U.S.NRC
United States Nuclear Regulatory Commission
Protecting People and the Environment

HABIT v2.2.1

Testing Documentation

December 12, 2024

Prepared by:
S. Edwards

Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Rockville, MD 20852

U.S.NRC
United States Nuclear Regulatory Commission
Protecting People and the Environment

Table of Contents

U.S.NRC
United States Nuclear Regulatory Commission
Protecting People and the Environment

List of Tables

List of Figures

U.S.NRC
United States Nuclear Regulatory Commission
Protecting People and the Environment

1 Introduction

The Computer Codes for Evaluation of Control Room Habitability (HABIT) package is designed to assist in the evaluation of control room (CR) habitability in the event of accidental spills of toxic chemicals.

This document outlines and verifies the modifications, additions, and/or removal of features from HABIT v2.2 to HABIT v2.2.1. Additionally, regression testing is conducted to ensure that results are consistent between the two versions.

This update was intended as a patch to fix various bugs and issues with the installation process and operation of the graphical user interface (GUI). Therefore, computations and results between the two versions should be identical.

This document contains testing that both (a) verifies that the issues have been correctly implemented and (b) ensures that results are consistent with the previous version. These can be found in Sections 3 and 5, respectively.

2 Abbreviations

Table 2-1 Abbreviations

Term	Definition
HABIT	Computer Codes for Evaluation of Control Room Habitability
CR	control room
GUI	graphical user interface

3 Verifying Updates

This section provides screen shots to verify that the reported updates are correctly implemented in HABIT v2.2.1. The default design that is loaded into HABIT (labelled Test Case 1) is used in this demonstration for all issues except when creating new designs to display certain behavior. **Note** that some issues have been saved for future updates or closed as duplicates, so certain numbers will be skipped in the issue list below.

Table 3-1 Summary of Resolved Issues in HABIT v2.2.1

Issue #	Description	Section
1	Corrected scaling of EXTRAN, DEGADIS, and SLAB tabs	3.1
4	Clarified a DEGADIS error when default input does not exist	3.2
5	Corrected Exposure Plot 'X-axis in seconds' button behavior	3.3
7	Corrected the 'Adjust Time Scale' slider behavior to properly handle the minimum and maximum data value	3.4
8	Allowed HABIT to be installed and operate out of any directory	3.5
10	Handled exceptions raised when trying to view outputs that do not exist	3.6
11	Fixed 'Load Input' behavior in DEGADIS tab to load the selected file	3.7
12	Handled exceptions when attempting to run DEGADIS and SLAB before loading inputs	3.8
13	Standardized the exponent notation in GUI text	3.9
14	Corrected the DEGADIS Concentration Graph	3.10

3.1 Issue 1: Scaling of EXTRAN, DEGADIS, and SLAB Tabs

When maximizing the HABIT window on larger screens, the automatic scaling of certain tabs caused input fields to become inaccessible. Figures 3-1 through 3-8, demonstrate that maximizing HABIT v2.2.1 no longer cuts off the input screens of the previously afflicted tabs.

Additionally, the ‘Plot Exposure’ button on the EXTRAN tab may be cut off on smaller monitors, such as those on a laptop. In HABIT v2.2.1, the legend was moved to the empty space in the lower left of the window to allow the buttons to shift up.

Note that the presence of the ‘Restore’ button (two overlapping squares) on the title bar in the top right corner indicates that all screens are maximized.

