream dimension to a given concentration. This field is not required for EXTRAN but is an additional dense gas parameter required for DEGADIS and SLAB. Surface roughness is in units of m. This field is editable by the user. The valid range of values for this field is from 0.001 to 10 m.

- <u>Vapor Phase Heat Capacity</u>: This field is an additional required dense gas parameter that is editable by the user. The units are joules per kilogram per Kelvin (J/kg/K). The valid range of values for this field is from -1×10^4 to 1×10^4 J/kg/K.

- <u>(Gauge) Storage Pressure</u>: This field is an additional required dense gas parameter without upper bounding values that is editable by the user. The units are newtons per square meters (N/m^2).

4.1.2.6   EXTRAN Tab Output Buttons

The **EXTRAN** tab contains several output buttons that allow the user to examine EXTRAN output data in separate windows and export the EXTRAN output data for other uses, as shown in Figure 4-16.
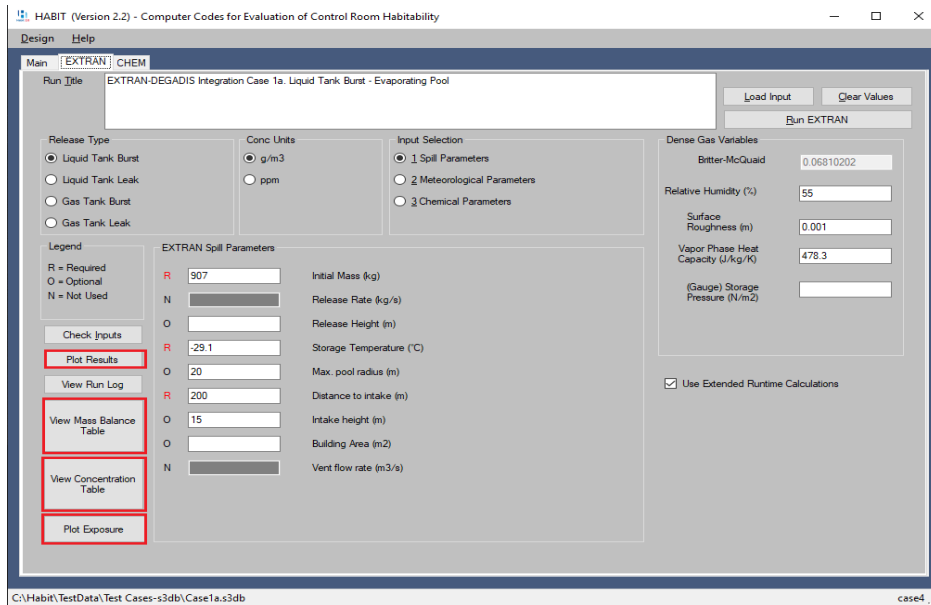
Figure 4-16   EXTRAN Tab Output Results Buttons

- The **Plot Results** button will open the **HABIT Concentration Plot** window and create a graph plotted with the concentration output results for all the HABIT 2.2 codes, as shown in Figure 4-17. This window contains the following user-friendly features:

    – three quick use icons in the upper right of the **HABIT Concentration Plot** window (Figure 4-17) that allow the user to save the plot as a picture file (.jpeg), copy the plot to the clipboard for use in another program (i.e., MS Word), and directly print the plot

    – convenient slider bars that allow the user to quickly adjust the time scale and the toxic limit (the toxic limit can also be adjusted manually by entering the values into the field)

    – displays of the maximum concentrations at the CR intake and in the CR, along with the time at which these maximum concentrations occur

    – easy-to-use graph legend options that include (1) check boxes allowing the user to change the Y-axis to a logarithmic scale or the X-axis units from minutes to seconds and (2) check boxes allowing the user to plot just the concentration output from the desired code or all of the codes
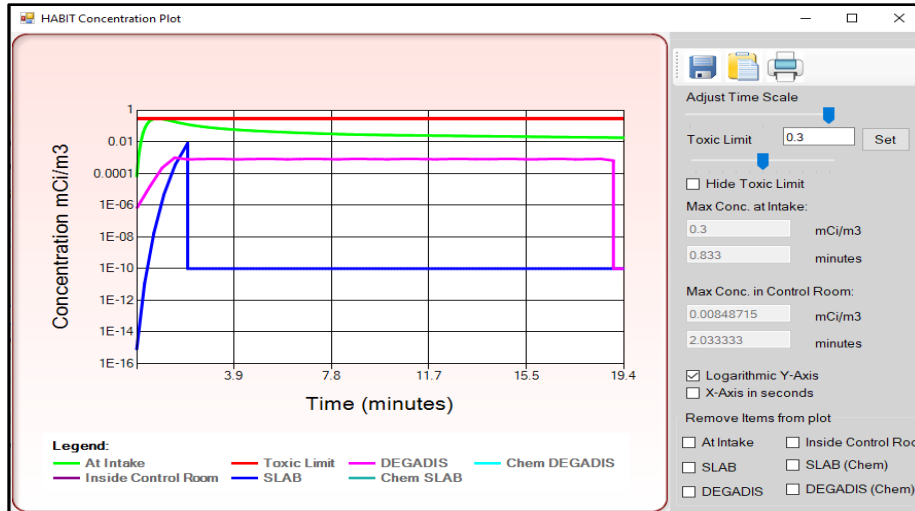
Figure 4-17   HABIT Concentration Plot Window

- The **View Mass Balance Table** button will open the **Mass Balance Table Form** window shown in Figure 4-18. This table displays the time-dependent characteristics of the chemical release.

- The **View Concentration Table** button will open the **Concentration Table Form** window shown in Figure 4-19. This table displays the time-dependent concentrations and exposures of the chemical release. A drop-down menu allows the user to choose to display the time-dependent concentrations for whichever computer model (e.g., EXTRAN, DEGADIS, SLAB) desired.

Id	ExtranModelId	Time	NPuffs	TankVolume	CurrentReleas	Pool	Flashed	Evaporated	Volume	Radius
1	1	0	2	0	907	713.59	161.18	32.23	0.48	3.89
2	1	0.1667	3	0	0	691.39	0	22.2	0.45	3.8
3	1	0.3333	4	0	0	673.58	0	17.8	0.44	3.74
4	1	0.5	5	0	0	658.39	0	15.19	0.43	3.7
5	1	0.6667	6	0	0	644.98	0	13.41	0.42	3.65
6	1	0.8333	7	0	0	632.88	0	12.1	0.41	3.62
7	1	1	8	0	0	621.79	0	11.08	0.4	3.58
8	1	1.1667	9	0	0	611.53	0	10.26	0.4	3.55
9	1	1.3333	10	0	0	601.95	0	9.58	0.39	3.52
10	1	1.5	11	0	0	592.95	0	9	0.38	3.49
11	1	1.6667	12	0	0	584.44	0	8.51	0.38	3.47
12	1	1.8333	13	0	0	576.36	0	8.08	0.37	3.44
13	1	2	14	0	0	568.67	0	7.7	0.37	3.42
14	1	2.1667	15	0	0	561.31	0	7.36	0.36	3.4
15	1	2.3333	16	0	0	554.26	0	7.05	0.36	3.37
16	1	2.5	17	0	0	547.49	0	6.77	0.35	3.35
17	1	2.6667	18	0	0	540.97	0	6.52	0.35	3.33
18	1	2.8333	19	0	0	534.68	0	6.29	0.34	3.31
19	1	3	20	0	0	528.6	0	6.08	0.34	3.29
20	1	3.1667	21	0	0	522.72	0	5.88	0.34	3.27

Figure 4-18   Mass Balance Table Form Window

Figure 4-19   Concentration Table Form Window

- The **Plot Exposure** button will open the **HABIT Exposure Plot** window shown in Figure 4-20. This window has three quick use icons at the top left that allow the user to save the plot as a picture file (.jpeg), copy the plot to the clipboard for use in another program (i.e., MS Word), and directly print the plot. The window also contains (1) a convenient slider bar enabling quick adjustment of the time scale and (2) graph legend option check boxes allowing the user to change the Y-axis to a logarithmic scale or the X-axis units from minutes to seconds.
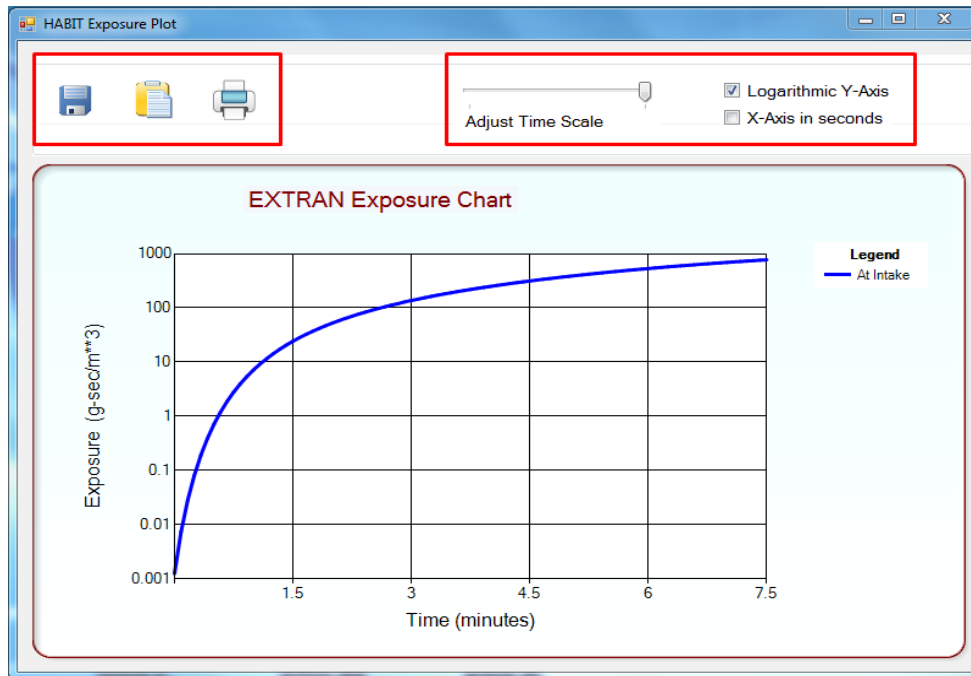
Figure 4-20   HABIT Exposure Plot Window

4.2　　　CHEM Module

4.2.1　　CHEM Code Description

As used in HABIT 2.2, the CHEM module receives the EXTRAN-calculated toxic substance concentration at the CR intake and calculates the exposure to the CR personnel. The CHEM module computes the mass balance within the CR between the toxic concentration rate through the intake and the vented rate by outflow. The **CHEM** tab in the TDI provides a user-friendly method to calculate the concentrations from accidental releases of toxic substances in nuclear power plant CRs.

4.2.1.1　General Description

CHEM is essentially a simplified version of the CONHAB code [4] [11]. All features pertaining to radioactive decay and daughter formation have been removed. The CR filters are assumed to not be effective against the toxic chemicals in question, and the concentrations at the CR intakes are computed by EXTRAN. The only process that needs to be modeled within CHEM is the conservation of chemical mass associated with inflow and outflow to the CR.

The toxic chemical concentration at the CR intakes is obtained from the mean concentration during each time step produced by EXTRAN. This concentration is assumed to be the same at all CR intakes; typically, this includes filtered CR intakes 1 and 2 and unfiltered CR intakes 1 and 2. The CR filtered intakes are assumed to be ineffective in removing the toxic, and the CR may also have a designed bottled air inflow. The only mechanism for removal of the toxic chemical from the CR is assumed to be outflow.

Section 7.2 of NUREG/CR-6210 [4] discusses the equations and parameters affecting the concentration of the toxic chemical in the CR. Equations (7.1) through (7.3) of NUREG/CR-6210 [4] display how CHEM calculates the chemical exposure to the CR occupants using the flow and concentrations into the CR, the flow and concentrations out of the CR, and bottled air flow into the CR.

4.2.2　　CHEM TDI Features

4.2.2.1　General Features of the CHEM TDI Tab

The user should be aware of some of the basic features of the **CHEM** tab in the HABIT 2.2 TDI shown in Figure 4-21. The values for the parameters will be pre-populated when imported from a previous design; otherwise, the user can enter the appropriate values. When the mouse pointer is hovered over an input field, the code will display the valid range for that field.
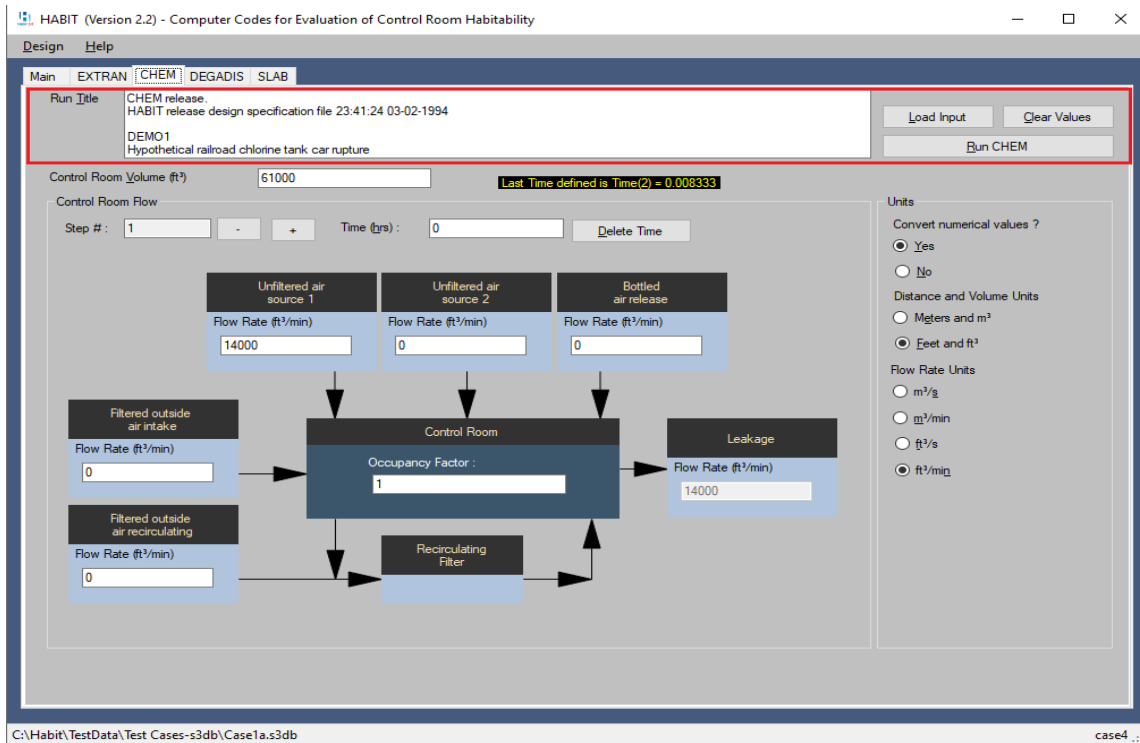
Figure 4-21   CHEM Tab General Features

The other general features on the **CHEM** tab include the following:

- The **Run Title** input text box enables the user to input a title and a brief description of the CHEM run. This input text box has an 80-character limit.

- The **Load Input** button opens an File Explorer display, as shown in Figure 4-4. The user can browse to the location of an existing folder and select the CHEM input file (i.e., "DesignCH.inp") to open. Click the **Open** button to open the existing design.

- The **Clear Values** button clears all values of CHEM input parameters from the tab and starts over with blank parameter input fields. Selecting this button will open the **Clear Form** window as shown in Figure 4-5. Selecting the **Yes** button on the **Clear Form** window will clear all the current values from the tab and return the user to a blank **CHEM** tab. Selecting the **No** button will retain the current values and return the user to the **CHEM** tab.