3.1.1 HABIT v2.2 Screenshots

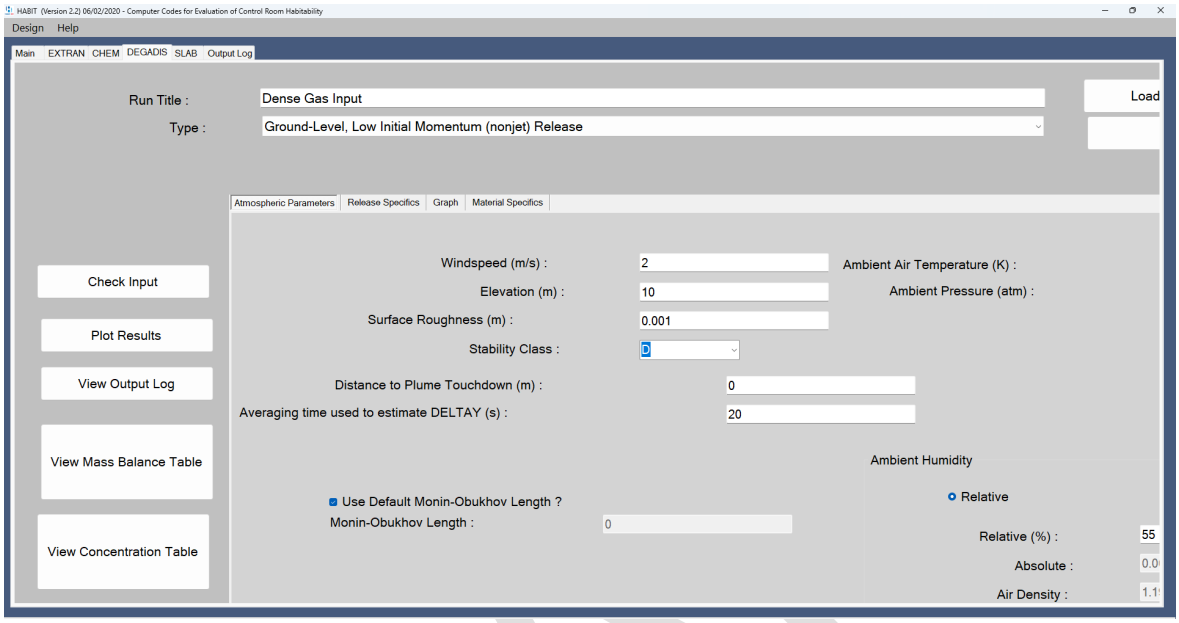

Figure 3-1 HABIT v2.2 DEGADIS Tab with Scaling Issues

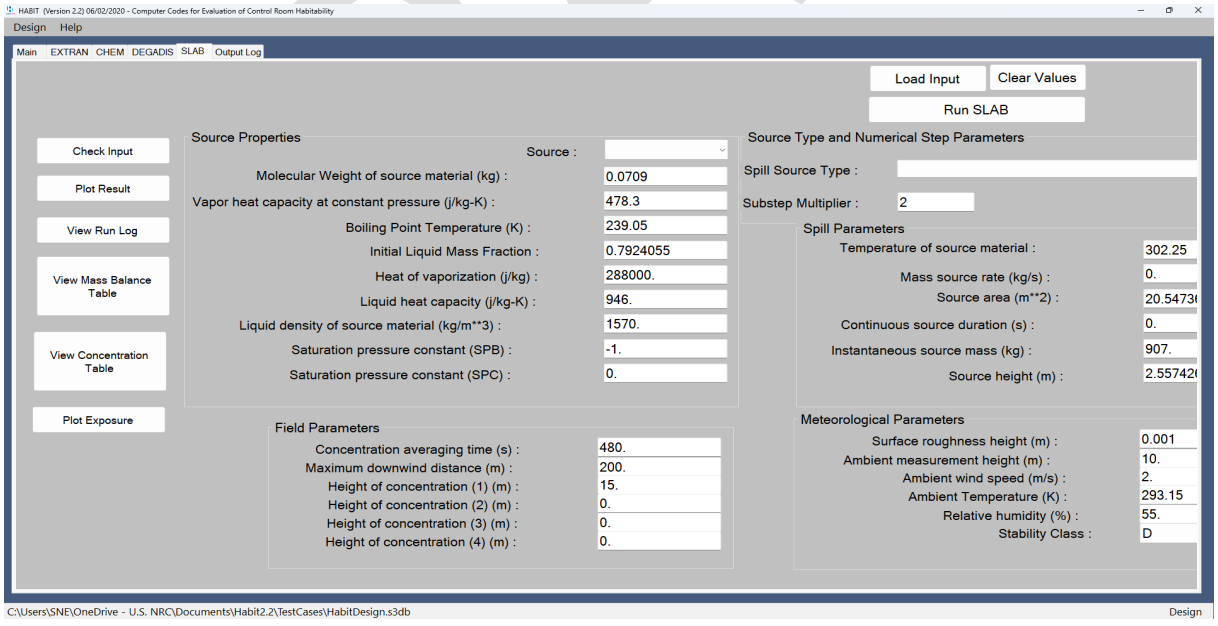

Figure 3-2 HABIT v2.2 SLAB Tab with Scaling Issues

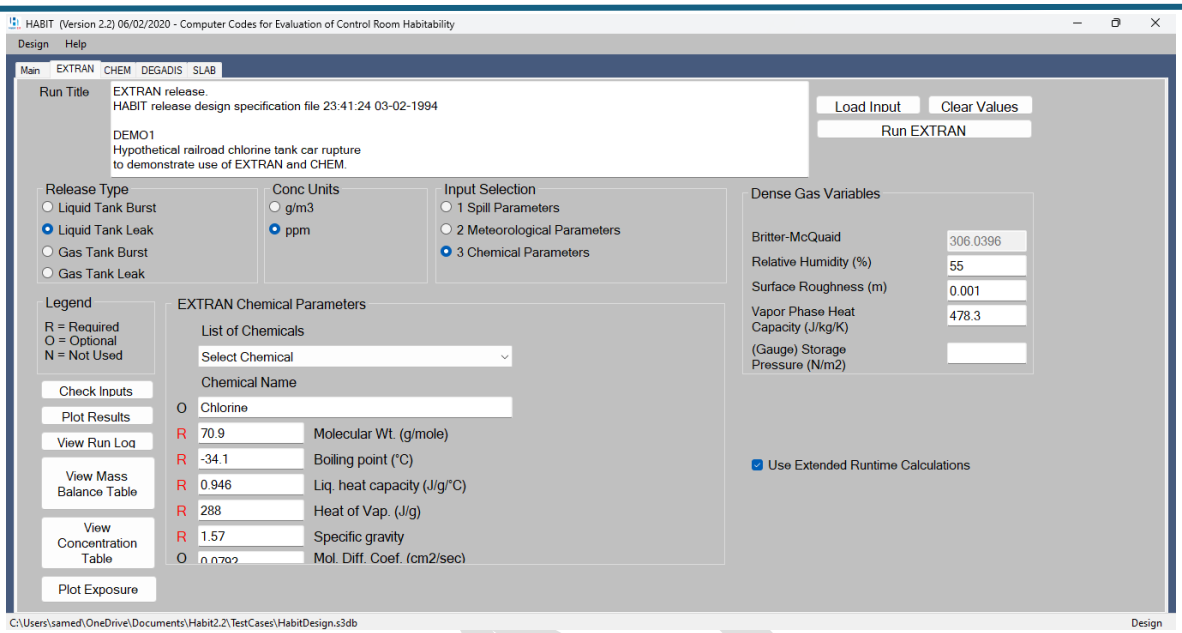

Figure 3-3 HABIT v2.2 EXTRAN Tab with Scaling Issues

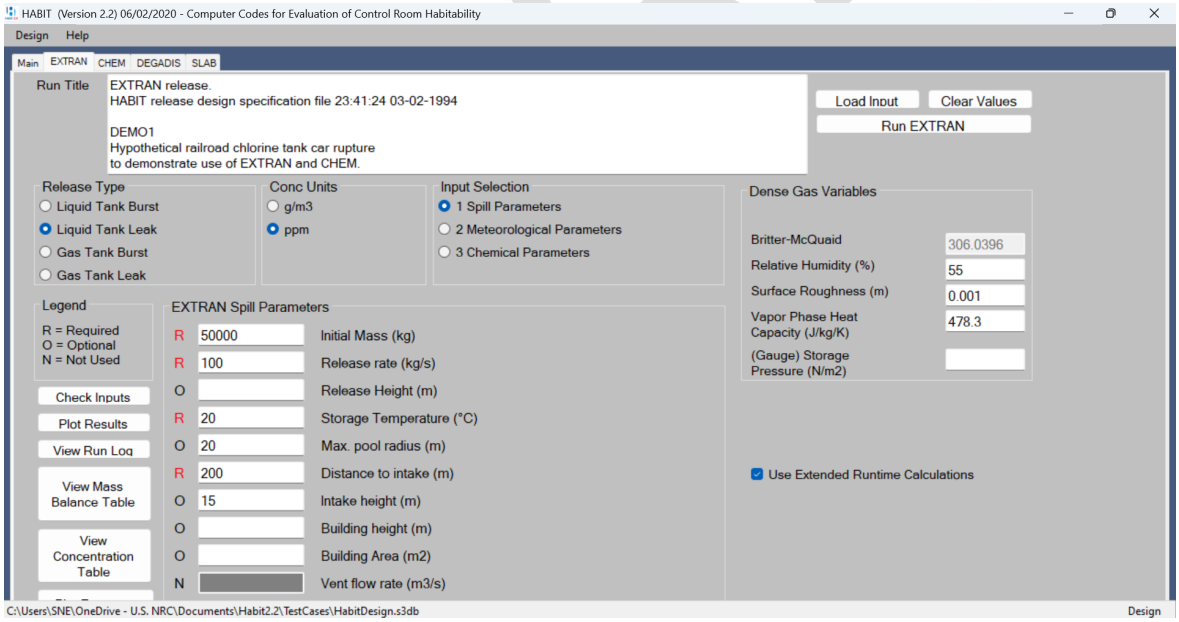

Figure 3-4 HABIT v2.2 EXTRAN Tab with Buttons Cut Off

3.1.2 HABIT v2.2.1 Screenshots

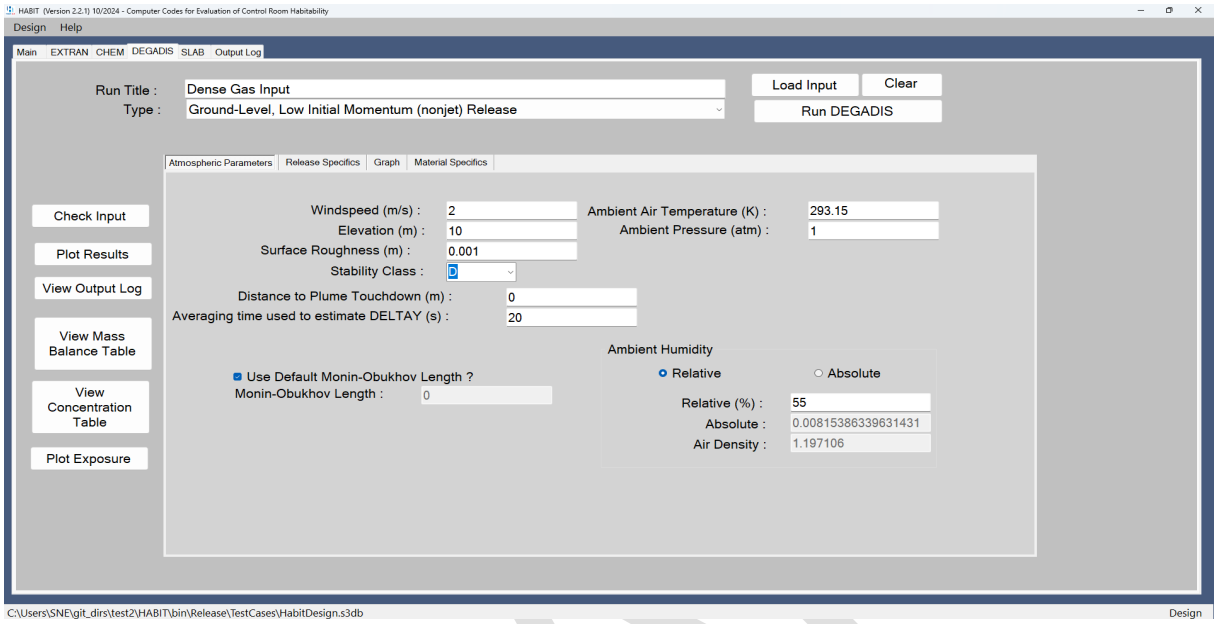

Figure 3-5 HABIT v2.2.1 DEGADIS Tab Properly Scaled

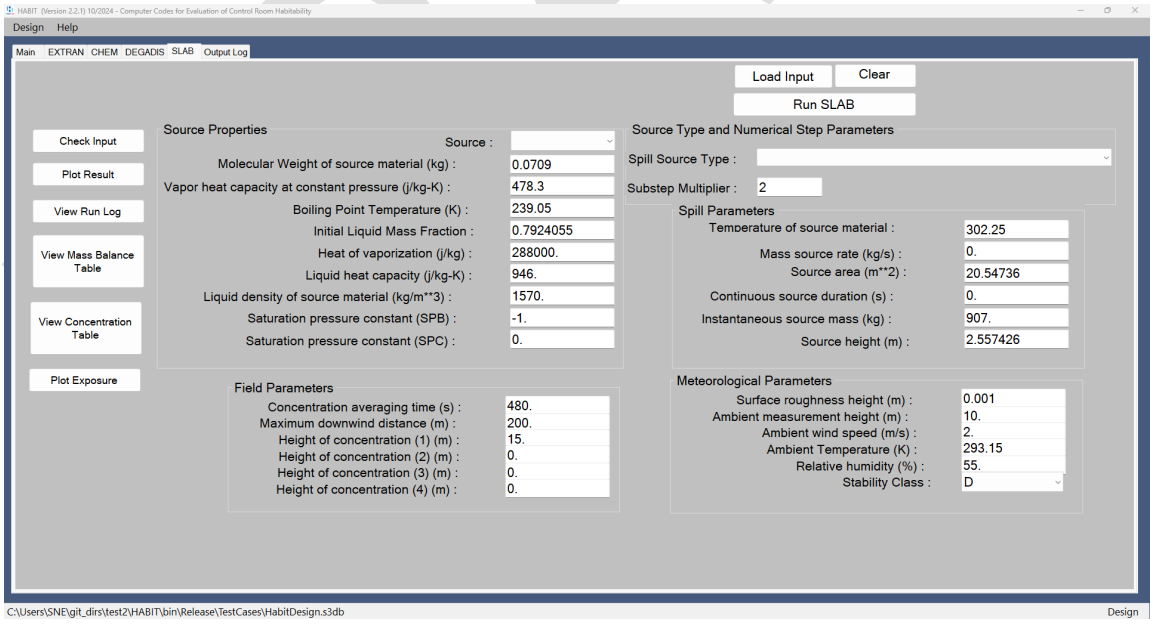

Figure 3-6 HABIT v2.2.1 SLAB Tab Properly Scaled

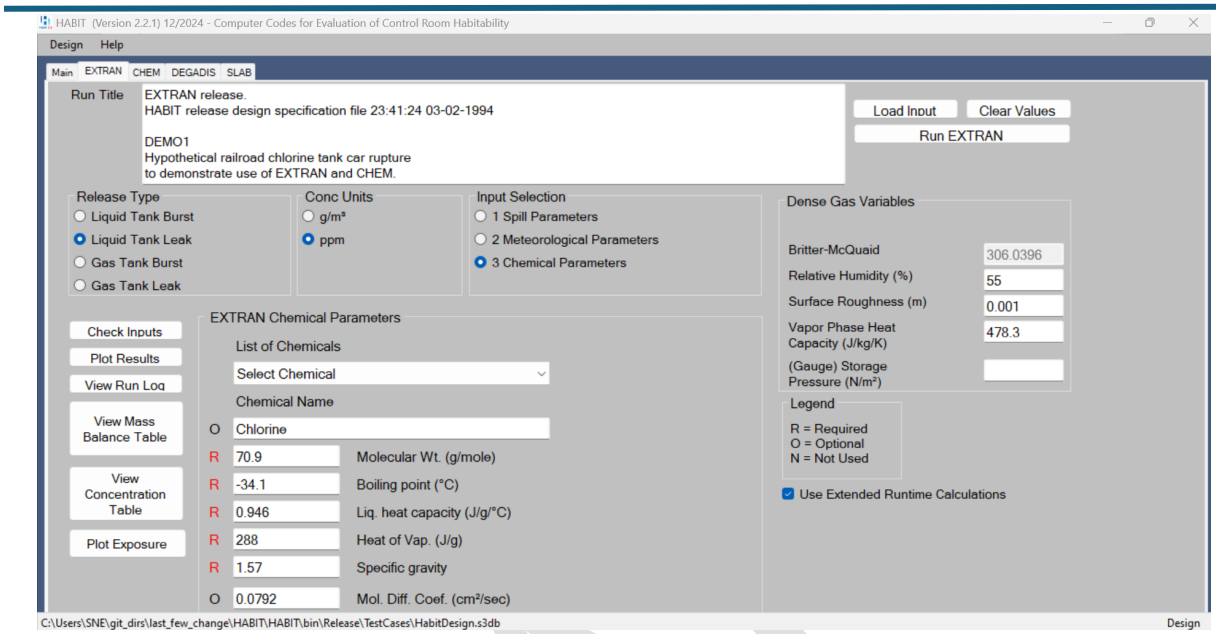

Figure 3-7 HABIT v2.2.1 EXTRAN Tab Properly Scaled

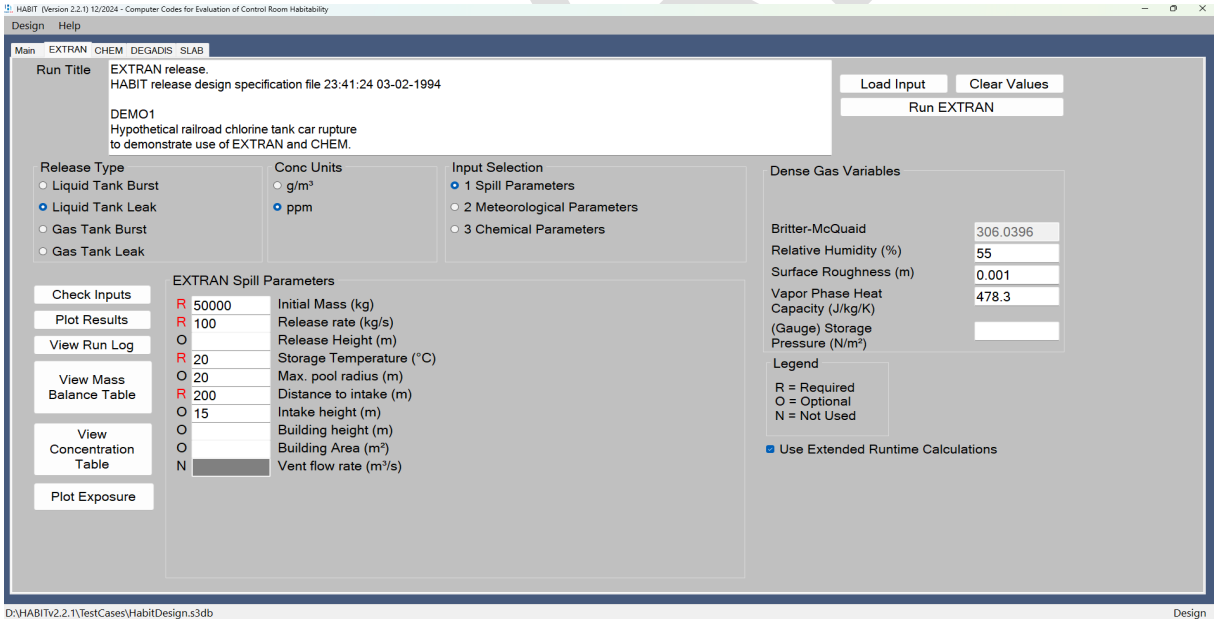

Figure 3-8 HABIT v2.2.1 EXTRAN Tab New Layout

3.2 Issue 4: Nonspecific DEGADIS Error

The DEGADIS module relies on having default parameters stored in the installation directory in the file Data/DefaultDG.inp. This allows the code to prepopulate the input fields of the DEGADIS tab when adding the DEGADIS module to an input case for the first time. Previously, if the DefaultDG.inp file was missing from the Data directory, an error message displayed which did not properly indicate the problem as shown in Figure 3-9. HABIT v2.2.1 was updated so that the error message accurately describes the issue as shown in Figure 3-10.

To verify this issue, a new design was created and selected to include DEGADIS on the Main tab. The DefaultDG.inp file was temporarily removed from the Data directory to trigger the error message.

3.2.1 HABIT v2.2 Screenshots

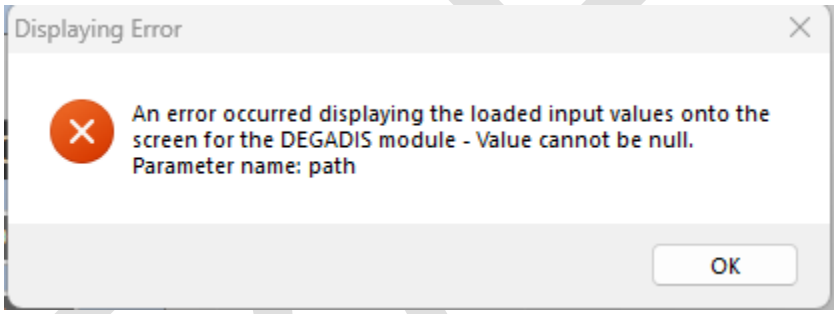

Figure 3-9 HABIT v2.2 DEGADIS Nonspecific Error

3.2.2 HABIT v2.2.1 Screenshots

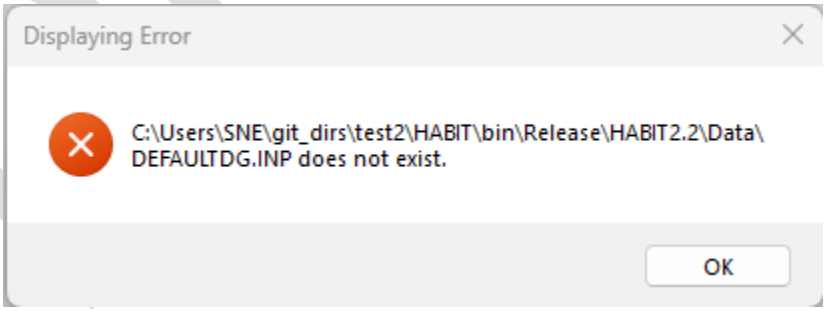

Figure 3-10 HABIT v.2.2.1 Clarified Error

3.3 Issue 5: X-axis in Seconds Button Changing Exposure Plot

Each module in the code has an Exposure Plot button to display a plot of the exposure over time as shown in Figures 3-11 and 3-12. If the button ‘x-axis in seconds’ is checked for any module, the depicted plot is changed with that of the EXTRAN module. This functionality has been modified to retain the displayed plot and only modify the units on the x-axis.

3.3.1 HABIT v2.2 Screenshots

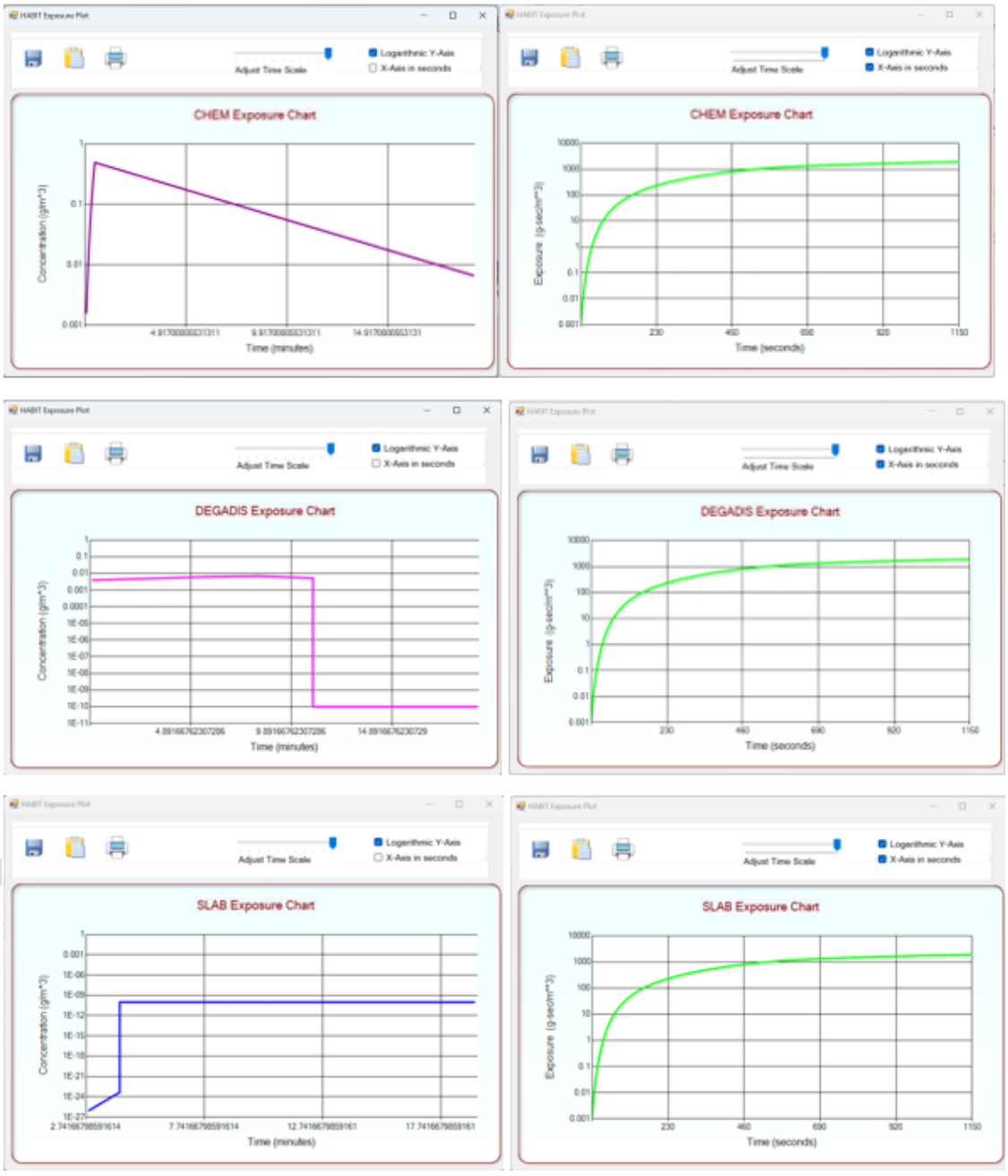

Figure 3-11 HABIT v2.2 Exposure Plots Changing when Selecting 'X-axis in Seconds

3.3.2 HABIT v2.2.1 Screenshots

Figure 3-12 HABIT v2.2.1 Exposure Plots Remaining Unchanged after Selecting 'X-Axis in Seconds

3.4 Issue 7: 'Adjust Time Scale' Slider in Exposure Plot Not Properly Handling Minimum and Maximum Data Value

Two separate errors have arisen from the 'Adjust Time Scale' slider in the Exposure Plot window. Moving the slider down by any increment prevents the user from returning the slider to the maximum value of the plot. Additionally, if the minimum time of the plot is significantly greater than 0 and the slider is moved below the minimum, an unhandled exception is raised. Both of these issues have been addressed and corrected in HABIT v2.2.1.

3.4.1 HABIT v2.2 Screenshots

Figure 3-13 displays the baseline window that appears, in HABIT v2.2, when clicking on the 'Exposure Plot' button. The maximum time in the plot is greater than 14 minutes.

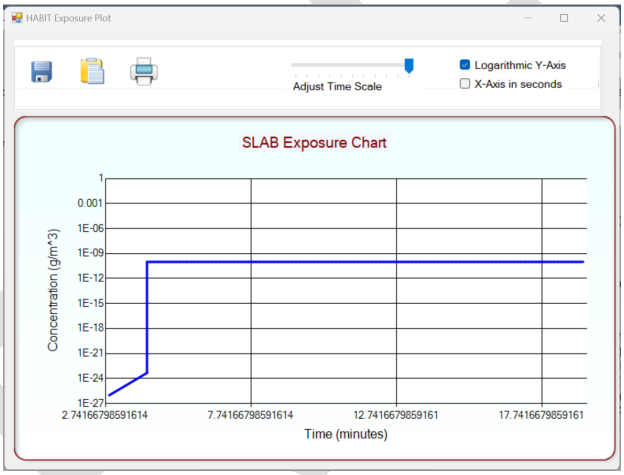

Figure 3-13 HABIT v2.2 Baseline Exposure Plot for the SLAB Module

Figure 3-14 displays this error in HABIT v.2.2. After moving the 'Adjust Time Scale' slider to the left (see first image), the maximum value that the slider is allowed to achieve is around 10 minutes (see second image). Note in the left image that the slider bar cannot move further to the right, yet the plot has not been restored to its original maximum.

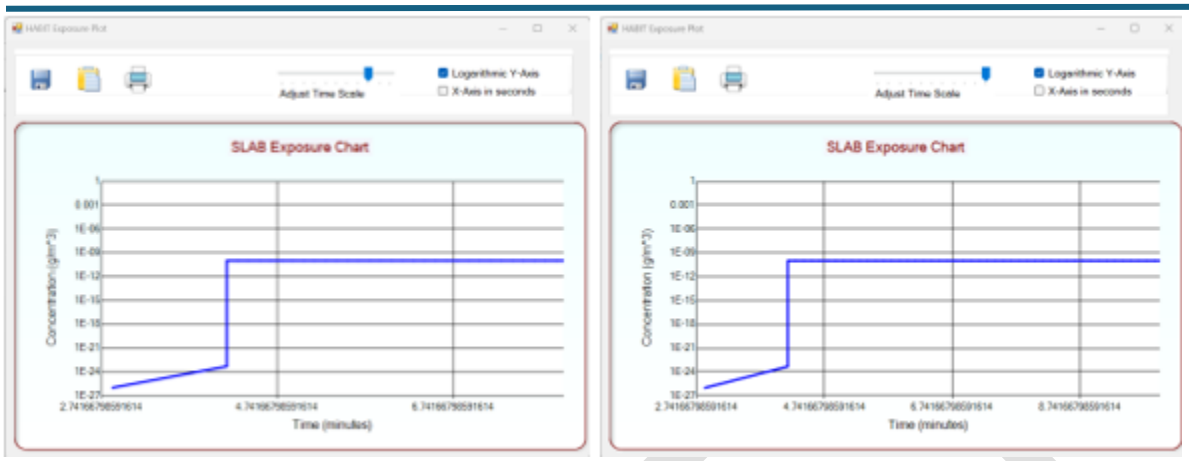

Figure 3-14 HABIT v2.2 Maximum Value Inaccessible after Moving 'Adjust Time Scale' Slider

Additionally, moving the slider bar to the left when the minimum is significantly above zero causes an unhandled exception and the plot to no longer display, as shown in Figure 3-15.