- The **Run CHEM** button will execute the program against the user-provided input parameters in the **CHEM** tab. Since CHEM uses the EXTRAN results, EXTRAN must run as a prerequisite. An error message (Figure 4-22) will display if the user attempts to run CHEM without first running EXTRAN. If there are any input errors the user has not corrected before clicking this button, the application will display a warning message as shown in Figure 4-6. To clear this message window, the user selects the **OK** button, and a red exclamation point icon will appear to the right of the missing required input parameters field.
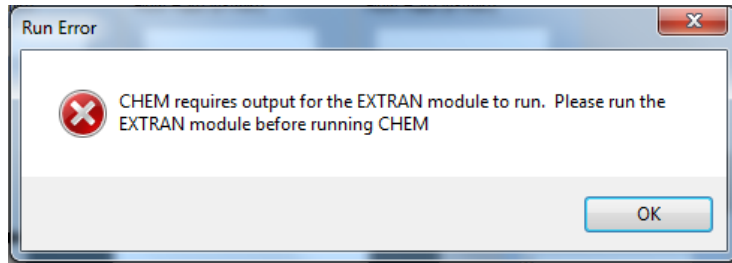
Figure 4-22   CHEM Run Error Window

4.2.2.2   CR Flow Section

The **Control Room Flow** section on the **CHEM** tab displays a schematic representation of the flows into and out of the CR, as shown in Figure 4-23. These input CR flow paths include two unfiltered CR intake paths, two filtered CR intake paths, and the bottled air flow intake path. The chemical concentration is assumed to be the same for all four inflow paths and is given by EXTRAN. Flows through all four paths are treated identically, so the user may choose to simply set the flow rate for any one of these paths to the total CR inflow rate and leave the others blank. The input parameter fields in the CR flow schematic are used as follows:

- The **Unfiltered air source 1** and **Unfiltered air source 2** input fields are user-specified fields for the flow of air into the CR from unfiltered air sources 1 and 2. **Bottled air release** is a user-specified input field for the flow rate of bottled air into the CR. The **Filtered outside air intake** (aka "Filtered air source 1") and **Filtered outside air recirculating** (aka "Filtered air source 2," which feeds the recirculating filter) input fields are user-specified fields for the flow that are used to specify the flow of air into the CR from filtered air sources 1 and 2. Note that intake filters are assumed to have no effect on the chemical concentrations in CHEM. The schematic also displays a box indicating the position of the CR recirculating filter; however, this filter has no effect on the chemical concentration in the CR and is included only for flow path accuracy. Section 4.2.2.3 discusses the units and valid ranges for these flow paths.

- The **Control Room Occupancy Factor** input field specifies the occupancy factor for CR operators (a typical value for occupancy factors is 1.0). This input field is unitless. The valid range of values for this field is from 0 to 1.0.

- The **Leakage** box indicates the CR leakage. This shows the total rate at which air must leak from the CF to offset the inflow. This value is simply the sum of the inflow rates; the interface provides it for information purposes only.
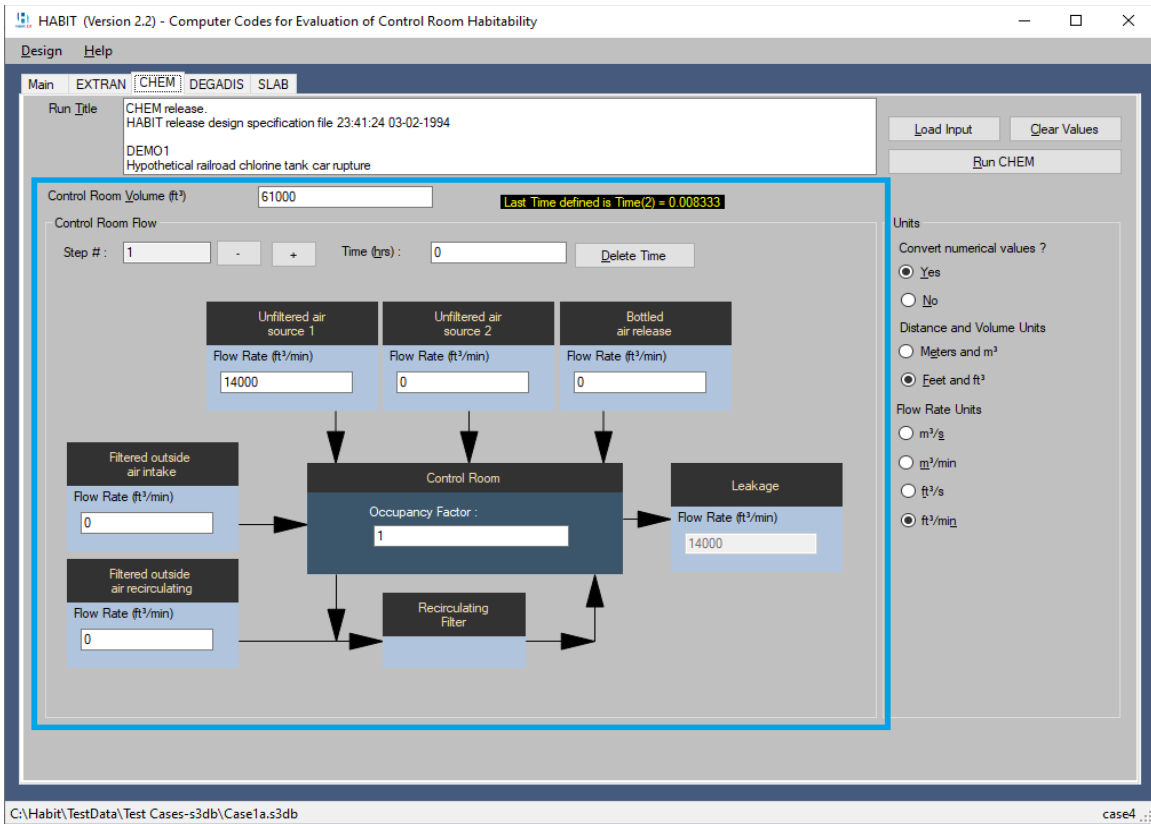
Figure 4-23   CHEM Tab Control Room Flow Section

To the right of the **Control Room Volume** input field is the **Last Time Defined** label, which displays the last time step number in parenthesis and time for the last defined time step in seconds. The **Control Room Flow** section of the **CHEM** tab also contains the **Step #** input field, which displays the number of the current time step. The user can select either the ─ or the **+** button to move to the previous or next time step. Selecting a time step beyond the last time step defined causes the program to display the **Step Time Missing** window, as shown in Figure 4-24. Select the **OK** button to return to the **CHEM** tab and use the ─ or the **+** buttons to return to the last time step defined.
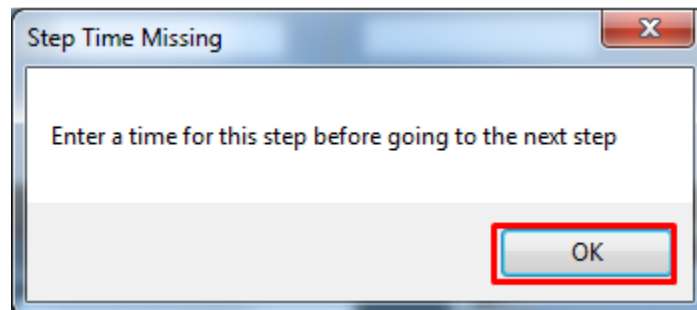
Figure 4-24   Step Time Missing Window

The **Delete Time** button, when accessible and clicked, will display the **Confirm Delete** window (Figure 4-25) warning the user that data for the current time step on the **CHEM** tab will be deleted. Select the **Yes** button to delete the data and the **No** button to cancel the deletion of the

time step data. The user can use the **Delete Time** button in conjunction with the ─ or **+** buttons to select a time step to be deleted.
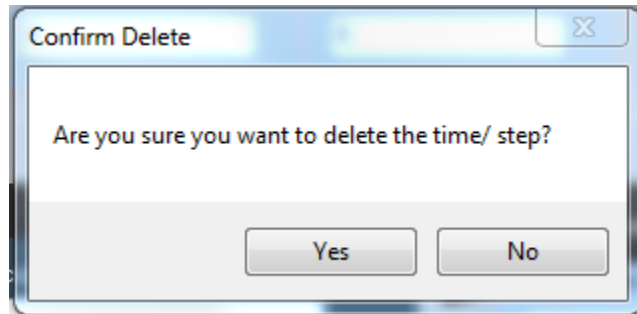
Figure 4-25   Confirm Time Step Deletion Warning Window

4.2.2.3   Units Selection Section

The **Units** selection section on the **CHEM** tab allows the user to change the volume and flow rate units used in CHEM, as shown in Figure 4-26. The **Units** selection section works in conjunction with the input fields on the schematic in the **Control Room Flow** section of the **CHEM** tab. The **Units** selection section contains three sets of user options:

- The first option enables the user to convert numerical values. Two radio button choices are available. If the user selects the **Yes** radio button (the default option), all numerical values already in the input will be converted from the old units to the new volume and flow rate units selected by the user in the sections below this option. If the user selects the **No** radio button, the new units with the original numerical values will be used. The user should take care when selecting this option because any subsequent changes in volume or flow rate units will not result in the conversion of the numerical values to the new volume or flow rate units chosen.

- The second option enables the selection of volume units. Two radio button options are available, either units of cubic meters (m^3) (the default option) or cubic feet (ft^3). The valid range for all the volume values for this field is between 3,531.467 and 706,293.6 m^3 and ft^3.

- The third option enables the selection of flow rate units. Four radio button options are available: m^3/s (the default option), cubic feet per second (ft^3/s), cubic meters per minute (m^3/min), and cubic feet per minute (ft^3/min). The valid range for all the flow rate values for this field is from 0 to 20 m^3/s, 0 and 1,200 m^3/min, 0 and 706 ft^3/s, and 0 and 42,400 ft^3/min, respectively.
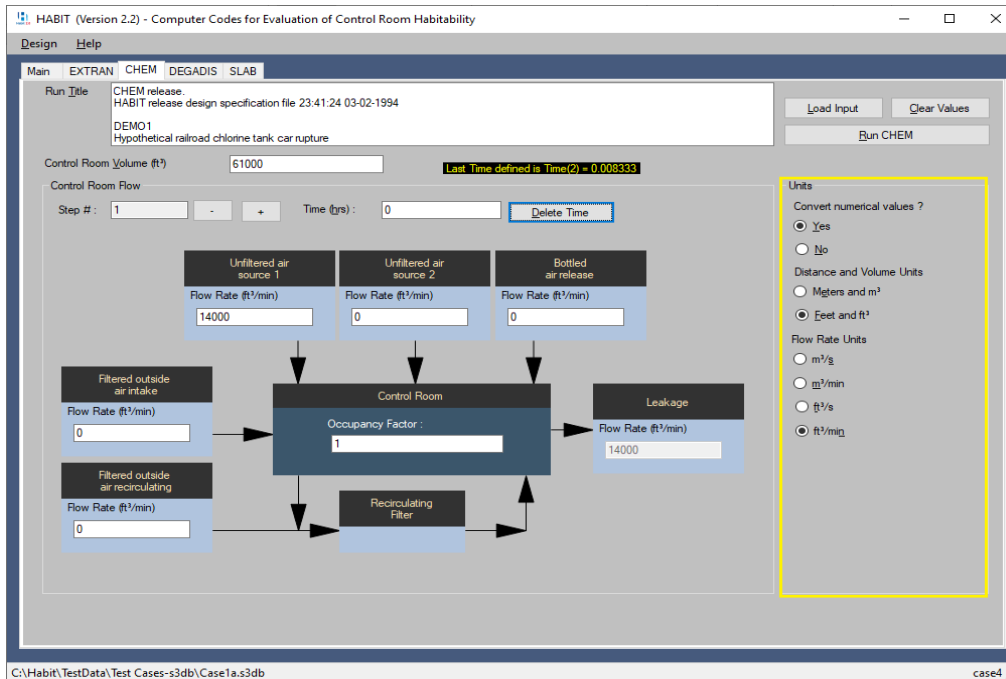
Figure 4-26   CHEM Tab Units Selection Section

4.3   DEGADIS Module

As mentioned in Section 1.0, HABIT 2.2 incorporates DEGADIS version 2.1 as one of calculation models available to evaluate the effects of denser-than-air chemical releases. According to the EPA's DEGADIS user's guide [13], DEGADIS is designed to model the atmospheric dispersion of ground-level, area-source dense gas (or aerosol) clouds released with zero (initial) momentum into an atmospheric boundary layer over flat, level terrain. DEGADIS describes the dispersion processes that accompany the ensuing gravity-driven flow and entrainment of the gas into the atmospheric boundary layer. Releases with significant vertical momentum can also be modeled, including the case where the resulting plume comes back to ground level. DEGADIS has been verified by comparison with a wide range of laboratory and field-scale heavy gas release/dispersion data.

As discussed previously, HABIT 2.2 will not automatically run the denser-than-air models of DEGADIS and SLAB but will inform the user that an evaluation of the release using the BMW criteria has determined that the dense gas effects are important to this run (Figure 4-2). With the buttons in the **Choose Dense Gas Model** window (Figure 4-2), the user can choose to have HABIT 2.2 run either DEGADIS, SLAB, both dense gas codes, or none of the dense gas codes. When the option to run either DEGADIS or all dense gas models is selected, HABIT 2.2 will use the EXTRAN spill, meteorological, and chemical input parameters along with the dense gas input variables provided by the user to perform the DEGADIS model calculations. The input parameters used in DEGADIS calculations are displayed on the **DEGADIS** tab shown in Figure 4-27 and described in Section 4.3.2.

4.3.1   DEGADIS Code Description

4.3.1.1   General Description

As described in the EPA DEGADIS user's guide [13], the atmospheric dispersion of gas releases may involve one of four fluid flow regimes. All four regimes, which may be present in different degrees depending on the rate and (characteristic) dimensions of the release, gas density, and characteristics of the atmospheric flow, should be accounted for in a general application dispersion model. These four fluid flow regimes include the following:

- jet
- buoyancy-dominated
- stably stratified
- passive dispersion

If a chemical gas release rate does not exceed the potential atmospheric take-up rate, the gas is taken up directly by the atmospheric flow and dispersed downwind. If the vertical momentum of the source is significant, it can be modeled in DEGADIS using the release type option **Jet of Elevated Simulation** (jet-plume model). This release type option in DEGADIS allows for modeling the dispersion of vertical jets perpendicular to the wind flow direction.

If a gas release rate exceeds the potential atmospheric take-up rate (rapid releases of large quantities of dense gas with low initial momentum), a denser-than-air "secondary source" blanket is formed over the primary source. In the near field, a buoyancy-dominated regime is modeled using a lumped parameter model (spatially averaged properties) that incorporates air entrainment at the gravity-spreading front using a frontal entrainment velocity. The gravity-induced slumping and lateral spreading motion ensues until the kinetic energy of the buoyancy-driven flow is dissipated. The gravity-induced flow, which may affect mixing primarily at the advancing vapor cloud front, can be an important determinant of the shape and extent of the gas cloud. After the kinetic energy of the buoyancy-driven flow is dissipated, the dispersion process can be described as a stably stratified plume embedded in the mean wind flow. This density stratification, which can be much stronger than that occurring naturally in the atmospheric boundary layer, will tend to dampen turbulence and reduce vertical mixing. As the dispersion proceeds, the stable stratification due to the dense gas decreases until the dispersion process can be represented as a neutrally buoyant plume in the mean wind flow, resulting in a passive dispersion regime. This can be modeled in DEGADIS using the release type option **Ground-level, Low Initial Momentum (nonjet) Release**.

The equations and theory behind both the **Jet of Elevated Simulation** and the **Ground-level, Low Initial Momentum (nonjet) Release** model are described in great detail in the EPA user's guide [13].

4.3.2   DEGADIS TDI Features

4.3.2.1   General Features of the DEGADIS TDI Tab

The user should be aware of some of the basic features associated with the **DEGADIS** tab in the HABIT 2.2 TDI, as shown in Figure 4-27. The values for the parameters will be pre-populated when imported from a previous design; otherwise, the user can enter the appropriate values. When the mouse pointer is hovered over an input field, the code will display the valid range for that field.
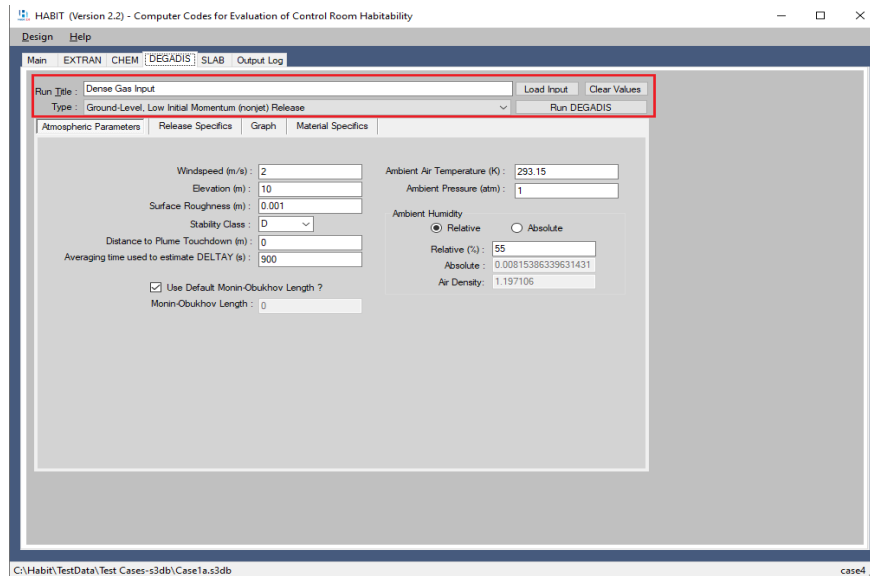
Figure 4-27   DEGADIS Tab General Features

The other general features on the **DEGADIS** tab include the following:

- The **Run Title** input text box enables the user to add a title or a brief description of the DEGADIS run. The size of input text box is unlimited.

- The **Type** drop-down menu provides the user with the two model options available in DEGADIS: (1) **Jet of Elevated Simulation** and (2) **Ground-level, Low Initial Momentum (nonjet) Release**. The EPA user's guide describes both [13].

- The **Load Input** button opens an MS Windows OS File Explorer window, as shown in Figure 4-4. The user can then browse to the location of an existing folder and select the DEGADIS input file (i.e., "DesignDG.inp") to open in that folder. Select the **Open** button to open the existing design.

- The **Clear Values** button clears all values in the DEGADIS input parameters from the tab and starts over with blank parameter input fields. Selecting this button will open the **Clear Form** window, as shown in Figure 4-5. Selecting the **Yes** button in the **Clear Form** window will clear all the current values from the tab and return the user to a blank **DEGADIS** tab. Selecting the **No** button will retain the current values and return the user to the **DEGADIS** tab.

- The **Run DEGADIS** button will execute the program against the user-provided input parameters in the **DEGADIS** tab. It will also open the **Output Log** tab (Figure 3-13) displaying MS-DOS output from the Fortran formulations and computations so they are visible from within the application.

As shown in Figure 4-27, the **DEGADIS** tab also contains four input tabs: **Atmospheric Parameters**, **Release Specifics**, **Graph**, and **Material Specifics**. The values for the parameters in these tabs will be pre-populated when imported from a previous design or when available from running the EXTRAN module; otherwise, the user can enter the appropriate values.

4-28

4.3.2.2 DEGADIS Atmospheric Parameters Tab

The **Atmospheric Parameters** tab under the **DEGADIS** tab displays two columns of data related to the atmospheric input parameters, as shown in Figure 4-28. These columns are the general atmospheric input parameters and the ambient humidity input parameters. The meteorological parameters and dense gas variables that were input to EXTRAN will automatically be passed to this tab and will be displayed as pre-populated fields. The input atmospheric parameters are as follows:

- Wind Speed: This is the wind speed at the elevation specified in the next field in units of m/s and is same value used in the meteorological parameters for EXTRAN (which uses an elevation of 10 m as described in Section 4.1.2.4). The valid range of values for this field is between 0 and 30 m/s.

- Elevation: This is the level above the ground in units of m at which the wind speed was measured. As noted in Section 4.1.2.4, the wind speed value used for EXTRAN is usually the wind speed reported at an elevation of 10 m. The valid range of values for this field is from 10 to 30 m.

- Surface Roughness: This is the same parameter as described in the **Dense Gas Variables** input parameter section of the **EXTRAN** tab (Section 4.1.2.5). DEGADIS uses the site surface roughness to parameterize air entrainment into the dispersing cloud (via the friction velocity, which includes the effect of atmospheric stability). This field is an additional required dense gas parameter in units of m and is editable by the user. It has a valid range of values between 0.001 and 99 m.

- Atmospheric Stability Class: Atmospheric stability classes are defined in Table 2-2 of RG 1.23 [21]. This parameter field has a drop-down menu with options **A** through **F**, ranging from extremely unstable **A** to extremely stable **F**. The **EXTRAN** tab includes the option for atmospheric stability class **G**, which is considered sufficiently rare that it is no longer typically used. Since DEGADIS only has provisions for atmospheric stability classes **A** through **F**, if atmospheric stability class **G** is selected in the **EXTRAN** tab, DEGADIS will use atmospheric stability class **F** to best approximate it.
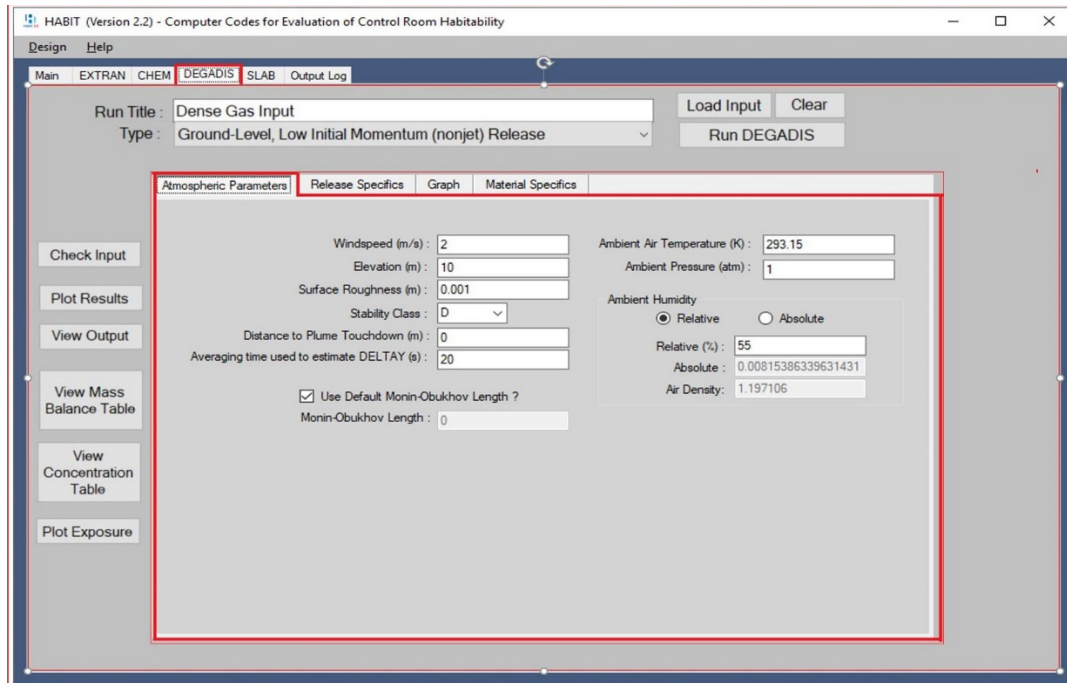
Figure 4-28   DEGADIS Tab Atmospheric Parameters

- Distance to Plume Touchdown (m): This is the downwind distance calculated in DEGADIS. It includes the distance to touchdown calculated using the Ooms model [13]. This field is in units of m and is editable by the user. The valid range of values for this field is between 0 and 999 m.

- Averaging time used to estimate DELTAY: This the averaging time in seconds for the lateral similarity coefficient. Changes to the values of DELTAY (δy) are calculated assuming that the effect of averaging time only influences the lateral plume meander of a steady-state release. This field is editable by the user. The valid range of values for this field is between 0 and 999 s.

- Use Default Monin-Obukhov Length?: This check box works in conjunction with the **Monin-Obukhov Length** input field. This parameter describes the effects of buoyancy on turbulent flows. The code can compute it based on the atmospheric stability and the surface roughness.

- Monin-Obukhov Length: This parameter describes the effects of buoyancy on turbulent flows. A Monin-Obukhov length value is required to calculate the friction velocity and is in units of m. It can be automatically estimated by DEGADIS. For direct input, the range of values for this field is between 0 and 50 m.

- Ambient Air Temperature: This is the environmental ambient air temperature in units of K. EXTRAN converts the air temperature entered in units of °C to K as needed within the code to perform calculations. The converted air temperature from EXTRAN is used

for DEGADIS calculations. This field is editable by the user. The valid range of values for this field is between 233.15 and 333.15 K.

- Ambient Pressure: This is the environmental atmospheric pressure in units of atmospheres (atm). DEGADIS will convert the atmospheric pressure entered in EXTRAN from mmHg to units of atm using the factor 1 atm/760 mmHg. This is a required atmospheric input parameter for DEGADIS. The valid range of values for this field is between 0.79 and 1.05 atm.

- Ambient Humidity Input Section: This section of the DEGADIS **Atmospheric Parameters** tab provides the user with two radio button selection options for humidity. DEGADIS considers the effect of ambient humidity, which can be important when evaluating the release of cryogenic materials (e.g., liquified natural gas). The default selection is the **Relative** humidity radio button, which works in conjunction with the **Relative (%)** humidity input field and uses the value for percent relative humidity entered on the **Dense Gas Variables** input section of the **EXTRAN** tab. The **Relative (%)** humidity input field is editable by the user; the valid range of values for this field is between 0 and 100 percent. When the **Relative** humidity radio button is selected, the input fields for **Absolute** humidity and **Air Density** are greyed out and not editable by the user. When the **Absolute** humidity radio button is selected, the **Absolute** humidity input field (in units of kg water/kg dry air) becomes active and editable by the user. The valid range of values for this field depends on ambient temperature and pressure; it should be chosen so that the calculated relative humidity is between 0 and 100 percent. Finally, the **Air Density**, for information only, is calculated using the ideal gas law and the sum of densities of the two gases, dry air and water vapor, in proportion with their partial pressures.

4.3.2.3   DEGADIS Material Specifics Tab

The **Material Specifics** tab under the **DEGADIS** tab contains check boxes that could change the view of the **Materials Specifics** tab see Figures 4-29; 4-30; and 4-31. The elements of Figure 4-30, which is presented as what happens when the user checks this box. The Heat transfer and Water transfer check boxes are also invisible which will be furtherly discussed. In Figure 4-29, it shows the location for "**Is isothermal spill?"** check box at the upper-left corner. The center section of the **Material Specifics** tab contains the **Contaminant** input section, which collects the characteristics of the contaminant needed for executing DEGADIS. The **Contaminant** input section fields are as follows:
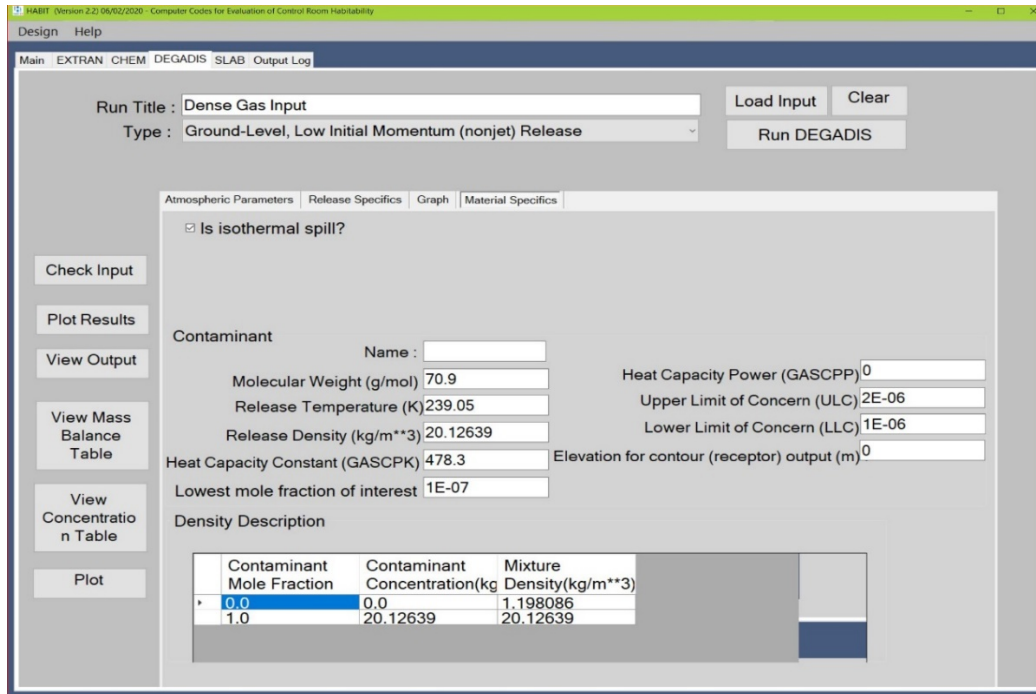
Figure 4-29   DEGADIS Tab Material Specifics

- Name: This input field is for the name of the contaminant. The chemical parameters entered for EXTRAN will not automatically be passed to this tab. Some chemical will be pre-populated from the EXTRAN data.

- Molecular Weight (g/mol): This parameter provides the molecular weight in units of g/mol for the chemical or the chemical compound. The valid range of values for this field is from 2.0 to 200 g/mol.

- Release Temperature (K): This is the environmental ambient air temperature in units of K. This value is passed from the **EXTRAN** tab; EXTRAN converts the air temperature to K as needed within the code to perform calculations. The valid range of values for this field is from 233.15 to 333.15 K.

- Release Density (kg/m³): This parameter provides the density in units of kilograms per cubic meter (kg/m³) for the chemical or the chemical compound. HABIT 2.2 converts the density (specific gravity) entered on the **EXTRAN** tab from units of g/ml to kg/m³ for use in the dense gas calculations. The valid range of values for this field is from 1 to 50 kg/m³.

- Heat Capacity Constant: This is the vapor phase heat capacity in units of J/kg/K at a constant pressure. The vapor phase heat capacity is a required input for DEGADIS, but it is not required for EXTRAN. DEGADIS uses this parameter in the energy balance to determine cloud temperature. DEGADIS is also able to use a temperature-dependent vapor heat capacity, but as this capability is likely only important for cryogenic liquids,

assuming a constant liquid heat capacity is adequate. The valid range of values for this field is from 0 to 999 J/kg/K.

- Lowest Mole Fraction of Interest: This is the lowest mole fraction of interest for the contaminant in units of mole fractions. Its value typically set to one-tenth the lower limit of concern (GAS_LCL) value. The fraction range of values for this field is from 1×10^{-7} to 1 mole.

- Heat Capacity Power (GASCPP): This field is the power for contaminant heat capacity, which is a unitless value from 0 to 1.

- Upper Limit of Concern (ULC): This is the upper contaminant concentration level (GAS_UFL) for estimating contours in units of mole fraction. Its value is typically set to twice the lower limit of concern (GAS_LCL) value. The fraction range of values for this field is from 1×10^{-6} to 1 mole.

- Lower Limit of Concern (LLC): This is the lower contaminant concentration level (GAS_LFL) for estimating contours, in units of mole fraction. This parameter will depend on whether a toxic or flammable gas is under evaluation. For toxic gases, this should be the level of concern, such as the threshold limit value–short-term exposure limit (TLV-STEL). For flammable gases, a concentration of 1×10^{-3} mole fraction should be adequate. The fraction range of values for this field is from 1×10^{-6} to 1 mole.

- Elevation for Contour (Receptor) Output: This is the elevation above ground for concentration output in units of m. It is typically set to 0 m. The valid range of values for this field is from 0 to 100 m.