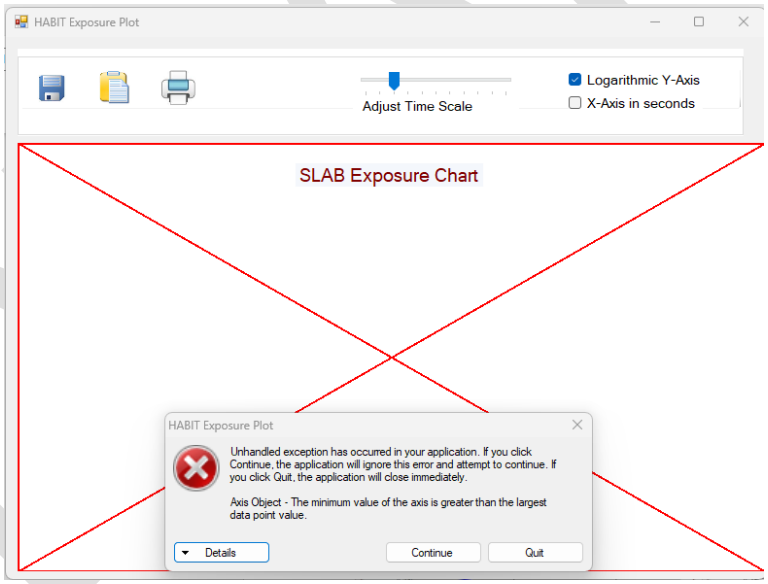

Figure 3-15 HABIT v2.2 Unhandled Exception when Moving 'Adjust Time Scale' Slider to Zero

3.4.2 HABIT v2.2.1 Screenshots

Figure 3-16 displays the baseline window that appears, in HABIT v2.2.1, when clicking on the 'Exposure Plot' button. In this version, the maximum of the plot was explicitly set to the ceiling of the latest time, so the axis on the plot is slightly different in the new version.

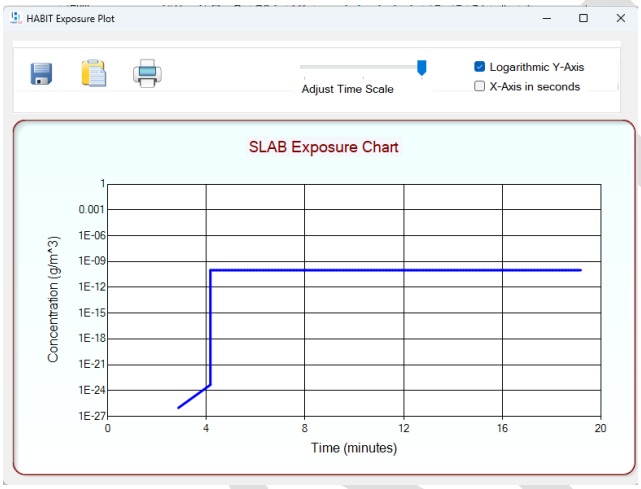

Figure 3-16 HABIT v2.2.1 Baseline Exposure Plot for the SLAB Module

In HABIT v2.2.1, after moving the 'Adjust Time Scale' slider to the left, the original maximum can be reached by moving the slider completely to the right, as shown in Figure 3-17.

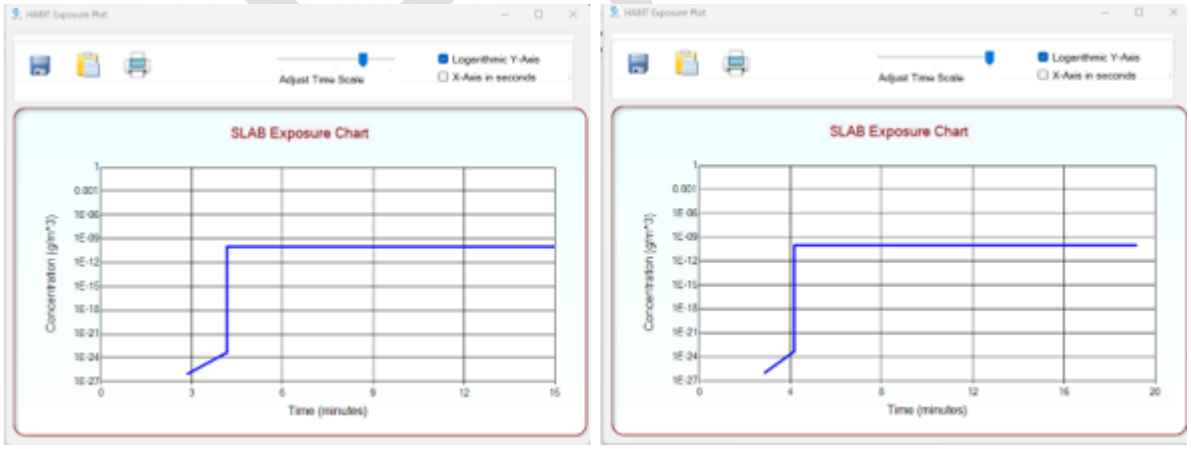

Figure 3-17 HABIT v2.2.1 Corrected 'Adjust Time Scale' Slider Behavior: Maximum Value

Additionally, Figure 3-18 displays that an unhandled exception error no longer occurs in HABIT v2.2.1 when the minimum of the plot is explicitly set so the plot does not crash when moving the slider down to 0. In the screenshot below, the plot is still displayed when the 'Adjust Time Scale' slider is moved completely to the left.

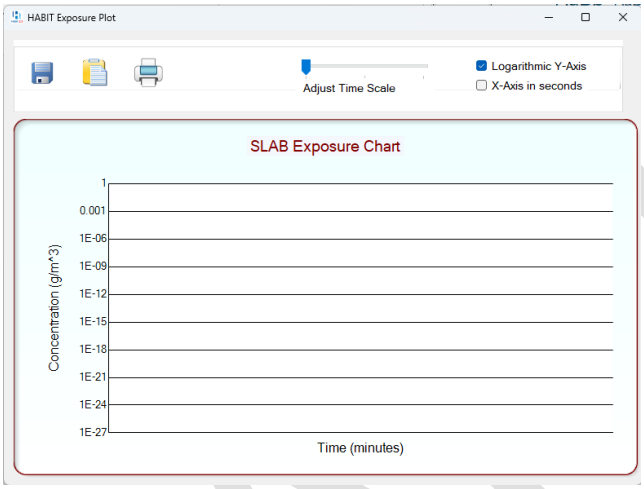

Figure 3-18 HABIT v2.2.1 Corrected 'Adjust Time Scale' Slider Behavior: Minimum Value

3.5 Issue 8: Directory for Install and Operation Hard-coded to 'Documents'

Previous versions of the code were configured to only run from the Documents directory. HABIT v2.2 was specifically configured to only operate from Documents\Habit2.2\. Certain required files were coded with the Documents directory; therefore, if HABIT or one of those files was not in the Documents directory, several errors would be presented, and the modules would ulitmately not execute properly. As shown in Figure 3-19, this error was tested by removing the HABIT2.2 directory (renaming the folder to HABIT2.2_test_not_here).

Figure 3-19 Removing the HABIT v2.2 Folder from Documents

3.5.1 HABIT v2.2 Screenshots

Figure 3-20 displays the error message –The nuclide data file was not found– in HABIT v2.2 when using the new folder, Habit2.2_test_not_here and when clicking on a 'Load Default Design'.

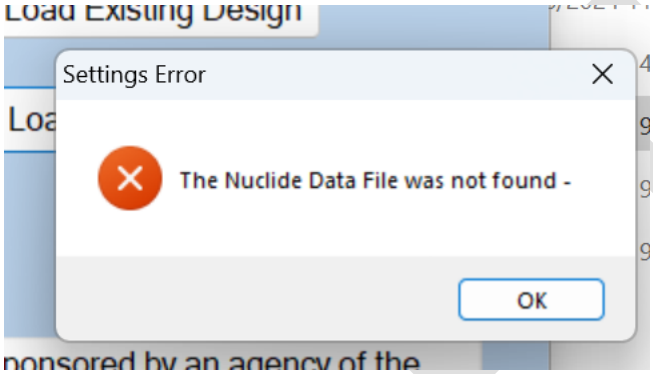

Figure 3-20 HABIT v2.2 Nuclide Data File Not Found Error for Default Case

Furthermore, when loading in an input file and attempting to run, an unhandled exception is thrown stating that no database is currently loaded, as shown in Figure 3-21.

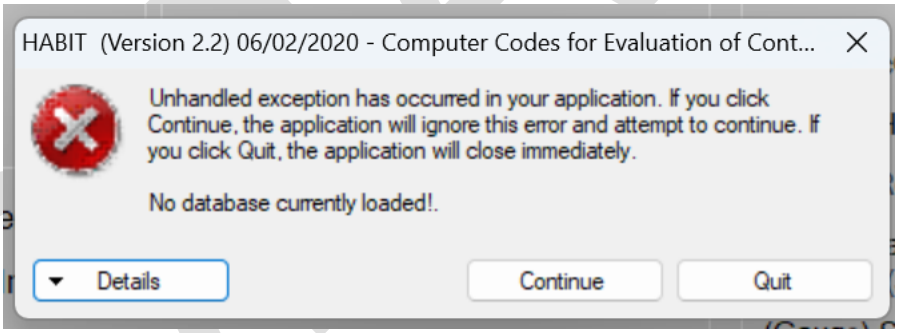

Figure 3-21 HABIT v2.2 Unhandled Exception: No Database Loaded

Similarly, when trying to load in an existing HABIT case, the following error is presented as shown in Figure 3-22.

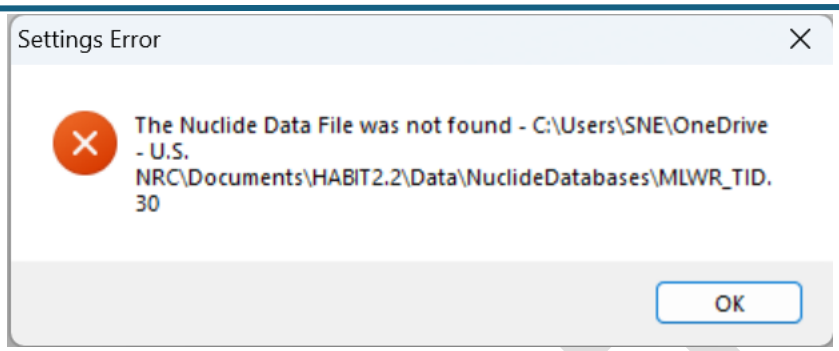

Figure 3-22 HABIT v2.2 Nuclide Data File Not Found Error for Existing Case

When any of the 'Run' buttons is selected, no errors are thrown but nothing executes. Furthermore, the installation file for HABIT v2.2 does not provide an option for the user to select the directory to which the code can be downloaded, as shown in Figure 3-23.

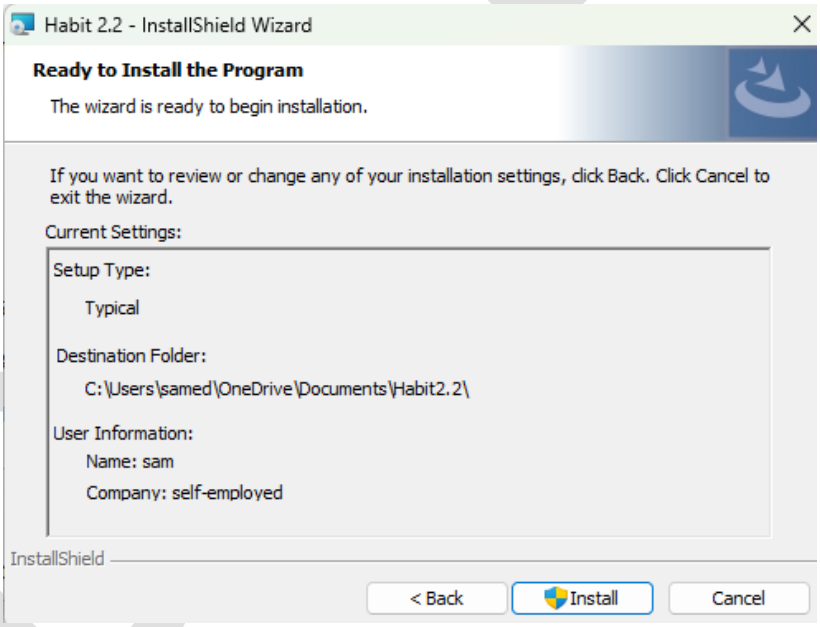

Figure 3-23. HABIT v2.2 Installation Directory Selection

3.5.2 HABIT v2.2.1 Screenshots

HABIT v2.2.1 has been modified so no errors are thrown and all modules can run when the executable and downloaded files are included in any folder, as shown in Figure 3-24.

Furthermore, in HABIT v2.2.1, the code will now operate without errors from any directory. Additionally, the installer will now prompt the user to select the installation folder.

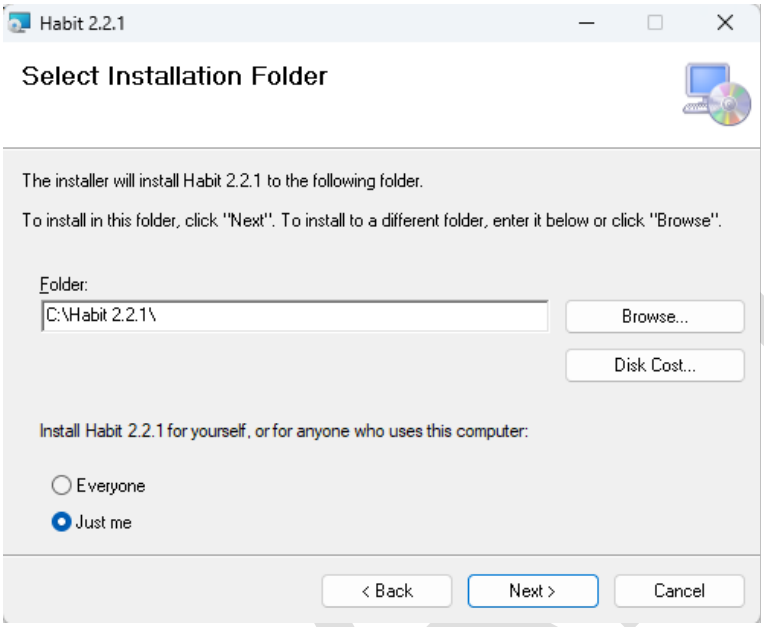

Figure 3-24 HABIT v2.2.1 Installation Directory Selection

3.6 Issue 10: Unhandled Exceptions when Outputs Do Not Exist

As shown in Figures 3-25 and 3-26, In HABIT v2.2 there are two unhandled exceptions that occur with new designs that do not have outputs created yet.

3.6.1 HABIT v2.2 Screenshots

The buttons 'View Run Log' in the EXTRAN and SLAB tabs and 'View Output Log' in the CHEM and DEGADIS tabs will cause an unhandled exception on a new design before running the respective module.

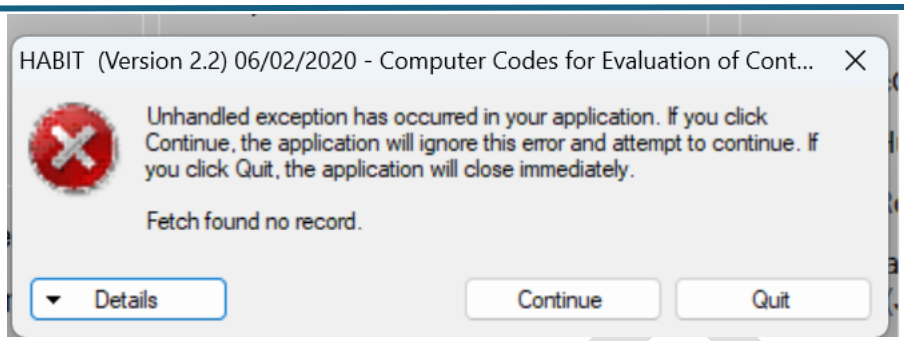

Figure 3-25 HABIT v2.2 Unhandled Exception: Viewing Outputs with no Outputs Generated

The button 'Plot Results' on all tabs will cause an unhandled exception.

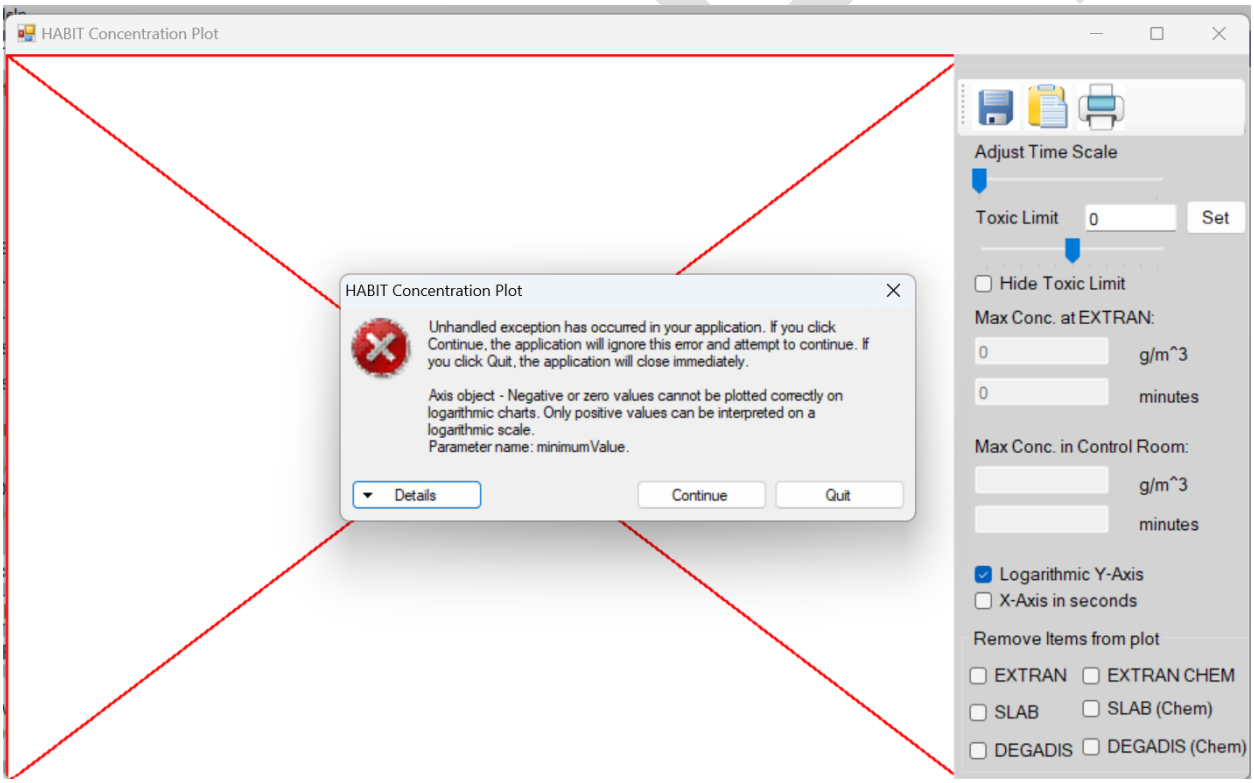

Figure 3-26 HABIT v2.2 Unhandled Exception: Plotting with no Outputs

3.6.2 HABIT v2.2.1 Screenshots

As shown in Figures 3-27 and 3-28, in HABIT v2.2.1, these errors are handled and do not cause any errors or pop-up messages. The output log now states, “the output does not exist.”

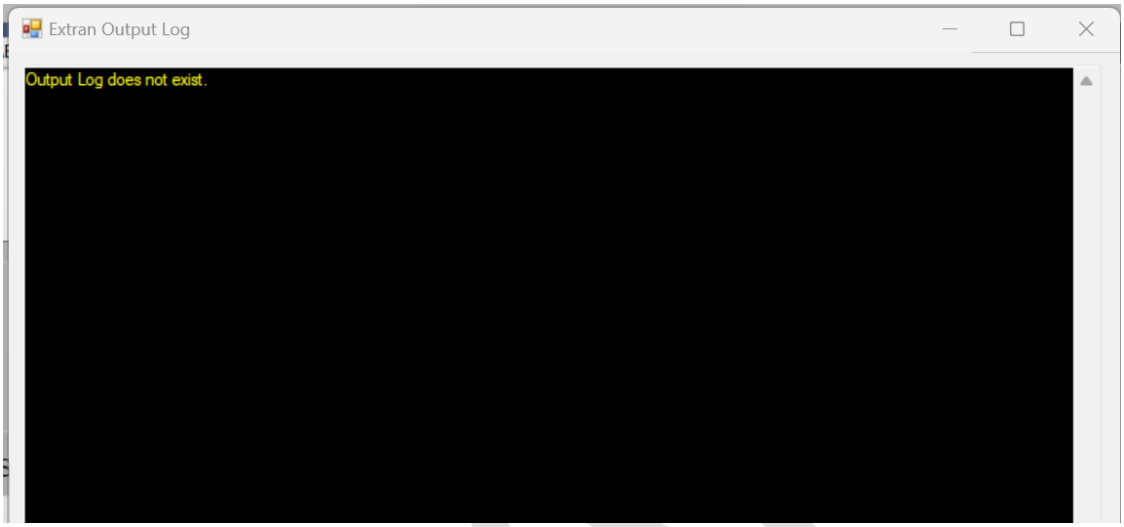

Figure 3-27 HABIT v2.2.1 Viewing Outputs with no Outputs Generated

In HABITv2.2.1, the plot now displays an empty chart as shown in Figure 3-28..

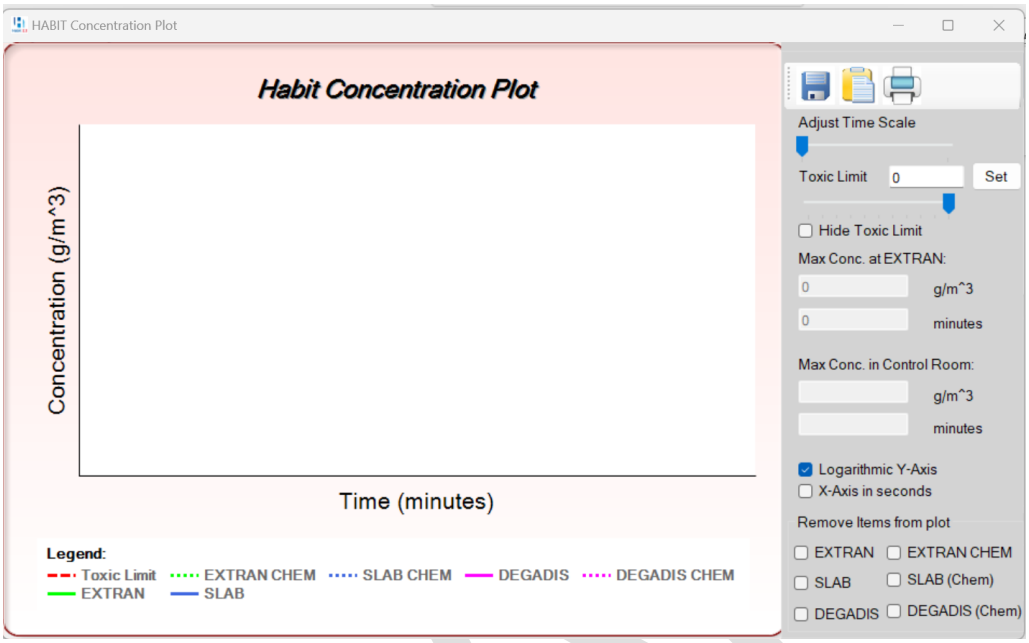

Figure 3-28 HABIT v2.2.1 Plotting with no Outputs Generated

3.7 Issue 11: Loading in DEGADIS Input Files

The DEGADIS module has a 'Load Input' button analogous to the other modules. However, despite producing a prompt for the user to select an input file to load, the default DefaultDG.inp file is always loaded. For example, a test file was created with the following parameters: windspeed: 2 m/s and stability class: D.