When the user selects the **Is isothermal spill?** check box, DEGADIS assumes that the spill temperature remains at ambient temperature throughout evaporation. Additionally, as shown in Figure 4-30, the **Density Description** section appears at the bottom of the **Material Specifics** tab. The **Density Description** section includes a table that displays in columns the **Contaminant Mole Fraction**, **Contaminant Concentration**, and **Mixture Density**.
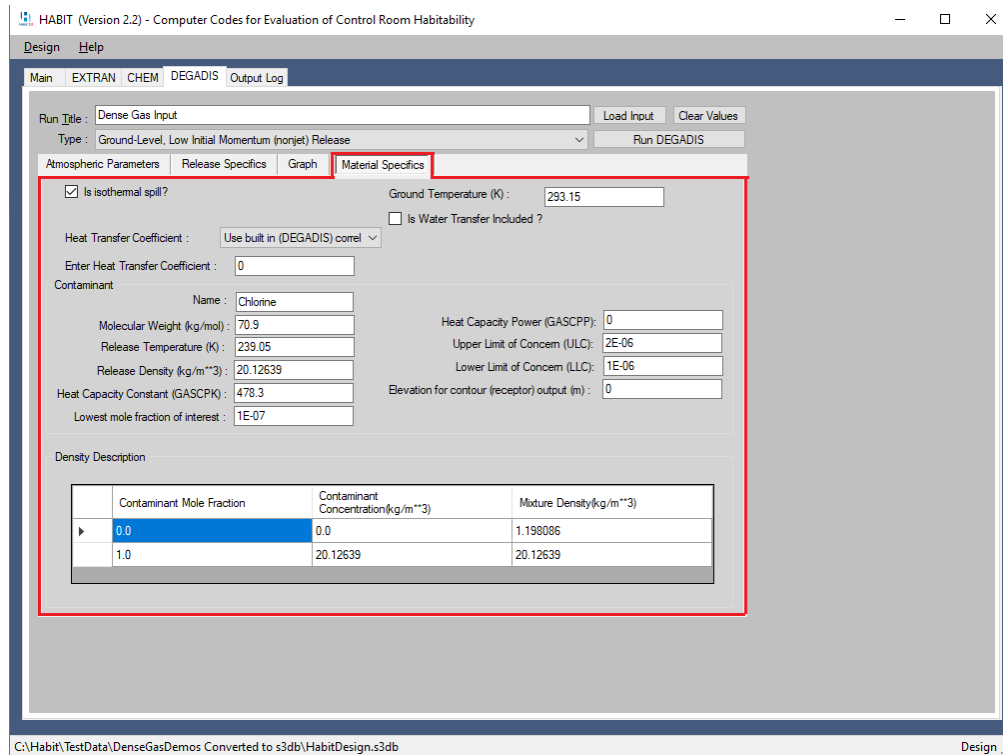
Figure 4-30   DEGADIS Tab Material Specifics (Isothermal Spill Checked)

Further, see Figure 4-31: When the user selects the **Is Heat Transfer to be included?** Check box, DEGADIS calculates thermal energy balances downwind, and the options in the upper portion of the **Material Specifics** tab change as shown in Figure 4-31. This check box is used for some simulations of cryogenic gas releases, when heat transfer to the plume in the downwind dispersion calculation may be important, particularly in low-wind conditions as discussed in the DEGADIS user's guide [13]. The additional inputs added to the **Material Specifics** tabs are as follows:

- Heat Transfer Coefficient Input Section: This section of the **Material Specifics** tab contains two input fields that work in conjunction with each other. The first input field is the **Heat Transfer Coefficient** drop-down menu, with the following three options available to the user (based on page 31 of the DEGADIS manual [13]):

  – **Use built in (DEGADIS) correlation**
  – **Use LLNL correlation**
  – **Manual Entry**

  This section also includes the **Heat Transfer Coefficient** input field, which works in conjunction with the **Manual Entry** option in the drop-down menu to allow the user to enter a heat transfer coefficient in units of joules per square meter Kelvin (J/m^2 K).

- Ground Temperature: This is the ground temperature value used for the **Liquid Tank Leak** and the **Liquid Tank Burst** release types in the **EXTRAN** tab. EXTRAN converts the air temperature to K as needed within the code to perform calculations. The valid range of values for this field is between 233.15 and 333.15 K.

4-34
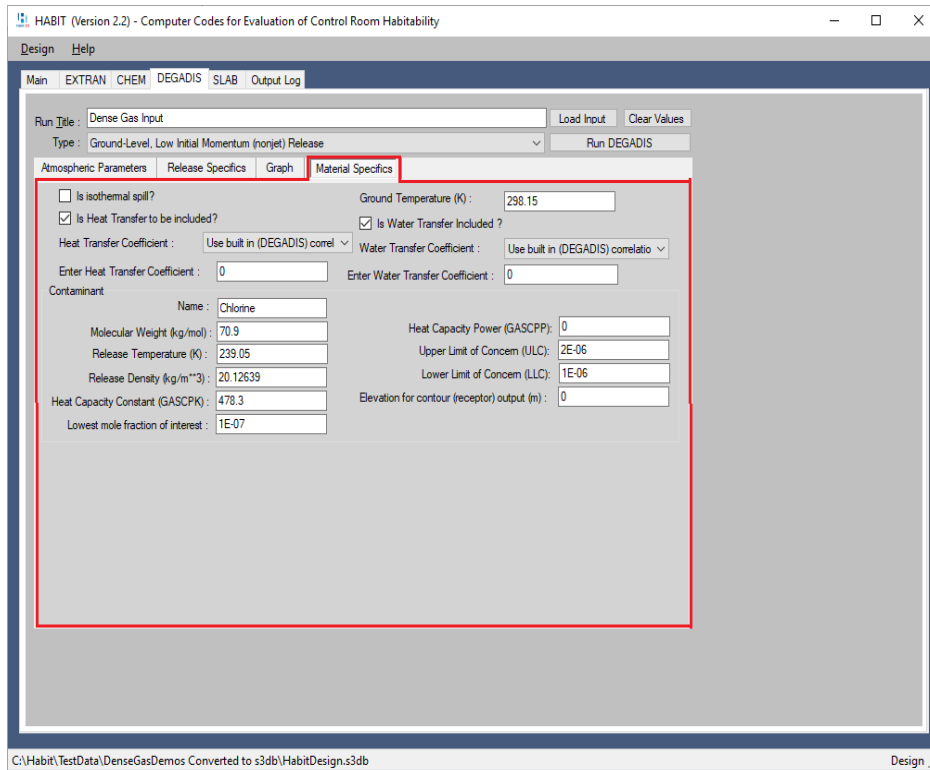
Figure 4-31   DEGADIS Tab Material Specifics (Heat and Water Transfer Included Checked)

- Water Transfer Coefficient Input Section: This section allows the user to take the water transfer effects to the cloud from the water surface under the source parameter. When the check box is selected, two additional input selection fields for the water transfer coefficient appear on the **Material Specifics** tab. The first input field is the **Water Transfer Coefficient** drop-down menu, with the following two options available to the user:

  – **Use built in (DEGADIS) correlation**
  – **Manual Entry**

  This section also includes the **Enter Water Transfer Coefficient** input field, which works in conjunction with the **Manual Entry** option in the drop-down menu to allow the user to enter a water transfer coefficient in units of kilograms per square meter second (kg/m^{2}s). The valid range of values for this field is better between 0 and 1 kg/m^{2}s.

4.3.2.4   DEGADIS Release Specifics Tab

The **Release Specifics** tab under the **DEGADIS** tab contains two drop-down menu selections related to the contaminant release parameters, as shown in Figure 4-32. The **Contaminant Released Is** drop-down menu has the options **Pure** or **Diluted with air**. The **Release can be considered** drop-down menu has the options **Steady State** or **Transient**. The **Release**

Specifics tab also contains a **Source Description** section whose input entries change according to the options selected in each drop-down menu, as described below.
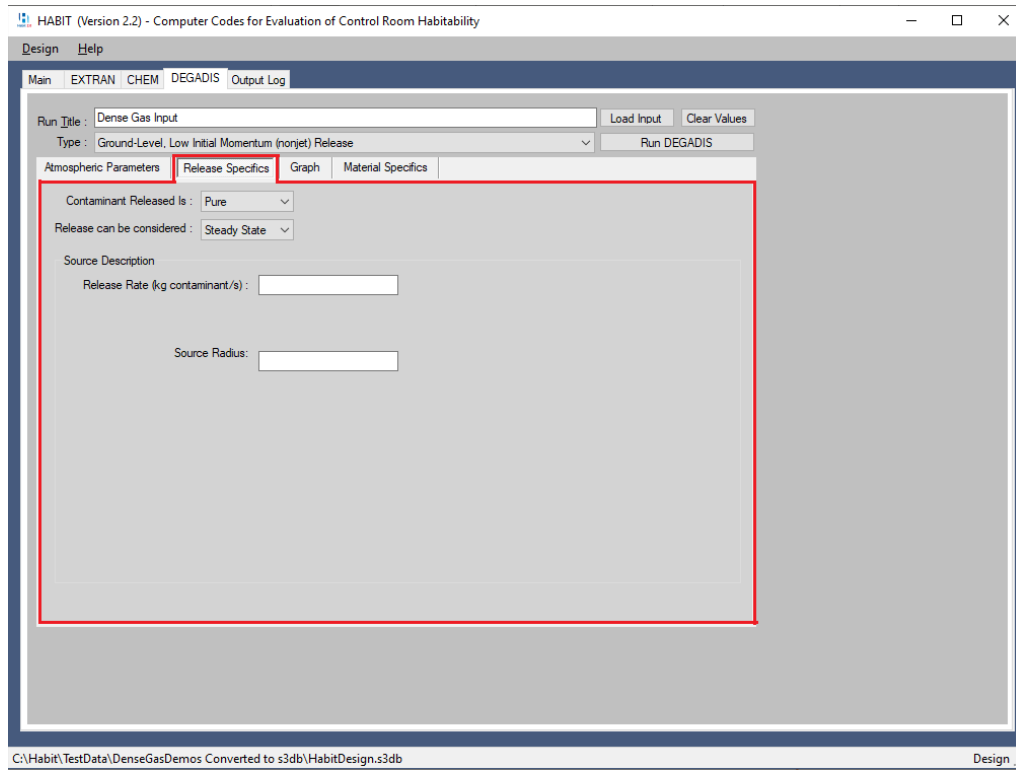
Figure 4-32   DEGADIS Tab Release Specifics (Pure/Steady State Options)

As show in Figure 4-32, when the **Pure**/**Steady State** options are selected on the two drop-down menus, there are two parameter input fields in the **Source Description** section:

- Release Rate: This input parameter is the steady state release rate for the contaminant in units of kg/s. The valid range of values for this field is between 0 and 5.0E+05 kg/s.

- Source Radius: This input parameter is the steady state source radius for the contaminant in units of m. The valid range of values for this field is between 0 and 100 m.

Figure 4-33 displays the **Release Specifics** tab with the **Diluted with Air**/**Steady State** options selected in the two drop-down menus. Notice that there are now two additional input parameter fields besides the **Release Rate** and **Source Radius** in the **Source Description** section:

- Source Contaminant Mass Fraction: This input parameter is the steady state contaminant mass fraction in units of mass fraction. The valid range of values for this field is between 0 and 100 mass fractions.

- Source Temperature: This input parameter is the steady state source temperature for the contaminant in units of K. The valid range of values for this field is between 233.15 and 333.15 K.
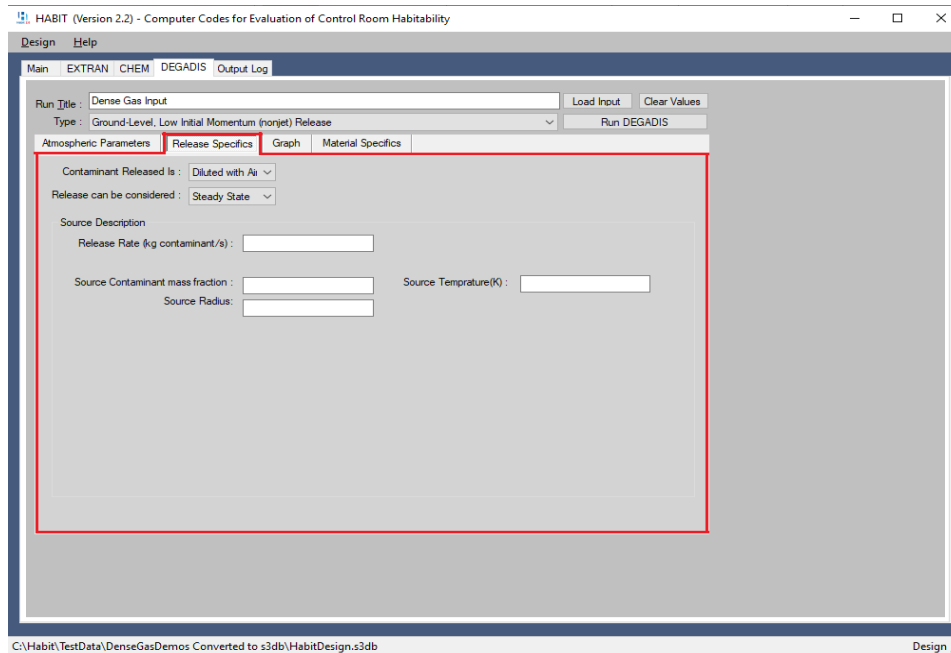
Figure 4-33   DEGADIS Tab Release Specifics (Diluted with Air Option)

Figure 4-34 displays the **Release Specifics** tab with the **Pure/Transient** options selected in the two drop-down menus. Notice that there is now a new input field in the upper right of the tab, **Initial Mass of Pure Contaminant over the source**, and that the input fields in the **Source Description** section are replaced by a table. The new input field in the upper right of the tab is the initial mass of pure contaminant over the source in units of kg. The valid range of positive values for this field is up to 5,000 kg. The table in the **Source Description** section shows **Release Rate** and **Source Radius** values for various time periods during the transient and cannot be changed in the interface. The valid ranges of values for both fields are the same as those discussed above.
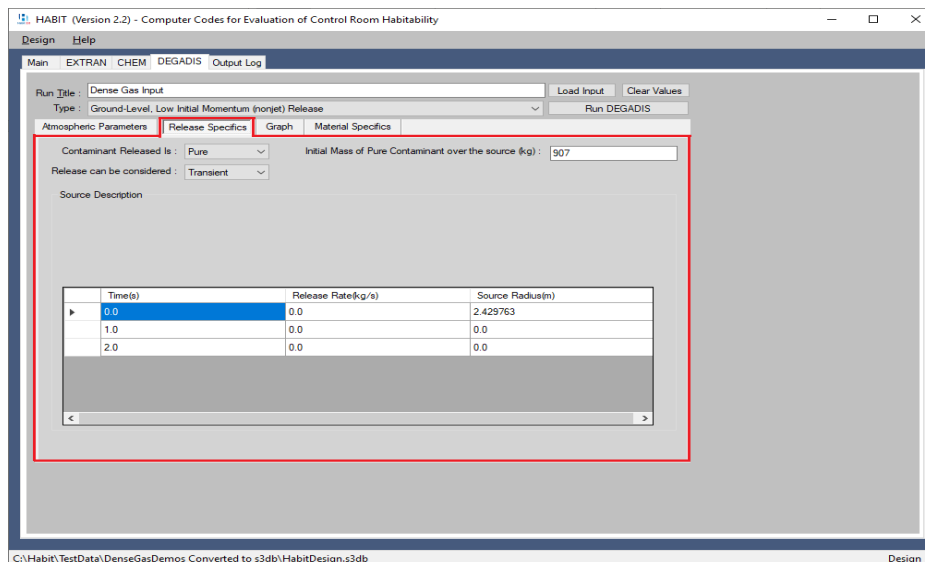
Figure 4-34   DEGADIS Tab Release Specifics (Transient Option)

4.3.2.5 DEGADIS Graph Tab

The **Graph** tab under the **DEGADIS** tab allows the user to create a graph plotted with the concentration output results for DEGADIS, as shown in Figure 4-35. This tab contains the following user-friendly features:

- Chart Type: This drop-down menu provides users with four chart options: (1) **Line**, (2) **Spline**, (3) **Step Line**, and (4) **Fast Line**.

- Point Labels: This drop-down menu provides users with 11 options for the position of the data point labels.

- Show X Axis Margin: This check box causes the X-axis to appear in the left-hand side margin.