3.7.1 HABIT v2.2 Screenshots

Loading in this file in HABIT v2.2 results in the following in correct information from default file (i.e., windspeed 4 m/s), as shown in Figure -3-29. There are many other instances of incorrect fields, such as the Molecular Weight in the Material Specifics tab as well.

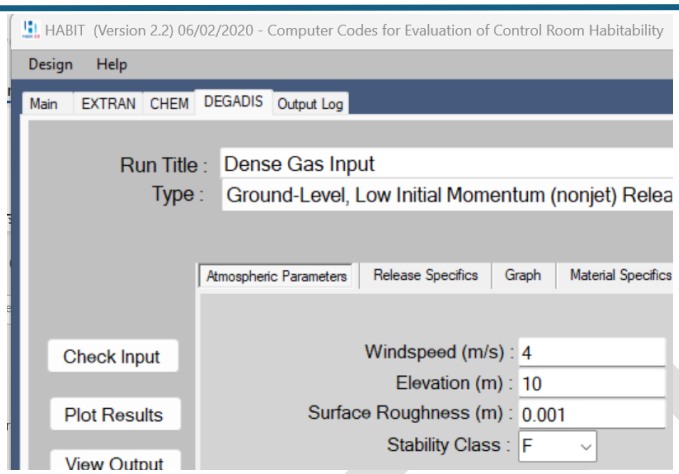

Figure 3-29 HABIT v2.2 Loading in Default DEGADIS Input File instead of Selected File

3.7.2 HABIT v2.2.1 Screenshots

HABIT v2.2.1 has been corrected so the input file selected by the user gets loaded into DEGADIS as shown in Figure 3-30.

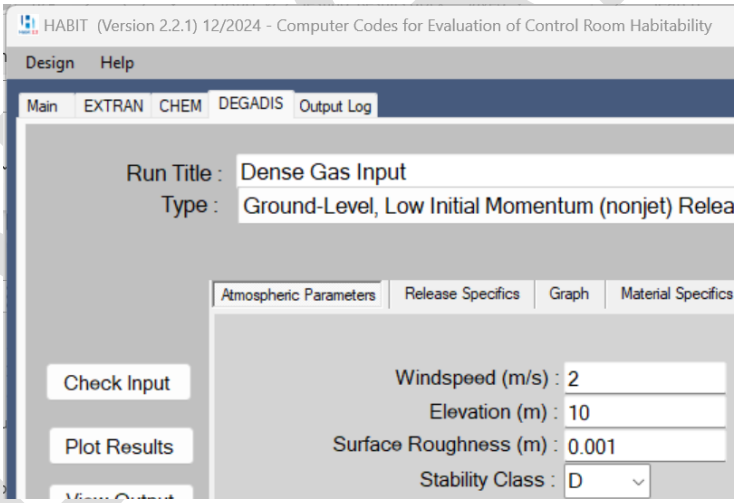

Figure 3-30 HABIT v2.2.1 Loading in Selected DEGADIS File

3.8 Issue 12: Running DEGADIS & SLAB Modules before Loading Inputs

In order to run the DEGADIS and SLAB modules, additional files need to be generated, specifically a .bat file for each module. This is typically handled by running the EXTRAN module

first. In HABIT v2.2, if the 'Run' button is selected, an unhandled exception is thrown, as shown in Figure 3-31, indicating that this .bat file is inaccessible.

3.8.1 HABIT v2.2 Screenshots

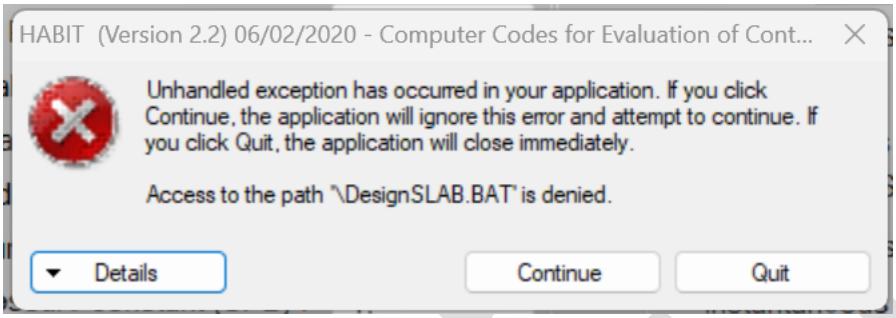

Figure 3-31 HABIT v2.2 Unhandled Exception: Running DEGADIS or SLAB without Inputs

3.8.2 HABIT v2.2.1 Screenshots

Figure 3-32 shows that in HABIT v2.2.1, this error is handled and gives a message on how to proceed (indicating that the user should run the Extran module).

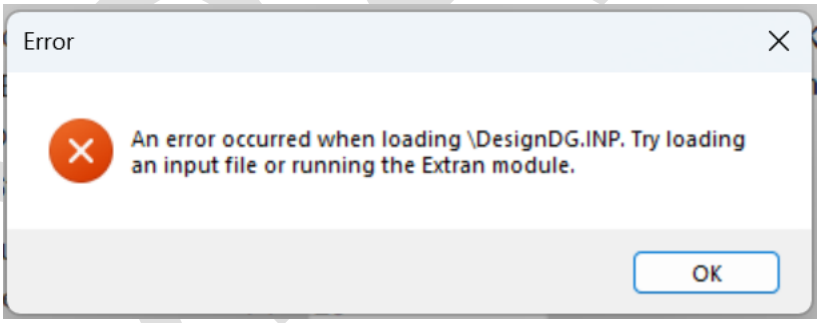

Figure 3-32 HABIT v2.2.1 Running DEGADIS or SLAB without Inputs

3.9 Issue 13: Standardizing Exponent Notation in GUI Text

Three modules in HABIT v2.2 have different methods of showing exponents (as shown in Figure 3-33):

- In EXTRAN, no character is used, such as m3/s.
- In CHEM, exponents are displayed as superscripts.
- In DEGADIS and SLAB: exponents appear using two asterisks, such as kg/m**3.

For clarity and consistency, the exponent text in the GUI was updated to all display as superscritps in HABIT v2.2.1 as shown in Figure 3-34.

3.9.1 HABIT v2.2 Screenshots

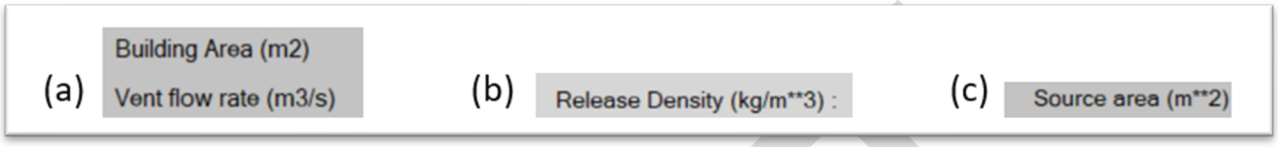

Figure 3-33 HABIT v2.2 Exponents Examples: (a) EXTRAN, (b) DEGADIS, (c) SLAB

3.9.2 HABIT v2.2.1 Screenshots

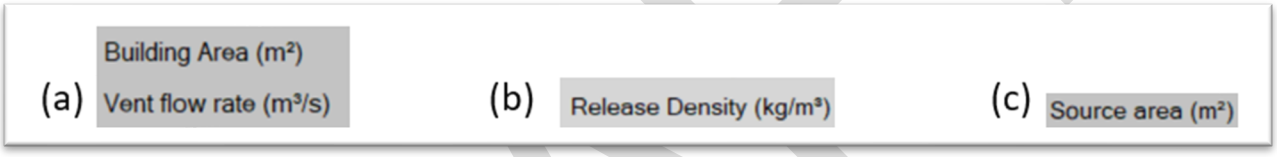

Figure 3-34. HABIT v2.2.1 Exponents Examples: (a) EXTRAN, (b) DEGADIS, (c) SLAB

3.10 Issue 14: DEGADIS Concentration Graph

The DEGADIS module has a Graph tab that is intended to depict a plot of the data from the *.SR4 file. However, the implementation of the plot in HABIT v2.2 does not properly read in the data. As an example, Figure 3-35 demonstrates what is to be plotted for the default case included in the code. Specifically, HABIT v2.2 plots the data twice and includes the timestamp of any missing data at time 0.

```
Records for 2038.0 s are missing - see source
Records for 2202.0 s are missing - see source
Records for 2366.0 s are missing - see source
Records for 2530.0 s are missing - see source
Records for 2694.0 s are missing - see source
Records for 2858.0 s are missing - see source
Records for 3022.0 s are missing - see source
Records for 3186.0 s are missing - see source
Records for 3350.0 s are missing - see source
Records for 3514.0 s are missing - see source
Records for 3678.0 s are missing - see source
Records for 3842.0 s are missing - see source
Records for 4006.0 s are missing - see source
Records for 4170.0 s are missing - see source
Records for 4334.0 s are missing - see source
4.498E+03 1.726E-03 5.096E-03 1.2029 293. 691. 1.90 33.6 783. 779.
4.662E+03 1.634E-03 4.823E-03 1.2026 293. 670. 1.93 66.7 851. 842.
4.826E+03 1.538E-03 4.539E-03 1.2024 293. 659. 1.96 86.0 892. 881.

4.990E+03 1.301E-03 3.841E-03 1.2017 293. 650. 2.00 103. 925. 911.
5.154E+03 7.237E-04 2.134E-03 1.2001 293. 641. 2.05 116. 939. 923.
```

Figure 3-35 DEGADIS Output File DesignDG.SR4 for the Default Case in HABIT v2.2

3.10.1 HABIT v2.2 Screenshots

The plot of this data in HABIT v2.2 is demonstrated below in Figure 3-36.

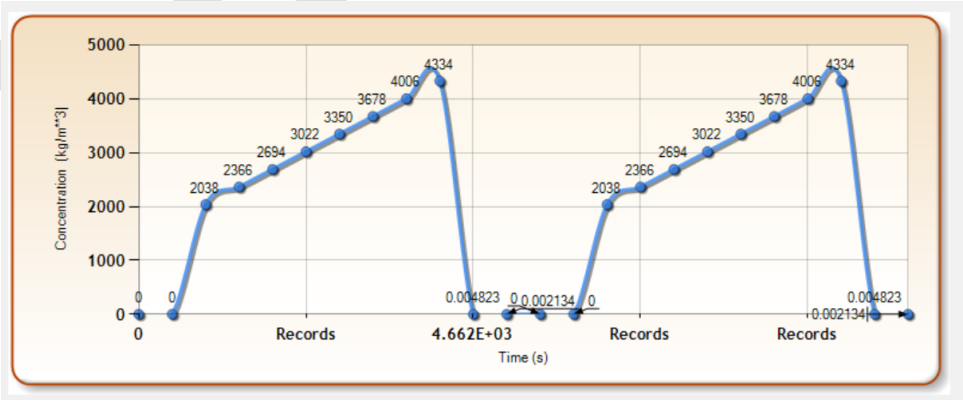

Figure 3-36 HABIT v2.2 DEGADIS Graph Tab Concentration Plot

3.10.2 HABIT v2.2.1 Screenshots

This behavior was corrected in HABIT v2.2.1. More specifically, only numerical data is parsed and included in the plot, and the points on the plot are not repeated. The corrected plot is included below in Figure 3-37.