- Display Chart as 3D: This check box shifts the chart from a two-dimensional image to a three-dimensional image.
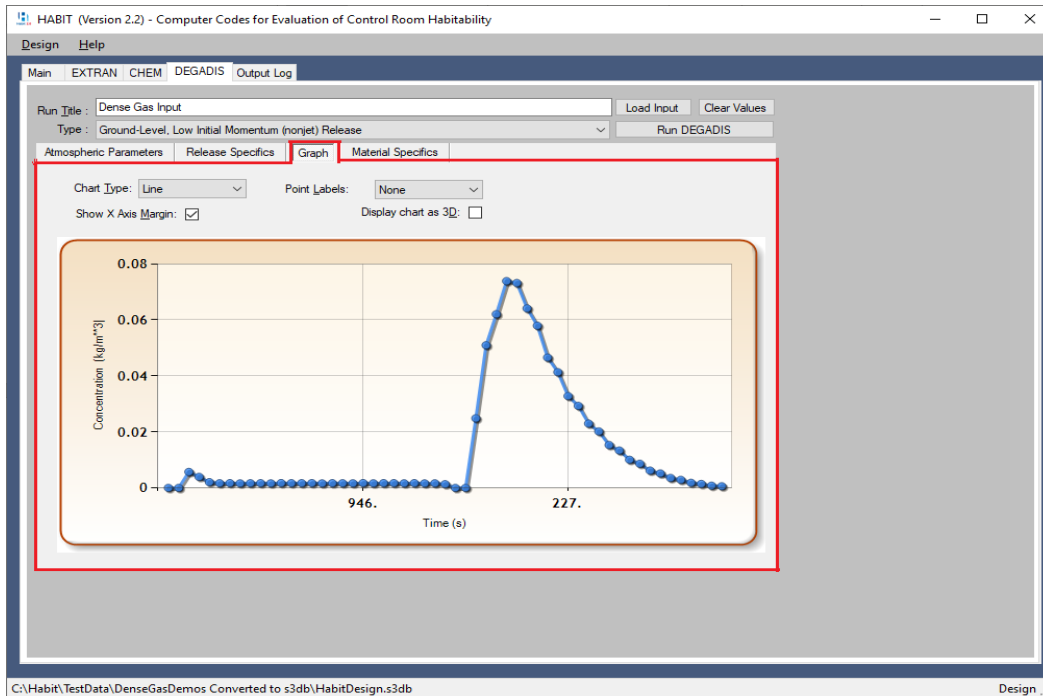
Figure 4-35   DEGADIS Graph Tab

4.4   SLAB Module

As mentioned in Section 1.0, HABIT 2.2 incorporates SLAB as one of the calculation models available to the user to evaluate the effects of denser-than-air chemical releases. As described in its user's manual [14], SLAB simulates the atmospheric dispersion of denser-than-air releases. The types of releases treated by SLAB include a ground-level evaporating pool, an elevated horizontal jet, a stack or elevated vertical jet, and an instantaneous volume source. SLAB models all of these sources as either pure vapor or a mixture of vapor and liquid droplets, with the exception of the evaporating pool source, which is assumed to be all vapor.

HABIT 2.2 will not automatically run the denser-than-air models of DEGADIS and SLAB but will inform the user that an evaluation of the release using the BMW criteria has determined that the dense gas effects are important to this run (Figure 4-2). With the buttons shown in Figure 4-2, the user can choose to have HABIT 2.2 run either DEGADIS, SLAB, both dense gas codes, or none of the dense gas codes. When the option to run either SLAB or all dense gas models is selected, HABIT 2.2 will use the EXTRAN spill, meteorological, and chemical input parameters along with the dense gas input variables provided by the user to perform the SLAB model calculations. Unlike DEGADIS, the input parameters used in the SLAB calculations can be fitted in one page that is displayed on the **SLAB** tab as shown in Figure 4-36 and described in Section 4.4.2.

4.4.1   SLAB Code Description

4.4.1.1   General Description

As described in its user's manual [14], SLAB calculates the atmospheric dispersion of the release by solving the conservation equations of mass, momentum, energy, and species. Additionally, the conservation equations are spatially averaged to treat the cloud as either a steady state plume, a transient puff, or a combination of the two depending upon the duration of the release. SLAB models a continuous release (very long source duration) as a steady state plume. In the case of a finite duration release, cloud dispersion is initially described using the steady state plume mode and remains in the plume mode if the source is actively releasing the chemical. Once the source stops, SLAB models the cloud as a puff, and subsequent dispersion is calculated using the transient puff mode. For instantaneous releases, SLAB models the release using the transient puff dispersion model for the entire duration of the release calculation. SLAB can model continuous, finite duration, and instantaneous releases from four types of sources:

- a ground-level evaporating pool release
- an elevated horizontal jet release
- a vertical jet or stack release
- a ground-based instantaneous or short-duration evaporating pool release

While SLAB is designed to model denser-than-air releases, it will also simulate cloud dispersion of neutrally buoyant releases and includes lofting of the cloud if it becomes lighter than air. The equations and theory for the models used in SLAB are described in detail in the SLAB user's manual [14]. Additionally, SLAB uses the stability class to simplify the inverse Monin-Obukhov length values. Table 4 of Section 3.1.5.6 of the user's manual [14] lists the values SLAB used for stability class, not the inverse Monin-Obukhov length values.

4.4.2   SLAB TDI Features

4.4.2.1   General Features of the SLAB TDI Tab

The user should be aware of some of the basic features associated with the **SLAB** tab in the HABIT 2.2 TDI as shown in Figure 4-36. The values for the parameters will be pre-populated when imported from a previous design; otherwise, the user can enter the appropriate values. When the mouse pointer is hovered over an input field, the code will display the valid range for that field. The other general features on the **SLAB** tab include the following:

- The **Load Input** button opens an MS Windows OS File Explorer window, as shown in Figure 4-4. The user can then browse to the location of an existing folder and select the SLAB input file (i.e., "DesignSLAB.inp") to open in that folder. Select the **OK** button to open the existing design.

- The **Clear Values** button clears all values in the SLAB input parameters from the tab and starts over with blank parameter input fields. Selecting this button will open the **Clear Form** window shown in Figure 4-5. Selecting the **Yes** button on the **Clear Form** window will clear all the current values from the tab and return the user to a blank **SLAB** tab. Selecting the **No** button will retain the current values and return the user to the **SLAB** tab.

- The **Run SLAB** button will execute the program against the user-provided input parameters in the **SLAB** tab. Additionally, this will open the **Output Log** tab (Figure 3-13) displaying MS-DOS output from the Fortran formulations and computations so they are visible from within the application.
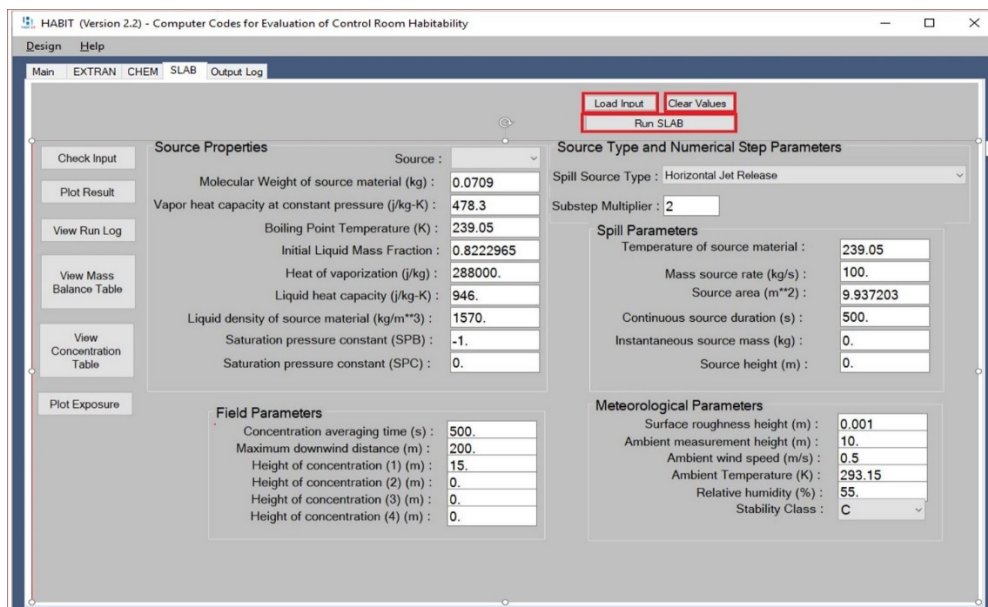
Figure 4-36   SLAB Tab General Features

As shown in Figure 4-36, the **SLAB** tab also contains five parameter input sections: **Source Properties**, **Field Parameters**, **Source Type and Numerical Step Parameters**, **Spill Parameters**, and **Meteorological Parameters**. The values for the parameters in these sections will be pre-populated when imported from a previous design or when available from running the EXTRAN module; otherwise, the user can enter the appropriate values.

4.4.2.2   Source Properties Section

The **Source Properties** section contains the parameters used to define the physical characteristics of the source material released, as shown in Figure 4-37. The input source properties are as follows:

- Source: HABIT 2.2 comes with a SLAB source data file, "SLABSources.XML," which contains information about the physical characteristics for 14 chemicals. The **Source** field is a drop-down menu with the names of the 14 chemicals in the "SLABSources.XML" file. The user can either select one of these chemicals or select **blank field**. When a chemical from the drop-down list is selected. the required chemical parameters will be automatically entered in the **Source Properties** section. When the **blank field** option is selected from the drop-down menu, the user will have to manually enter the values in the parameter fields. Note that all units written as "[j]" on the interface shown in Figure 4-37 should be read as "[J]" for joule.

Figure 4-37   SLAB Tab Source Properties Input Section

- Molecular Weight of source material: This parameter provides the molecular weight in units of kilograms per mole (kg/mol) for the chemical or the chemical compound. The valid range of values for this field is from 0.02 to 0.2 kg/mol.

- Vapor Heat Capacity at Constant Pressure: This is the vapor phase heat capacity in units of J/kg/K at a constant pressure. The vapor phase heat capacity is a required input for SLAB, but it is not required for EXTRAN. SLAB uses this parameter (i.e., CPSL) in the energy balance to determine cloud temperature. The valid range of values for this field is from 1,000 to 5,000 J/kg/K.

- Boiling Point Temperature: This parameter provides the boiling point for the chemical in units of K. EXTRAN converts temperatures entered in units of °C to K as needed within the code to perform calculations. Boiling point temperatures are a function of pressure and should be the boiling point at 1 atm pressure (760 mmHg). The valid range of values for this field is from 18.5 to 773.15 K.

- Initial Liquid Mass Fraction: This field is the mass fraction of the liquid phase of the release. It is a unitless field. The valid range of values is from 0 to 1.0.

- Heat of Vaporization: The heat of vaporization is the energy used in calculating the evaporation of liquids. The heat of vaporization is in units of joules per kilogram (J/kg). The valid range of values for this field is from $1x10^5$ to $2x10^6$ J/kg.

- Liquid Heat Capacity: The liquid heat capacity determines the fraction of a liquefied gas that flashes upon release and temperature change in the spill pool. Liquid heat capacity is in units of J/kg/K. The valid range of values for this field is from 500 to 5,000 J/kg/K.

- Liquid Density of Source Material: This parameter provides the density in units of kg/m^3 for the chemical or the chemical compound. HABIT 2.2 converts the density (specific gravity) entered on the **EXTRAN** tab from units of g/ml to kg/m^3 for use in the dense gas calculations. The valid range of values for this field is from 50 to 5, 000 kg/m^3.

- Saturation Pressure Constant (SPB): This input field is the source material-specific saturation pressure constant B as expressed in Equation (43a) of the SLAB user's manual [14] and denoted as variable SPB in SLAB. It is the basic property of the released source material. Both SPB and variable SPC described in the next bullet are unitless constants and required for SLAB calculations. Table 2 of the user's manual [14] provides SPB and SPC values. The suggested SPB values for this field are between 500 and 5,000. A default SPB value can be obtained using Equation (43b) of the user's manual [14].

- Saturation Pressure Constant (SPC): This input field is the source material-specific saturation pressure constant C as expressed in Equation (43a) of the SLAB user's manual [14] and denoted as variable SPC in SLAB. Table 2 of the user's manual [14] provides SPC values in units of K. The valid range of values for this field is from 0 to 500 K.

- Saturation Pressure Constant (A): This field is not visible in Figure 4-37. However, it is the source material-specific saturation pressure constant A as expressed in Equation (43a) of the SLAB user's manual [14] and denoted as variable SPA in SLAB. This constant can be computed by Equation (43c) in the user's manual [14] with a given boiling point temperature of the substance.

4.4.2.3   Field Parameters Section

The **Field Parameters** section contains the inputs used to define the physical characteristics of the chemical effluent, as shown in Figure 4-38. The input parameters are as follows:

- Concentration Averaging Time: The concentration averaging time is the appropriate averaging time, in units of s, for the safety standard of interest. For example, if the safety standard of interest for a particular material is a maximum average concentration of 100 ppm for a 1-hour exposure, then the concentration averaging time would be 3,600 s. For a single toxic material, there are generally a number of safety levels of

interest, each corresponding to a different exposure time. Thus, there might be 8-hour, 1-hour, 15-minute, and less-than-1-minute exposure levels. In this case, SLAB would have to be run four times, each with different values for the concentration averaging time corresponding to the appropriate duration of exposure. The valid range of values for this field is between 10 and 600 s.

- Maximum Downwind Distance: This distance is the maximum downwind distance, in units of m, for which the user is interested in identifying the cloud concentration. The valid range of values for this field is from 50 to 2,000 m.
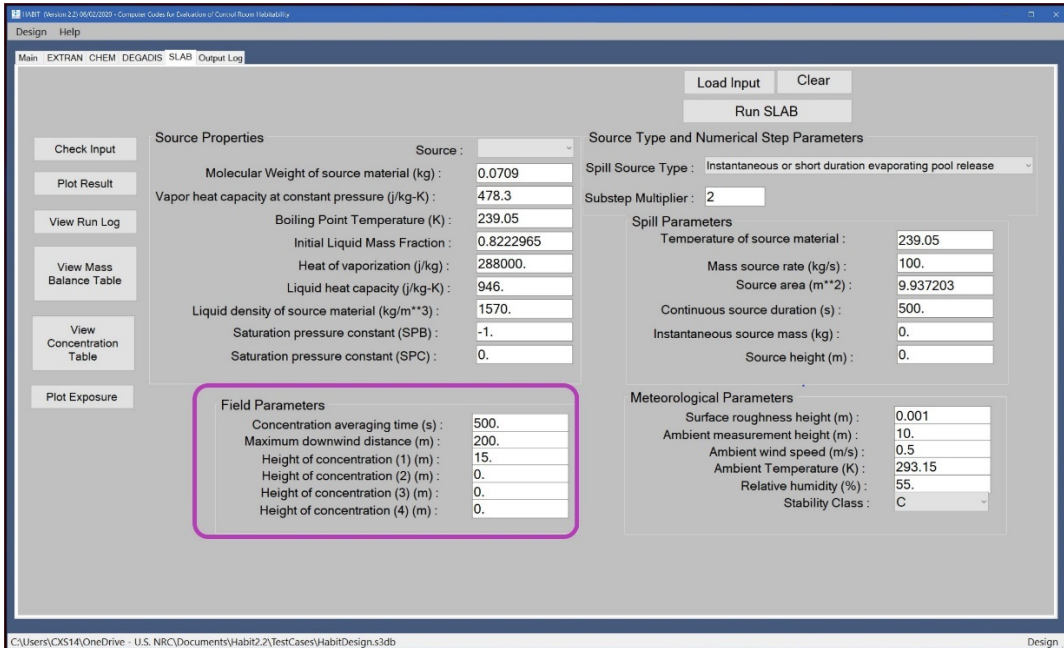
Figure 4-38   SLAB Tab Field Parameters Input Section

- Height of Concentration (1) through (4): This is the height, in units of m, at which the concentration is calculated as a function of downwind distance. No matter how many heights are to be used in the concentration calculation, four values of height must be specified in the input file even if all four values are equal to zero. The valid range of values for this field is from 0 to 30 m.

4.4.2.4   *Source Type and Numerical Step Parameters Section*

The **Source Type and Numerical Step Parameters** section contains the spill type inputs and the substep multiplier, as shown in Figure 4-39.
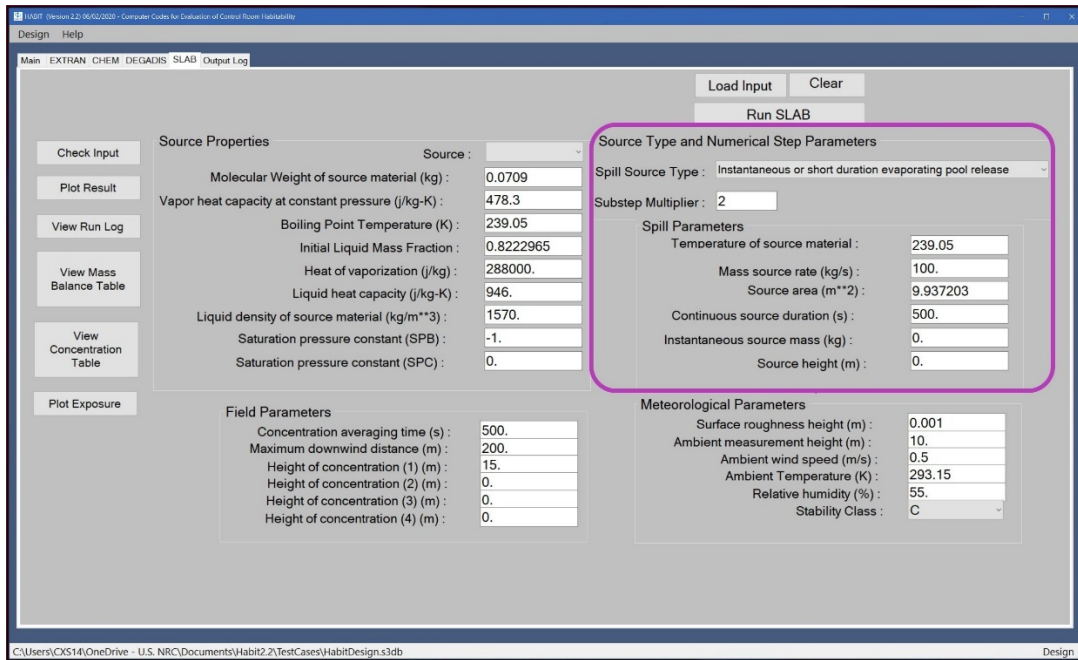
**Figure 4-39   SLAB Tab Source Type and Numerical Step Parameters and
Spill Parameters Input Sections**

The input source type and numerical step parameters are as follows:

- Spill Source Type: This is a drop-down menu that contains the four types of spills model by SLAB. The four drop-down menu options are as follows:

  (1)   Evaporating Pool Release: This is a ground-level, area source of finite duration. The center of the source is located at x, y, z coordinates 0.0, 0.0, 0.0; where x is downwind distance, y is crosswind distance, and z is height. When the spill duration is sufficiently short, a steady state plume does not form at any downwind distance. When SLAB determines that this is the case, it will automatically stop the calculation, redefine the source type as a short-duration evaporating pool release, and start the calculation over.

  (2)   Horizontal Jet Release: The horizontal jet release is an area source with the source plane perpendicular to the ambient wind direction and source velocity pointing directly downwind. The center of the jet is located at x = 1.0, y = 0.0, and z = the input spill parameter **Source height**, with the initial liquid mass fraction equal to 1.0.

  (3)   Vertical Jet or Stack Release: The vertical jet or stack release is an area source with the source plane parallel to the ground and the source velocity pointing directly upward. The center of the source is located at x = 0.0, y = 0.0, and z = the input spill parameter **Source height**, with the initial liquid mass fraction equal to 1.0.

  (4)   Instantaneous or Short Duration Evaporating Pool Release: The instantaneous or short duration evaporating pool release is a combination of two sources: an

instantaneous volume source with a total mass given by the input spill parameter **Instantaneous source mass** and a short-duration, ground-level, area source with a source rate and spill duration given by the input spill parameters **Mass source rate** and **Continuous source duration**, respectively. When an instantaneous volume release is to be simulated, **Instantaneous source mass** is specified, and the **Mass source rate** and **Continuous source duration** are both set equal to zero. In SLAB, the pressure within the cloud is always equal to 101,325 N/m^2 (1 atm). Consequently, if an expanding source release (explosion) is to be simulated, the SLAB calculation begins after the source is fully expanded and the pressure has been reduced to the ambient atmospheric level. The short-duration evaporating pool release is intended to be a default for the **Spill Source Type**>**Evaporating Pool Release** when the spill duration is so short that steady state is not reached anywhere within the dispersing cloud. While this type of source can be run directly by setting the **Spill Source Type** to **Instantaneous or Short Duration Evaporating Pool Release** and specifying input spill parameters **Mass Source Rate** and **Continuous Source Duration**, the NRC recommends that an evaporating pool release of any finite duration be run with the **Spill Source Type** set to **Evaporating Pool Release**. If a steady state cloud is not achieved (due to short spill duration), the code will automatically change the **Spill Source Type** to **Instantaneous or Short Duration Evaporating Pool Release** and indicate this change in the code output.

- Substep Multiplier: This input parameter is an integer substep multiplier that specifies the number of calculational substeps performed during the integration of the conservation equations. A value of 1.0 is generally recommended to provide computational stability and sufficient numerical accuracy. However, if numerical stability problems are encountered, the value can be increased. For example, a default value of 2.0 doubles the number of substeps and decreases the size of the integration step by a factor of one-half. Similarly, a value of 3.0 triples the number of substeps and decreases the size of the integration step by a factor of one-third. The overall effect of change to this input value, from 1 to 9, will result in an increase in computational time roughly equal this input value.

4.4.2.5   Spill Parameters Section

The **Spill Parameters** section contains the inputs used to define the physical characteristics of the spill or chemical release, as shown in Figure 4-39. The input spill parameters are as follows:

- Temperature of Source Material: This is the temperature of the source material released in units of K. This value depends upon the **Spill Source Type** selected in Section 4.4.2.4. When the source is an evaporating pool, as indicated by the selection of either **Evaporating Pool Release** or **Instantaneous or Short Duration Evaporating Pool Release**, this value is the same as the temperature entered for the boiling point in the **Source Properties** section. When the release is instantaneous, as indicated by the spill source type **Instantaneous or Short Duration Evaporating Pool Release**, the source temperature is either the temperature of the material at the instant it is released or, when the source is the result of an explosion, the temperature of the material after it is fully expanded and reduced to a pressure of 1 atm. For situations where the release

is a pressurized jet release, as indicated by the use of either the **Horizontal Jet Release** or **Vertical Jet or Stack Release** types, the source conditions are the properties of the material after it has fully expanded. When the source material is stored as a vapor under pressure and, therefore, released as a vapor (i.e., the source parameter **Initial Liquid Mass Fraction** equals zero), the NRC recommends that the expansion be treated as adiabatic. The source temperature is then calculated as described in Section 3.1.3.1 of the SLAB user's manual [14]. The valid range of values for this field is from 18.5 to 773.15 K.

- Mass Source Rate: This is the release rate of the spill source in units of kg/s. It is dependent upon the **Spill Source Type** selected in Section 4.4.2.4. For the continuously releasing spill source types (i.e., the evaporating pool, either of the jet releases, and the short-duration evaporating pool), this is the spill source release rate. For the **Instantaneous Release** type, this value should be set equal to zero. The valid range of values for this field is from 0 to 5,000 kg/s.

- Source Area: This is the source area in units of m^2. It is dependent upon the **Spill Source Type** selected in Section 4.4.2.4. For an evaporating pool release (i.e., **Evaporating Pool Release** or **Short Duration Evaporating Pool**), the **Source area** is the area of the evaporating pool. If the **Source area** is not known, it can be calculated from the effective evaporation rate using the equations in Section 3.1.3.3 of the SLAB user's manual [14]. The valid range of values for this field is from 25 to 900 m^2.

- Continuous Source Duration: This is the duration from the release of an evaporating pool in units of s. It is dependent upon the **Spill Source Type** selected in Section 4.4.2.4. When an instantaneous release is to be simulated, the **Continuous source duration** is set equal to 0 s. The valid range of values for this field is from 0 to 9,999 s.

- Instantaneous Source Mass: This input value is the total mass for spill type **Instantaneous Release** in units of kg. When the source is either an evaporating pool or jet release, this value is set equal to 0 kg. The valid range of values for this field is from 0 to 9,999 kg.

- Source Height: The definition of the **Source height** differs for each source type and is in units of m. For the spill types for evaporating pools (i.e., **Evaporating Pool Release** and **Short Duration Evaporating Pool Release**), the **Source height** value is set equal to 0.0 m because the pool is assumed to be at ground level. For the spill type **Horizontal Jet Release**, the **Source height** value is set equal to the center of the jet. For the spill type **Vertical Jet or Stack Release**, the **Source height** value is set equal to the actual height of the jet or stack. Finally, when the spill type **Instantaneous Release** is simulated, the **Source height** value is the height of the instantaneous release, such that the product of the **Source height** and **Source area** is equal to the total volume released as discussed in Section 3.1.3.3 of the SLAB user's manual [14]. The valid range of values for this field is from 0 to 99 m.

4.4.2.6   Meteorological Parameters Section

The **Meteorological Parameters** section contains the inputs used to define the atmospheric conditions in the area of the chemical release, as shown in Figure 4-40. The meteorological parameter inputs are as follows:

- Surface Roughness Height: This is the same parameter as described in the **Dense Gas Variables** section of the **EXTRAN** tab (Section 4.1.2.5). Section 3.1.5.1 of the SLAB user's manual [14] discusses the surface roughness height, including a table of values for the **Surface roughness height** parameter based upon the type of surface. Surface roughness height is in units of m. The valid range of values for this field is from 0 to 5 m, for example, for ice and full-grown root crops, respectively (see Table 3 of the SLAB user's manual [14]).

- Ambient Measurement Height: This is the height at which the ambient wind speed is measured in units of m. As noted in Section 3.1.5.1 of the SLAB user's manual [14], this height should be significantly larger than the **Surface roughness height**. The valid range of values for this field is from 10 to 99 m.

- Ambient Wind Speed: This is the average wind speed at the **Ambient measurement height** in units of m/s. The valid range of values for this field is from 0 to 30 m/s.

- Ambient Temperature: This is the environmental ambient air temperature in units of K. EXTRAN converts the air temperature entered in units of °C to K as needed within the code to perform calculations. The converted air temperature from EXTRAN is used for SLAB calculations. This field is editable by the user. The valid range of values for this field is from 233 to 333 K.

- Relative Humidity: This parameter is the environmental relative humidity in units of percent humidity. This field is an input parameter from the **Dense Gas Variables** section of the **EXTRAN** tab. This field is editable by the user. The valid range of values for this field is from 0 to 100 percent.

- Stability Class: Atmospheric stability classes A through F are defined in Table 2-2 of RG 1.23 [21]. This parameter field has a drop-down menu with options **A** through **F**, ranging from extremely unstable **A** to extremely stable **F**. The **EXTRAN** tab includes the option for atmospheric stability class **G**, which is considered sufficiently rare that it is no longer typically used. Since SLAB only has provisions for atmospheric stability classes **A** through **F**, if atmospheric stability class **G** is selected in the **EXTRAN** tab, SLAB will use atmospheric stability class **F** to best approximate atmospheric stability class **G**.

Figure 4-40   SLAB Tab Meteorological Parameters Input Section

5   REFERENCES

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APPENDIX A   UNIFICATION FOR INPUT PARAMETER

As part of the U.S. Nuclear Regulatory Commission's (NRC's) effort to follow the Advisory Committee on Reactor Safeguards recommendation to consider and include the effects of denser-than-air contaminant cloud behavior in the HABIT code, the NRC staff recognized that many of the input parameters used in the EXTRAN computer code are also used in the denser-than-air models of the DEGADIS and SLAB codes. To facilitate workflow for the final user, this section summarizes the current inputs to EXTRAN and how they are used in DEGADIS and SLAB.

A.1   EXTRAN Code Dispersion Model Input Parameters

In HABIT version 2.2, EXTRAN models four basic release scenarios for accident chemical releases in the vicinity of the control room (CR):

(1)   Liquid Tank Burst
(2)   Liquid Tank Leak
(3)   Gas Tank Burst
(4)   Gas Tank Leak

All of these are treated as time dependent. (**Note** that DEGADIS and SLAB inputs can be changed to simulate continuous releases that do not stop, termed steady state releases.) HABIT 2.2 uses the convention that input parameters are listed as required (**R**), optional (**O**), or not used (**N**) depending on the release case or type. In general, DEGADIS and SLAB have the same input requirements, so that if EXTRAN has an input that is required, it will be required for both DEGADIS and SLAB as well. DEGADIS and SLAB also have input parameters that are not included in the current input parameters for EXTRAN, but these parameters can often be estimated or calculated from information already supplied to EXTRAN. One example of this type of input is the Monin-Obukhov length, which can be directly input to DEGADIS and SLAB. However, the atmospheric stability class and surface roughness that are (required) inputs to EXTRAN can be used to estimate the Monin-Obukhov length in both DEGADIS and SLAB.

For the four scenarios listed above, EXTRAN estimates the rate at which material becomes airborne so DEGADIS and SLAB can then calculate atmospheric dispersion calculations to determine the impact. DEGADIS and SLAB are both strictly atmospheric dispersion models in the sense that they require the airborne rate of the dispersing material, which must be provided by the user. For consistency, EXTRAN output is used in some cases to provide the rate the released material becomes airborne, particularly for evaporating liquid pools. EXTRAN models flashing liquid releases assuming the liquid phase completely rains out on the ground. This approach has been called into question, particularly given preliminary results from recent field-scale releases of chlorine. The sections that follow outline the approach that users can take, assuming that the liquid phase of a flashing two-phase release remains suspended as an aerosol.

A.2   BMW Criteria for Recommending Use of a Denser-than-Air Dispersion Model

After EXTRAN performs its calculation, HABIT 2.2 will evaluate the release to determine the importance of denser-than-air effects using the Britter-McQuaid Workbook (BMW) criteria [1] [2]. The BMW criteria proposed correlations for modeling the dispersion of denser-than-air

contaminants from area sources for plumes and puffs based on field test data. The analysis of the field test data identified the dominant independent variables as (1) density of the released contaminant after depressurization to atmospheric pressure, (2) volumetric release rate or total volume released, (3) characteristic wind speed, and (4) characteristic source dimension. The correlations proposed by the BMW criteria are also limited by the lowest concentrations that could be predicted (1,000 to 2,000 ppm), but they also proposed criteria by which the importance of denser-than-air effects can be assessed. Equations 4-1 and 4-2 are the BMW criteria for steady state plume releases and for instantaneous puff gas releases, respectively, determining when the denser-than-air effects consideration is recommended. The choice of the calculation is depending user's need. However, EXTRAN, DEGADIS and SLAB can be run simultaneously for comparison or validation purposes.

A.3　　Meteorological Input Parameters

Table A-1 shows the relationship between meteorological input parameters for EXTRAN, DEGADIS, and SLAB. As noted in Table A-1, the following important parameters are used by DEGADIS and SLAB, but not by EXTRAN:

- Ambient Humidity: DEGADIS and SLAB both consider the effect of ambient humidity, which can be important when considering cryogenic materials (e.g., liquified natural gas).

- Surface Roughness: DEGADIS and SLAB both use the site surface roughness to parameterize air entrainment into the dispersing cloud (via the friction velocity, which includes the effect of atmospheric stability).

The reverse Monin-Obukhov length can be estimated by both DEGADIS and SLAB models based on the atmospheric stability class and the surface roughness. Consequently, the following input parameters are fixed in DEGADIS and SLAB:

- DEGADIS (oodist): Offset distance for a vertical jet release not used (set oodist = 0.)

- DEGADIS (indvel): This variable indicates whether the default Monin-Obukhov length is used (indvel = 1) or whether a value has been input by the user (indvel = 2) (set indvel = 1)

- DEGADIS (frml): A user input value of the Monin-Obukhov length not used (set frml = 0.)

- DEGADIS (humid): The ambient humidity is based on the relative humidity (set humid = 0.)

- SLAB (ALA): The inverse Monin-Obukhov length is based on the input stability class and is not used (set ALA = 0.)

Table A-1   HABIT 2.2 Meteorological Input Parameters

Model Input	Common Variable	EXTRAN Model Type Input	DEGADIS	SLAB
Wind Speed (at 10 m) (m/s)	U_a	R – R – R – R	u0 (m/s) = U_a z0 (m) = 10 m	UA (m/s) = U_a ZA = 10 m
Atm. Stability Class	Note 1	R – R – R – R	istab (A=1, B=2, etc.)	STAB (A=1, B=2, etc.)
Air Temperature (°C)	T_a	R – R – R – R	tamb (K) = T_a + 273.15	TA (K) = T_a + 273.15
Atmospheric Pressure (mmHg)	P_a	R – R – R – R	pamb (atm) = P_a/760	not used
Solar Radiation (W/m²)	R_s Note 2	R – R – N – N	Note 3	Note 3
Cloud Cover (1/10)	cc Note 2	R – R – N – N	Note 3	Note 3
Ground Temperature (°C)	T_g Note 2	R – R – N – N	tsurf (K) = T_g + 273.15 Note 3	Note 3
Surface roughness (m)	None	R – R – R – R Note 4	z_R	ZO
Relative Humidity (%)	None	R – R – R – R Note 4	relhum	RH

Notes:

1   EXTRAN uses Pasquill-Gifford stability classes A–G. Stability class G is typically considered sufficiently rare that it is no longer used. DEGADIS and SLAB only have provision for classes A–F, so class G would be best approximated with class F in those models.

2   EXTRAN uses these inputs only for liquid releases to estimate the heat input to a liquid pool [4], and these can also be used to make similar estimates for DEGADIS and SLAB. DEGADIS uses the surface temperature (tsurf) to estimate ground-to-cloud heat transfer downwind of the source; this parameter is only relevant if the dispersing cloud is cold.