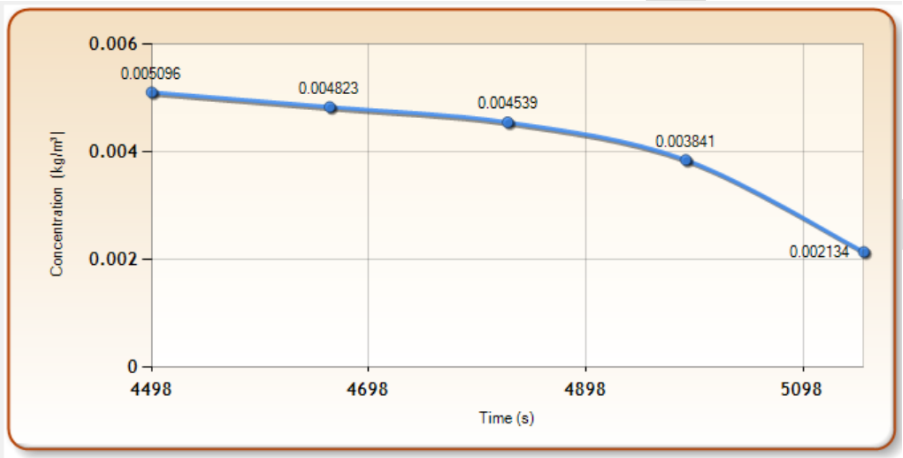

Figure 3-37 HABIT v2.2.1 DEGADIS Graph Tab Concentration Plot

4 Regression Test Cases

A series of seven test cases was compiled from existing HABIT runs at the NRC. Table 4-1 demonstrates which HABIT modules are tested in each run. The EXTRAN and CHEM file inputs are provided in Appendix A. Note that the DEGADIS and SLAB inputs can be generated by running EXTRAN through either HABIT v2.2 or HABIT v2.2.1.

Table 4-1 Modules Tested in Each Regression Test Case

Test Case	Description	EXTRAN	CHEM	DEGADIS	SLAB
1	Liquid Tank Leak of Chlorine	✓	✓	✓	✓
2	Liquid Tank Burst of Chlorine	✓	✓	✓	✓
3	Liquid Tank Burst of HCl	✓	✓		
4	Liquid Tank Burst of Acetic Acid	✓	✓	✓	✓
5	Gas Tank Burst of Carbon Dioxide	✓	✓	✓	
6	Gas Tank Burst of Acetic Acid	✓	✓		✓
7	Liquid Tank Burst of Chlorine	✓	✓	✓	✓

5 Regression Testing

For regression testing, the seven test cases were run through HABIT v2.2 and HABIT v2.2.1, and the outputs were compared. Since only changes to the graphical interface were implemented in HABIT v2.2.1, no variance in the outputs was expected. Therefore, the outputs had to perfectly match in order for the testing to be considered a success. A Python script was written to compare the text-based output files from each module. In Table 5-1, a green checkmark indicates that HABIT v2.2.1 produced identical outputs to HABIT v2.2 for the indicated module, confirming that HABIT v2.2 and HABIT v2.2.1 produced identical outputs from the same inputs.

Table 5-1 Regression Testing on HABIT v2.2.1

Test Case	EXTRAN	CHEM	DEGADIS	SLAB
1	✓	✓	✓	✓
2	✓	✓	✓	✓
3	✓	✓	—	—
4	✓	✓	✓	✓
5	✓	✓	✓	—
6	✓	✓	—	✓
7	✓	✓	✓	✓

5.1 Test Case 7 Plots

Figures 5-1 through 5-6, provide a visual comparison of the generated plots for Test Case 7. Figures 5-2 and 5-2 demonstrate the outputs of the ‘Plot Results’ button, which creates a graph plotted with the concentration output results for all of the included modules.

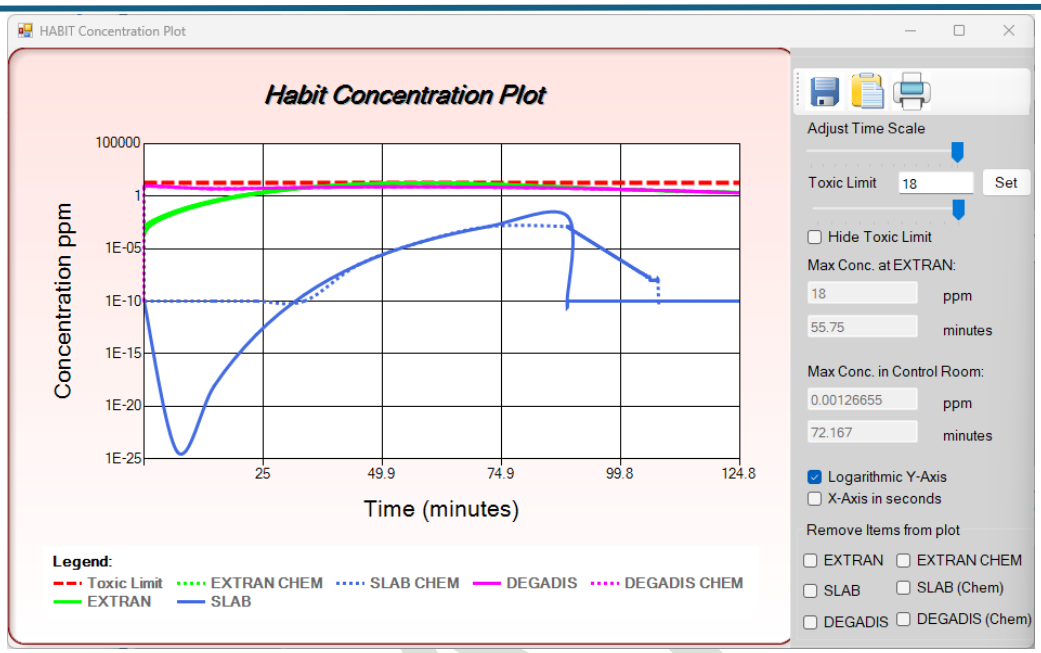

Figure 5-1 HABIT v2.2 Test Case 7 Plot Results Chart

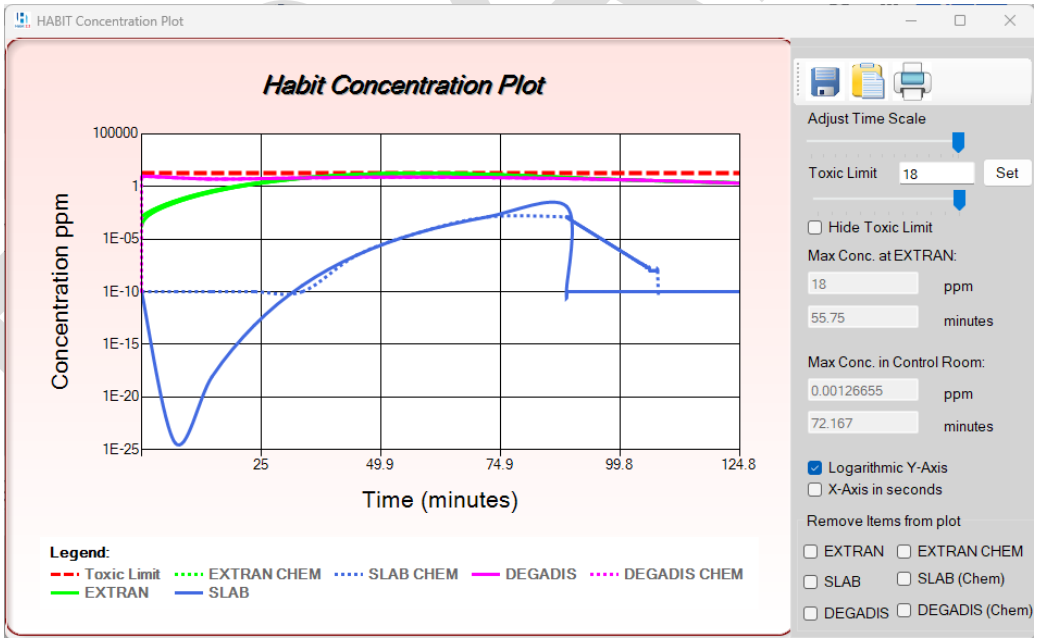

Figure 5-2 HABIT v2.2.1 Test Case 7 Plot Results Chart

Figures 5-3 through 5-6 demonstrate side-by-side comparisons of the graphs generated from the individual 'Plot Exposure' buttons of each module in both HABIT v2.2 and HABIT v2.2.1.