3   The pool evaporation model in EXTRAN uses these parameters. The EXTRAN-calculated mass evolution as a function of time is used to generate source input parameters for DEGADIS and SLAB.

4   Surface roughness and relative humidity are not used by EXTRAN but are required inputs for DEGADIS and SLAB.

A.4   Chemical Input Parameters

Table A-2 shows the relationship between chemical input parameters for EXTRAN, DEGADIS, and SLAB.

Table A-2   HABIT 2.2 Chemical Input Parameters

Model Input	Common Variable	EXTRAN Model Type Input	DEGADIS	SLAB
Chemical Name	None	O – O – O – O	Note 1	not used
Molecular Weight (g/mol)	mw_g	R – R – R – R	gas_mw (kg/kmol) = mw_g	WMS (kg/gmol) = $mw_g/1000$
Normal Boiling Point (°C)	T_b	R – R – N – N	Note 2	TBP (K) = $T_b + 273.15$ [3]
Liquid Heat Capacity (J/g/°C)	c_p	R – R – N – N	Note 2	DHE (J/kg) = $h_v *1000$
Heat of Vaporization (J/g)	h_v	R – R – N – N	Note 2	Note 3
Specific Gravity (liquid) (g/ml)	ρ_L	R – R – N – N	Note 2	RHOSL (kg/m³) = $\rho_L *1000$
Molecular Diffusion Coefficient (cm²/s)	D	O – O – N – N	Note 4	Note 4
Vapor Phase Heat Capacity (J/g/K)	c_{pv}	R – R – R – R [5]	gascpk = CPS gascpp = 0	CPS

Notes:

[1]   DEGADIS has a simple chemical database based that has appropriate property values, but these may not be useful for the other codes.

[2]   These parameters are not used to estimate other input parameters for DEGADIS and SLAB. For simplicity, input variable names used in SLAB (and common variables in the table) are used to describe DEGADIS inputs.

[3]   NUREG/CR-6210, "Computer Codes for Evaluation of Control Room Habitability (HABIT)," issued June 1996 [3], specifies that the normal boiling point should be specified at 1 atm ambient pressure. SLAB assumes the ambient pressure is always 1 atm; therefore, the values are the same.

[4]   The pool evaporation model in EXTRAN uses these parameters. The EXTRAN-calculated mass evolution as a function of time is used to generate source input parameters for DEGADIS and SLAB.

[5]   Vapor phase heat capacity is not used by EXTRAN but is a required input for DEGADIS and SLAB.

As noted in Table A-2, the vapor phase heat capacity is a required input for DEGADIS and SLAB; however, it is not required for EXTRAN. Both DEGADIS and SLAB use this parameter in the energy balance to determine cloud temperature. DEGADIS also has the capability of using a temperature-dependent liquid heat capacity, but this capability is likely only important for cryogenic liquids. Therefore, assuming a constant liquid heat capacity is adequate for DEGADIS.

The following input chemical parameters are required by DEGADIS and SLAB for calculations:

- Initial Vapor/Liquid Phase Mass Faction: For aerosol releases, the vapor flash fraction, f_v, can be calculated using $f_v = CPSL*(T_s – T_b)/DHE$ for both DEGADIS and SLAB. SLAB requires the liquid phase mass fraction (CMEDO) as input, and CMEDO = $1 – f_v$.

- Vapor Pressure Constants: SLAB uses the vapor pressure as a function of temperature, so these constants are necessary for cases involving liquids. The SLAB vapor pressure equation is $P_{SAT} = P_A \exp(SPA - SPB/(T + SPC))$, with P_A representing ambient pressure (newtons per square meter (N/m^2)), and T the temperature (Kelvin (°K)). This equation can be used in DEGADIS calculations as well. SLAB (which uses a constant atmospheric pressure of 101,325 N/m^2) allows for default values for saturation pressure constant B (SPB) and saturation pressure constant C (SPC) of -1.0 and 0.0, respectively. With these default values, SLAB calculates the value of SPA and SPB based on the normal boiling point (assuming SPC = 0).

A.5   Spill Input Parameters

Table A-3 shows the relationship between spill input parameters for EXTRAN, DEGADIS, and SLAB. Many of the EXTRAN inputs are used in both DEGADIS and SLAB, but the relationship between parameters is less direct than for meteorological and chemical parameters. Additional inputs required by SLAB and DEGADIS are also listed in Table A-3.

The remaining model parameters required to complete the SLAB input file are as follows:

- spill source type (IDSPL)
- numerical substep parameter (NCALC)
- temperature of source material (°K) (TS)
- mass source rate (kilogram per second (kg/s)) (QS)
- source area (square meter (m^2)) (AS)
- continuous source duration (seconds (s)) (TSD)
- instantaneous source mass (kilograms (kg)) (QTIS)
- source height (meters (m)) (HS)
- concentration averaging time (s) (TAV)

All these parameters depend on the source type (IDSPL) except for the numerical substep parameter (NCALC). When SLAB was originally written, there were often conflicts between accuracy and computational speed, and this value was recommended to be NCALC = 1. Given the speed of current computational resources, a value of NCALC = 2 may be preferred.

Table A-3 HABIT 2.2 Spill Input Parameters

Model Input	Common Variable	EXTRAN Model Type Input	DEGADIS	SLAB
Initial Mass (kg)	m Note 1	R – R – R – R		
Release Rate (kg/s)	dm	N – R – N – R		
Release Height (m)	h	O – O – O – O		
Storage Temperature (°C)	T_s Note 2	R – R – R – R		
Maximum Pool Radius (m)	R_{max}	O – O – N – N		
Distance to Intake (m)	X_p	R – R – R – R		XFFM = X_p
Intake Height (m)	Z_p	O – O – O – O		ZP(1) = Z_p/4; ZP (2) = 2*Z_p/4 etc.
Building Area (m²)	A_{wake}	O – O – O – O		
Ventilation Flow Rate (m³/s)	F_v	N – N – N – O		
Averaging Time (s)		N – N – N – N	avtime Note 3	TAV Note 3
Storage Pressure (Gauge) (N/m²)		N – N – N – N]	P_i	P_i

Notes:

1   The initial mass in EXTRAN is the entire inventory of material to be released.

2   NUREG/CR-6210 [3] states that the storage temperature is used to determine the expansion of gases upon release and the rate of evaporation of liquids. For pool evaporation, Witlox et al. (2010) [4] use T_p as the symbol for the pool temperature (calculated as a function of time), with an initial value of the lower of the boiling point (T_b) or the storage temperature.

3   The averaging time used in DEGADIS and SLAB accounts for the effect of plume meander and depends on the hazard time under consideration (t_h) as well as the amount of time required for the release to become airborne (t_d). For flammable materials, t_h can be taken to be zero; for toxic materials, t_h should be based on the criterion for comparison (e.g., TLV-STEL is based on an exposure duration of 15 minutes so t_h = 900 s). The length of time required for the release to become airborne depends on the spill scenario. DEGADIS and SLAB also have a lower limit of the averaging time (t_{min}) based on the model formulation (t_{min} = 20 s for DEGADIS and t_{min} = 10 s for SLAB). The averaging time input to the models should be taken as the max (min (t_h, t_d), t_{min}). The current implementation assumes that hazards under consideration are evaluated with the STEL; therefore, t_h = 900 s.

The remaining model parameters required to complete the DEGADIS input file are as follows:

- Computational flag to indicate if the gas phase energy balance is used (isofl = 0) or not (isofl = 1).

- Computational flag to indicate if ground-to-cloud heat transfer is used (ihtfl = 1) or not (ihtfl = 0).

- Ground-to-cloud heat transfer coefficient (watts per square meter Kelvin ((W/m^2K))) if the default value is not used (htco = 0).

- The parameters used for dispersion over water or not (iwtfl = 0 and wtco = 0).

- Gas temperature (°K) (gastem).

- Gas density (kilograms per cubic meter (kg/m^3)) (gasrho).

- Lower level of gas concentration concern (mole fraction) (gasllc). This parameter will depend on whether a toxic or flammable gas is under consideration. For toxic gases, this should be the level of concern, such as the threshold limie value–short-term exposure limit (TLV-STEL). For flammable gases, a concentration of 0.001 mole fraction should be adequate.

- Upper level of gas concentration concern (gasulc = 2*gasllc).

- Elevation above ground for concentration output (m) (gaszzc = 0).

- Lowest concentration for calculations (yclow = gasllc/10).

- Gas density as a function of concentration.

- Mass of gas initially over the area source (kg) (gmass).

- Area source parameters. Time (s), mass evolution rate (kg/s), source radius (m). For the source specification, default values can fill out each line: pwc = 1, ptemp = gastem, and pfracv = 1.

- Computational flag to indicate whether the simulation is for a steady, continuous release or for a transient release (check4 = F, because all cases simulated here are transient sources).

- A date/time stamp is included in the last line (24-character string).

All of these parameters depend on the source type except for the concentration output parameters (gasllc, gasulc, gaszzc, and yclow), the flag check4 (always F here because all cases simulated here are transient sources), and the date/time stamp.

A.6   EXTRAN Spill Type Summaries

The following sections summarize in detail the specifications for the remaining parameters for each spill type.

A.6.1   Liquid Tank Burst

In EXTRAN, this spill type generates a finite-duration release based on evaporation from a spreading liquid pool. If the vapor pressure at the storage conditions is higher than ambient pressure, there will be at least some flashing. NUREG/CR-6210 [3] indicates that the flash fraction is calculated using the ambient temperature, but the calculations may actually use the storage temperature. EXTRAN treats a flashing release assuming all of the liquid phase rains out and subsequently evaporates from a liquid pool; there are clear indications that such a treatment is neither realistic nor conservative.

The importance of flashing can be predicted based on several different approaches. Witlox et al. [4] considered data from several sources and concluded that there was a transition between mechanical breakup and fully flashing jets for superheats (temperature above the boiling point) between 10 and 20 degrees Celsius (°C). For the calculations proposed here, a conservative assumption would be to assume that jets fully flash with a superheat of 10 °C.

In DEGADIS, which uses units of atmosphere (atm) for ambient pressure, the normal boiling point should be adjusted to local atmospheric pressure using the Clausius-Clapeyron equation. Equation (A-1) uses the form of the equation in the SLAB code (Equation (43a) of the SLAB user's manual [5]):

$$P_{Sat} = P_A \, e^{\left(SPA - SPB/(T + SPC)\right)}$$
(A-1)

where P_{Sat} =   is the saturation pressure (atm)
        P_A =   is the ambient atmospheric pressure at 1 atm (atm)
        SPA =   a saturation pressure constant (unitless)
        SPB =   a saturation pressure constant (unitless)
        T =   is the local cloud temperature (K)
        SPC =   a saturation pressure constant (K)

The saturation pressure constants SPA, SPB, and SPC used in Equation (A-1) are basic properties of the released material. The constants SPB and SPC are required input parameters; however, a default option exists in SLAB in which the Clapeyron equation is used to specify SPB and SPC is assumed to be zero. When the SLAB default option is chosen, SPB is given by Equation (A-2):

$$SPB = DHE * \left(WMS/R_{gas}\right)$$
(A-2)

where SPB =   saturation pressure constant (unitless)
        DHE =   heat of vaporization (joules per kilogram (J/kg))
        WMS =   the molecular weight (kilogram per mole (kg/mol))
        R_{gas} =   ideal gas constant (8.314 joules per mole Kelvin (J/(mol K))

Note that Equation (A-2) was incorrect in the SLAB user's manual [5] but is correct in the SLAB code. When the default option is chosen, SPA is calculated from the normal boiling point and

SPB in Equation (A-2). The boiling point corrected to local ambient pressure is then given by Equation (A-3):

$$TBA = \left. SPB \middle/ \left(SPA - \ln\left(\frac{P_a}{760}\right)\right)\right.$$

(A-3)

where   *TBA* = the boiling point corrected to ambient pressure (K)
             P_a = is the ambient atmospheric pressure (mmHg)
             760 = the pressure conversion factor from mmHg to atm

In Equation (A-3), ambient pressure is in units of mmHg because those are the units used in EXTRAN.

A.6.1.1   Liquid Tank Burst—Two-Phase Flashing Release

In this spill type scenario, some liquid rainout may occur, but this case can be treated conservatively as if there is little or no liquid rainout.

The remaining model parameters required to complete the SLAB input file are as follows:

- Spill source type (IDSPL = 4).

- Temperature of source material (°K) (TS = TBP). Note that the normal boiling point is used in SLAB calculations.

- Mass source rate (kg/s) (QS = 0).

- Source area (m^2) (AS = $\pi^{1/3}(m/\rho)^{2/3}$).

- Continuous source duration (s) (TSD = 0).

- Instantaneous source mass (kg) (QTIS = mass of the tank inventory).

- Source height (m) (HS = $((m/\rho)/\pi)^{1/3}$).

- Source duration (s) (TSD = 0).

Values of source area (AS) and source height (HS) are set assuming that the height-to-diameter ratio of the initial cloud is 0.5, and the total volume is m/ρ, where m (or QTIS) is the total mass (kg) and ρ is the aerosol density given by Equation (A-4):

$$\rho = \left. 1 \middle/ \left[\left(\frac{f_v}{RHOV}\right) + \left(\frac{1 - f_v}{RHOSL}\right)\right]\right.$$

(A-4)

where ρ = the aerosol density (kg/m^3)
             F_v = is the crosswind friction term (unitless)
             RHOV   = is the volume-averaged cloud density (kg/m^3)
             RHOSL = the liquid density of the source material (kg/m^3)

The remaining model parameters required to complete the DEGADIS input file are as follows:

- Computational flags to model an aerosol release (isofl = 1 and ihtfl = 0).

- Ground-to-cloud heat transfer coefficient for an aerosol release (htco = 0).

- Gas temperature (°K) (gastem = TBA).

- Gas density (kg/m^3) (gasrho = ρ (aerosol density) as calculated in Equation (A-4)).

- Gas density as a function of concentration. Aerosol density is assumed to be a linear function of concentration. The input lines are as follows:

  2
  0.0   0.0   RHOA   0.0   TA
  1.0 ρ ρ 0.0   TBA

- Mass of gas initially over the area source (kg) (gmass = mass of the tank inventory).

- Area source parameters (including time (s), mass evolution rate (kg/s), and source radius (m)). The initial radius $R_0 = ((m/\rho)/\pi)^{1/3}$), where the height-to-diameter ratio of the cloud is assumed to be 0.5 as above. For an instantaneous release, the input lines are as follows:

  3
  0.0   0.0   R0   1.   TBA   1.0
  1.0   0.0   0.0   1.0   TBA   1.0
  2.0   0.0   0.0   1.0   TBA   1.0

The importance of denser-than-air effects on downwind dispersion can be confirmed using the BMW criterion for a puff with m as the total tank inventory and ρ_s as the aerosol density ρ as calculated in Equation (A-4).

A.6.1.2   Liquid Tank Burst—Evaporating Pool

In this spill type release scenario, the source parameters calculated by EXTRAN can be used to model the evaporating pool.

SLAB has no provision for an area source that changes over time, so representative source parameters must be determined from the EXTRAN output file. In the EXTRAN output file with extension "SPD," the continuous source duration (TSD) is taken to be the last entry in the column labeled "TIME" (the value of TIME is in minutes and must be converted to seconds for TSD), and the source area (AS) is taken to be the average of the column labeled "AREA."

The remaining model parameters required to complete the SLAB input file are as follows:

- Spill source type (IDSPL = 1).

- Temperature of source material (°K) (TS = Ts + 273.15 (from the EXTRAN storage temperature)).

- Mass source rate (kg/s) (QS = dm = m/TSD).

- Source area (m^2) (AS = average of the column labeled "AREA" from EXTRAN).

- Continuous source duration (s) (TSD = from EXTRAN).

- Instantaneous source mass (kg) (QTIS = 0).

- Source height (m) (HS = 0.0 m).

- Source duration (s) (TSD = 0).

The remaining model parameters required to complete the DEGADIS input file are as follows:

- Computational flags to model a gas release (isofl = 0 and ihtfl = 1).

- Ground-to-cloud default heat transfer coefficient (htco = 0).

- Gas temperature (°K) (gastem = TS).

- Gas density (kg/m^3) (gasrho = ideal gas vapor density (RHOV) in Eq. A-4).

- Gas density as a function of concentration (isofl = 0). Not used in this case.

- Mass of gas initially over the area source (kg) (gmass = 0).

- Area source parameters (including time (s), mass evolution rate (kg/s), and source radius (m)). The initial radius $R_0 = (AS/\pi)^{1/2}$ for consistency with the SLAB code. For a continuous release, the input lines are as follows:

  ```
  4
  0.0  dm  R0  1.0  TS  1.0
  TSD  dm  R0  1.0  TS  1.0
  TSD+1  0.0  0.0  1.0  TS  1.0
  TSD+2  0.0  0.0  1.0  TS  1.0
  ```

The importance of denser-than-air effects on downwind dispersion can be confirmed using the BMW criterion for a plume with dm as the average release rate, ρ_s as the gas vapor density RHOV as calculated above, and $D_s = 2 * R_0$.

A.6.2   Liquid Tank Leak

In EXTRAN, this spill type generates a finite-duration release based on evaporation from a spreading liquid pool for the duration of the release. For the tank burst, if the vapor pressure at the storage conditions is higher than ambient pressure, there will be some flashing.

The importance of flashing can be predicted as discussed in Section A.6.1 for Liquid Tank Burst.

Noticed that the Equation (A-1) is used to adjust a normal boiling point to the local atmospheric pressure and the Equation (A-3) is used to correct the boiling point to local ambient pressure.

A.6.2.1   Liquid Tank Leak—Two-Phase Flashing Release

In this spill type release scenario, some liquid rainout may occur, but this case can be treated conservatively as if there is little or no liquid rainout. This release scenario is simulated in SLAB as if the flashing release occurred from a ground-level, area source as a vertical jet (IDSPL = 3). For this scenario, DEGADIS and SLAB use the area of the release to predict several source parameters, but because this information is not currently requested by HABIT 2.2, the source parameters will be estimated assuming that the vertical jet velocity is the same as the ambient wind speed.

The remaining model parameters required to complete the SLAB input file are as follows:

- Spill source type (IDSPL = 3).

- Temperature of source material (°K) (TS = TBP). Note that the normal boiling point is used in SLAB calculations.

- Mass source rate (kg/s) (QS = dm).

- Source area (m^2) (AS = $dm/(U_a\rho)$ where ρ is the aerosol density as calculated in Equation (A-4)).

- Continuous source duration (s) (TSD = m/dm).

- Instantaneous source mass (kg) (QTIS = 0).

- Source height (m) (HS = 0).

- Source duration (s) (TSD = 0).

The remaining model parameters required to complete the DEGADIS input file are as follows:

- Computational flags to model an aerosol release (isofl = 1 and ihtfl = 0).

- Ground-to-cloud heat transfer coefficient for an aerosol release (htco = 0).

- Gas temperature (°K) (gastem = TBA).

- Gas density (kg/m^3) (gasrho = ρ (aerosol density) as calculated in Equation (A-4)).

- Gas density as a function of concentration. Aerosol density is assumed to be a linear function of concentration. The input lines are as follows:

  2
  0.0   0.0   RHOA   0.0   TA
  1.0 ρ ρ 0.0   TBA

- Mass of gas initially over the area source (kg) (gmass = 0).

- Area source parameters (including time (s), mass evolution rate (kg/s), and source radius (m)). The initial radius $R_0 = (AS/\pi)^{1/2}$ using the same source area used in the

SLAB calculations for liquid tank releases. For an instantaneous release, the input lines are as follows:

```
4
0.0   dm   R0   1.0   TBA   1.0
TSD   dm   R0   1.0   TBA   1.0
TSD+1   0.0   0.0   1.0   TBA   1.0
TSD+2   0.0   0.0   1.0   TBA   1.0
```

The importance of denser-than-air effects on downwind dispersion can be confirmed using the BMW criterion for a puff, with m as the total tank inventory, ρ_s as the aerosol density ρ as calculated in Equation (A-4), and $D_s = 2*R_0$.

A.6.2.2   Liquid Tank Leak—Evaporating Pool

In this spill type release scenario, the source parameters calculated by EXTRAN can be used to model the evaporating pool.

SLAB has no provision for an area source that changes over time, so representative source parameters must be determined from the EXTRAN output file. In the EXTRAN output file with extension "SPD," the continuous source duration (TSD) is taken to be the last entry in the column labeled "TIME" (the value of "TIME" is in minutes and must be converted to seconds for TSD), and the source area (AS) is taken to be the average of the column labeled "AREA."

The remaining model parameters required to complete the SLAB input file are as follows:

- Spill source type (IDSPL = 1).

- Temperature of source material (°K) (TS = Ts + 273.15 (from the EXTRAN storage temperature)).

- Mass source rate (kg/s): (QS = dm = m/TSD).

- Source area (m²): (AS = average of the column labeled "AREA" from EXTRAN).

- Continuous source duration (s) (TSD = from EXTRAN).

- Instantaneous source mass (kg) (QTIS = 0).

- Source height (m) (HS = 0.0 m).

- Source duration (s) (TSD = 0).

The remaining model parameters required to complete the DEGADIS input file are as follows:

- Computational flags to model a gas release (isofl = 0 and ihtfl = 1).

- Ground-to-cloud default heat transfer coefficient (htco = 0).

- Gas temperature (°K) (gastem = TS).

- Gas density (kg/m^3) (gasrho = ideal gas vapor density (RHOV).

- Gas density as a function of concentration (isofl = 0). Not used in this case.

- Mass of gas initially over the area source (kg) (gmass = 0).

- Area source parameters (including time (s), mass evolution rate (kg/s), and source radius (m)). The initial radius $R_0 = (AS/\pi)^{1/2}$ for consistency with SLAB. For a continuous release, the input lines are as follows:

```
4
0.0   dm   R0   1.0   TS   1.0
TSD   dm   R0   1.0   TS   1.0
TSD+1 0.0  0.0  1.0   TS   1.0
TSD+2 0.0  0.0  1.0   TS   1.0
```

The importance of denser-than-air effects on downwind dispersion can be confirmed using the BMW criterion for a plume with dm as the average release rate, ρ_s as the gas vapor density RHOV as calculated above, and $D_s = 2 *R_0$.

A.6.3   Gas Tank Burst

This spill type release scenario generates an instantaneous cloud that could be simulated by DEGADIS and SLAB. Such a scenario normally is simulated assuming some sort of initial dilution with air because of the explosive release, but EXTRAN does not make that assumption. For consistency with EXTRAN, the input file specifications listed in this section do not include initial cloud dilution due to an explosive release.

The remaining model parameters required to complete the SLAB input file are as follows:

- Spill source type (IDSPL = 4).

- Temperature of source material (K): TS = $(Ts + 273.15)[1 - (8314 \text{ J/kmol/K})/(CPS*mwg)*(P_i/P_a - 1)]$. This is consistent with the equation for adiabatic expansion of a pressurized gas in the SLAB user's manual [5]. The value of TS should never be made less than the boiling point at ambient pressure (TBA). At this temperature, RHOV = $(P_a/760 \text{ mmHg})*WMS/(8.314 \text{ J/gmol/K} * TS)$.

- Mass source rate (kg/s) (QS = 0).

- Source area (m^2) (AS = $\pi^{1/3}(m/RHOV)^{2/3}$).

- Continuous source duration (s) (TSD = 0).

- Instantaneous source mass (kg) (QTIS = mass of the tank inventory).

- Source height (m) (HS = $((m/RHOV)/\pi)^{1/3}$).

- Source duration (s) (TSD = 0).

Values of source (AS) and source height (HS) are set assuming that the height-to-diameter ratio of the initial cloud is 0.5 and the total volume is m/RHOV where m (or QTIS) is the total mass (kg).

The remaining model parameters required to complete the DEGADIS input file are as follows:

- Computational flags to model an aerosol release (isofl = 1 and ihtfl = 0).

- Ground-to-cloud heat transfer coefficient for an aerosol release (htco = 0).

- Gas temperature (°K) (gastem = TS).

- Gas density (kg/m^3) (gasrho = ideal gas vapor density (RHOV).

- Not used in this case for a gas tank burst (isofl = 0).

- Mass of gas initially over the area source (kg) (gmass = mass of the tank inventory).

- Area source parameters (including time (s), mass evolution rate (kg/s), and source radius (m)). The initial radius $R_0 = ((m/\text{RHOV})/\pi)^{1/3})$ where the height-to-diameter ratio of the cloud is assumed to be 0.5. For an instantaneous release, the input lines are as follows:

```
3
0.0  0.0  R0   1.0  TBA  1.0
1.0  0.0  0.0  1.0  TBA  1.0
2.0  0.0  0.0  1.0  TBA  1.0
```

The importance of denser-than-air effects on downwind dispersion can be confirmed using the BMW criterion for a puff with m as the total tank inventory and ρ_s as the gas vapor density RHOV calculated in Equation A-4.

A.6.4   Gas Tank Leak

This spill type release scenario can be simulated with SLAB as a horizontal (with the wind) or vertical jet. For DEGADIS, the jet can be vertical, or the release can be simulated so that the release momentum is dissipated at the source without dilution. If the release momentum is dissipated at the source without air dilution, this would be a conservative approach that is consistent with the treatment outlined above for a gas tank burst. In HABIT 2.2, the DEGADIS and SLAB and calculations can be made for this scenario for vertical (up) and for vertical (up) and horizontal cases, respectively. Taking the jet orientation into account would require additional input from the user (orientation and opening diameter).

For this scenario, DEGADIS and SLAB use the area of the release to predict several source parameters. However, because this information is not currently requested by HABIT 2.2, the source parameters are estimated assuming the vertical jet velocity is the same as the ambient wind speed.

The remaining model parameters required to complete the SLAB input file are as follows:

- Spill source type (IDSPL = 4).

- Temperature of source material (°K): $TS = (Ts + 273.15)[1 – (8314\ \text{J/kmol K})/(CPS*mwg)*(P_i/P_a – 1)]$. This is consistent with the equation for adiabatic expansion of a pressurized gas given in the SLAB user's manual [5]. The value of TS should never be made less than the boiling point at ambient pressure (TBA). At this temperature, $RHOV = (P_a/760\ \text{mmHg})*WMS/(8.314\ \text{J/gmol/K} * TS)$.

- Mass source rate (kg/s) ($QS = dm$).

- Source area (m^2) ($AS = dm/(U_aRHOV)$, where RHOV is the gas vapor density as calculated).

- Continuous source duration (s) ($TSD = m/dm$).

- Instantaneous source mass (kg) ($QTIS = 0$).

- Source height (m) ($HS = 0$).

- Source duration (s) ($TSD = 0$).

The remaining model parameters required to complete the DEGADIS input file are as follows:

- Computational flags to model a gas release (isofl = 0 and ihtfl = 1).

- Ground-to-cloud default heat transfer coefficient (htco = 0).

- Gas temperature (°K) (gastem = TS).

- Gas density (kg/m^3) (gasrho = ideal gas vapor density (RHOV) as calculated).

- Gas density as a function of concentration (isofl = 0). Not used in this case.

- Mass of gas initially over the area source (kg) (gmass = mass of the tank inventory).

- Area source parameters (including time (s), mass evolution rate (kg/s), and source radius (m)). The initial radius $R_0 = (AS/\pi)^{1/2}$ for consistency with SLAB. For a continuous release, the input lines are as follows:

  ```
  4
  0.0   dm   R0   1.0   TS   1.0
  TSD   dm   R0   1.0   TS   1.0
  TSD+1 0.0  0.0  1.0   TS   1.0
  TSD+2 0.0  0.0  1.0   TS   1.0
  ```

The importance of denser-than-air effects on downwind dispersion can be confirmed using the BMW criterion for a plume with dm as the average release rate, ρ_s as the gas vapor density RHOV as calculated in Equation A-4, and $D_s = 2 * R_0$.

A.7   Summary

This appendix has summarized inputs to DEGADIS and SLAB to estimate the hazard for a denser-than-air toxic material in a manner consistent with the current methods used by EXTRAN in HABIT 2.2. This discussion was based on the following major assumptions:

- EXTRAN uses Pasquill-Gifford atmospheric stability classes A–G. Stability class G is considered sufficiently rare that it is no longer typically used. SLAB and DEGADIS only have provision for classes A–F, so class G would be best approximated with class F in those models. Note that the Category F Pasquill stability class represents the worst 5th percentile meteorology observed at the majority of the nuclear power plant sites [6].

- The BMW criteria for predicting the importance of denser-than-air effects on dispersion are used as a condition for using DEGADIS and SLAB.

- DEGADIS and SLAB allow some parameters to assume default values. These default parameters have been used in the implementation of the models in HABIT 2.2 to minimize the requested amount of additional information. The default values are appropriate for the intended use in HABIT 2.2.

- The averaging time (t_{av}) used in DEGADIS and SLAB accounts for the effect of plume meander and depends on the hazard under consideration (t_h) as well as the amount of time required for the release to become airborne (t_d). For flammable materials, t_h can be taken to be zero; for toxic materials, t_h should be based on the criterion for comparison (e.g., TLV-STEL is based on an exposure duration of 15 minutes, so t_h = 900 s). The length of time required for the release to become airborne depends on the spill scenario. DEGADIS and SLAB also have a lower limit of the averaging time (t_{min}) based on the model formulation (t_{min} = 20 s for DEGADIS and t_{min} = 10 s for SLAB). The averaging time input to the models should be taken as the max (min (t_h, t_d), t_{min}), which limits the averaging time to no longer than the release duration. The current implementation assumes that hazards under consideration are evaluated with the TLV-STEL, so t_{haz} = 900 s.

- Witlox et al. [4] considered data from several sources and concluded that there was a transition between mechanical breakup and fully flashing jets for superheats (temperature above the boiling point) between 10 and 20 °C. For the calculations proposed here, a conservative assumption would be to assume that jets fully flash with a superheat of 10 °C.

- When an instantaneous cloud of gas or aerosol is formed, the height-to-diameter ratio of the initial cloud is assumed to be 0.5.

- When an instantaneous cloud of gas or aerosol is formed, the initial cloud is assumed to be pure gas or aerosol without any air addition.

- SLAB has no provision for an area source to change over time, so representative source parameters must be determined from the EXTRAN output file. In the EXTRAN output file with extension "SPD," the continuous source duration (TSD) is taken to be the last entry in the column labeled "TIME" (the value of "TIME" is in minutes and must be converted to s for TSD), and the source area (AS) is taken to be the average of the

column labeled "AREA." These representative parameters are used as input in both DEGADIS and SLAB.

- For two-phase flashing releases, some liquid rainout may occur, but this case can be treated conservatively as if there is little or no liquid rainout. This spill type release scenario is simulated in SLAB as if the flashing release occurred from a ground-level, area source as a vertical jet (IDSPL = 3). For this scenario, the DEGADIS and SLAB codes use the area of the release to predict several source parameters. However, because this information is not currently requested by HABIT 2.2, the source parameters are estimated assuming the vertical jet velocity is the same as the ambient wind speed.

- For pressurized gas releases, the gas temperature after depressurization is reduced during the process of adiabatic expansion against atmospheric pressure. With this assumption, the temperature of source material is calculated using $(Ts + 273.15)[1 - (8314 \text{ J/kmol K})/(CPS*mwg)*(P_i/P_a - 1)]$, which is the equation given in the SLAB user's manual [5] for these circumstances. The value of TS should never be made less than the boiling point at ambient pressure (TBA).

A.8   References

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11. ABSTRACT (200 words or less)

The HABIT code is based on the external transport (EXTRAN) computer code for estimating transient concentrations at a specific downwind location (i.e., CR air intake) for four release scenarios (i.e., liquid burst, liquid leak, gas burst, and gas leak). The toxic chemical or radioactive gas using Gaussian puff dispersion methods and building-wake diffusion algorithms. HABIT version 2.2 is the latest: It is an update to the previous version of the codes (i.e., HABIT 2.0) and could trace its development back to the original version of HABIT 1.1. It works in Microsoft 64-bit operating systems such as Windows 10 and has fully incorporated the Britter and McQuaid Workbook (BMW) criteria with both the DEGADIS and SLAB computer codes for auto-determination of the importance of denser-than-air effects. In addition, unlike the previous version, HABIT 2.2 removed all the radiological dose assessment calculations. Finally, the GUI screen for HABIT 2.2 was updated with easy-to-read color and fonts, improved waring and notification messaging, and a redesign of the graphing and plotting utilities and also has a full backward-compatibility to re-run the files from HABIT 1.1.

12. KEY WORDS/DESCRIPTORS (List words or phrases that will assist researchers in locating the report.)

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