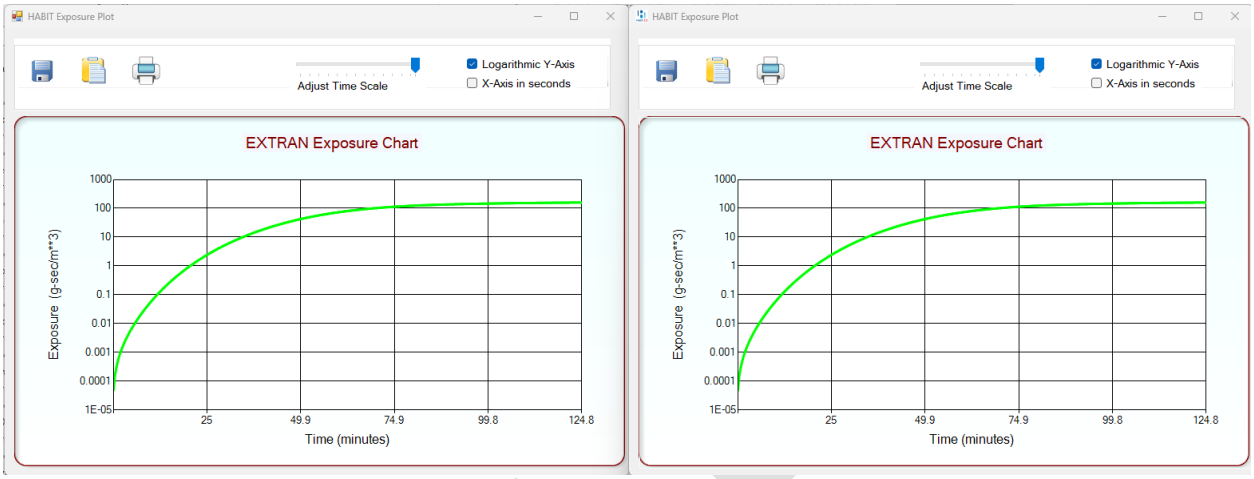

Figure 5-3 Comparison of EXTRAN Exposure Plots for Test Case 7

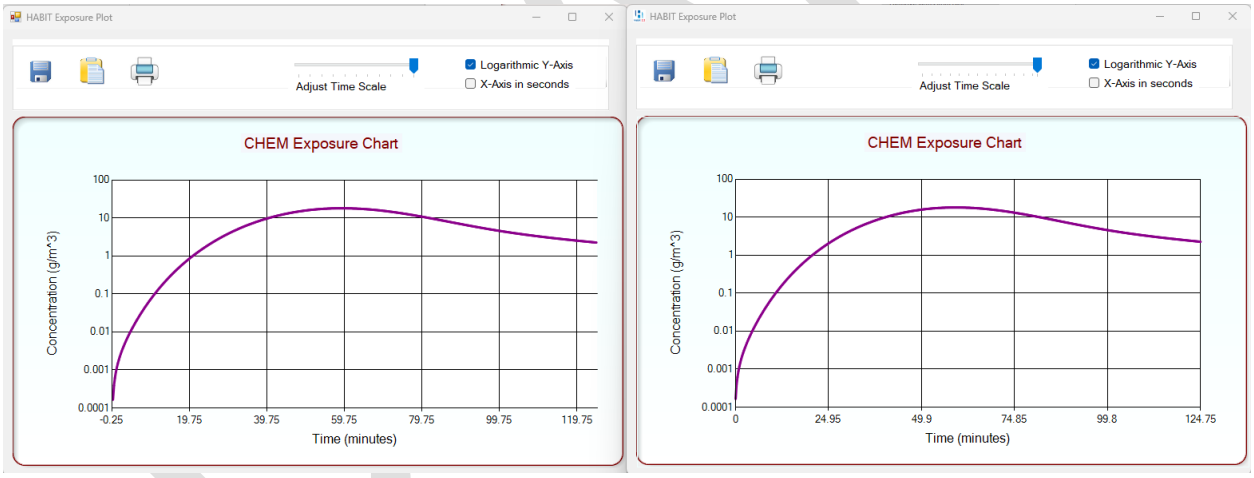

Figure 5-4 Comparison of CHEM Exposure Plots for Test Case 7

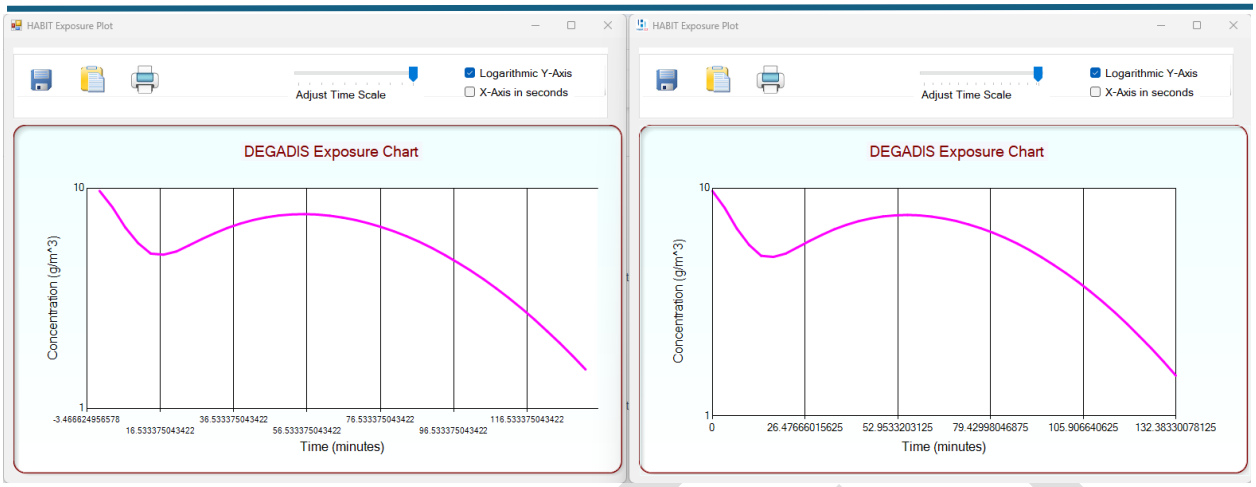

Figure 5-5 Comparison of DEGADIS Exposure Plots for Test Case 7

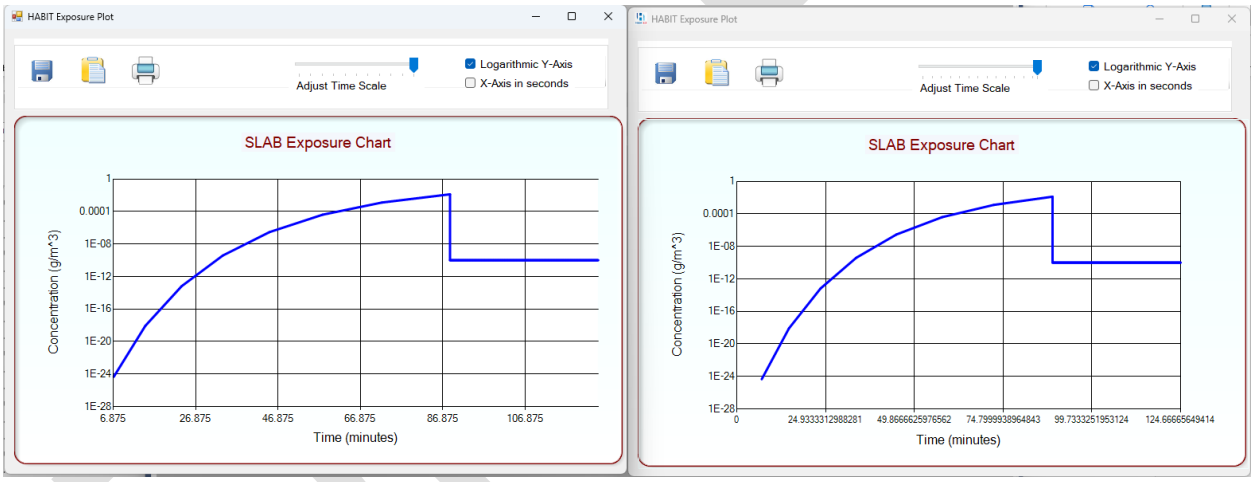

Figure 5-6 Comparison of SLAB Exposure Plots for Test Case 7

U.S.NRC
United States Nuclear Regulatory Commission
Protecting People and the Environment

Appendix A – Test Cases

In this appendix, provides the text of the EXTRAN and CHEM input files used for regression testing. The inputs for the DEGADIS and SLAB modules can be generated from running the EXTRAN module with the appropriate dense gas model.

A.1 Test Case 1

Test Case 1 demonstrates a Liquid Tank Leak of Chlorine. This is the default case that comes with HABIT v2.2 and HABIT v2.2.1.

A.1.1 EXTRAN Input File

```
STARTDATA:
        1       ! Concentration units
        2       ! ReleaseType
    50000         ! Initial Mass(kg or Ci)
      100         ! Release Rate (kg/s or Ci/s)
        0       ! Release Height (m)
       20        ! Storage Temperature (°C)
       20        ! Max. pool radius (m)
      200         ! Distance to intake (m)
       15        ! Intake height (m)
        0       ! Building Area (m2)
        0       ! Vent flow rate (m3/s)
        1       ! Wind speed (m/s)
        E       ! Atmospheric stability class
       20        ! Air temperature (°C)
      760         ! Atmos. Pressure (mm Hg)
      500         ! Solar radiation (W/m2)
        2       ! Cloud cover (tenths)
       25        ! Ground temperature (°C)
 Chlorine          ! Chemical Name
     70.9        ! Molecular Wt. (g/mole)
    -34.1        ! Boiling point (°C)
    0.946         ! Liq. heat capacity (J/g/°C)
      288        ! Heat of Vap. (J/g)
     1.57        ! Specific gravity
   0.0792          ! Mol. Diff. Coef. (cm2/sec)
```

A.1.2 CHEM Input File

```
STARTDATA:
      2        4        0      ! Distance units & Flow Units used in input, X/Q option flag
      0     ! Power level (MWt)
1727.328       ! Control room volume (m3)
      0        0        0      ! Core fractions:  Halogens (Elem., Org., Part.)
      0        0        0      ! Core fractions:  Nobles (Elem., Org., Part.)
      0        0        0      ! Core fractions:  Solids (Elem., Org., Part.)
      0        0        0      ! Core fractions:  Sodiums (Elem., Org., Part.)
      0        0        0      ! Core fractions:  Plutoniums (Elem., Org., Part.)
      0   0.008333       ! ====== Start of step 1,  StartTime (hrs), EndTime (hrs)
      0     ! Effluent Vertical velocity m/s
      0     ! Effluent flow rate (m3/s)
      0     ! Release height (m)
      0     ! Building height (m)
      0     ! Building cross sectional Area (m2)
      0     ! Horizontal Distance to receptor (m)
      0     ! Air intake height (m)
      0     ! Windspeed (m/s)
      4     ! Vertical dispersion class
      4     ! Horizontal dispersion class
6.607264       ! Flow rate from unfiltered intake source #1 (m3/s)
      0     ! Flow rate from unfiltered intake source #2 (m3/s)
      0     ! Bottled air flow rate (m3/s)
      0     ! Flow rate from filtered intake source #1 (m3/s)
      0        0        0      ! Filter efficiencies #1, (Elem., Org., Part.)(fraction)
      0     ! Flow rate from filtered intake source #2 (feeds recirc, m3/s)
      0        0        0      ! Filter efficiencies #2, (Elem., Org., Part.)(fraction)
      0     ! Recirculation flow rate (m3/s)
      0        0        0      ! Recirc. filter efficiencies , (Elem., Org., Part.)(fraction)
      1     ! Control room occupancy factor
0.008333   0.008333      ! ====== Start of step 2,  StartTime (hrs), EndTime (hrs)
      0     ! Effluent Vertical velocity m/s
      0     ! Effluent flow rate (m3/s)
      0     ! Release height (m)
      0     ! Building height (m)
      0     ! Building cross sectional Area (m2)
      0     ! Horizontal Distance to receptor (m)
      0     ! Air intake height (m)
```

```
     0      ! Windspeed (m/s)
     4      ! Vertical dispersion class
     4      ! Horizontal dispersion class
     0      ! Flow rate from unfiltered intake source #1 (m3/s)
     0      ! Flow rate from unfiltered intake source #2 (m3/s)
6.607264       ! Bottled air flow rate (m3/s)
     0      ! Flow rate from filtered intake source #1 (m3/s)
     0        0        0      ! Filter efficiencies #1, (Elem., Org., Part.)(fraction)
     0      ! Flow rate from filtered intake source #2 (feeds recirc, m3/s)
     0        0        0      ! Filter efficiencies #2, (Elem., Org., Part.)(fraction)
     0      ! Recirculation flow rate (m3/s)
     0        0        0      ! Recirc. filter efficiencies , (Elem., Org., Part.)(fraction)
     1      ! Control room occupancy factor
```

A.2 Test Case 2

Test Case 2 demonstrates a Liquid Tank Burst of Chlorine.

A.2.1 EXTRAN Input File

```
STARTDATA:
          1          ! Concentration units
          1          ! ReleaseType
        907          ! Initial Mass(kg or Ci)
          0          ! Release Rate (kg/s or Ci/s)
          0          ! Release Height (m)
         20          ! Storage Temperature (°C)
         20          ! Max. pool radius (m)
         20          ! Distance to intake (m)
        0.5          ! Intake height (m)
          0          ! Building Area (m2)
          0          ! Vent flow rate (m3/s)
          2          ! Wind speed (m/s)
          D          ! Atmospheric stability class
         20          ! Air temperature (°C)
        760          ! Atmos. Pressure (mm Hg)
        150          ! Solar radiation (W/m2)
          8          ! Cloud cover (tenths)
         25          ! Ground temperature (°C)
   Chlorine          ! Chemical Name
       70.9          ! Molecular Wt. (g/mole)
```

```
      -34.1          ! Boiling point (°C)
      0.946          ! Liq. heat capacity (J/g/°C)
        288          ! Heat of Vap. (J/g)
       1.57          ! Specific gravity
     0.0792          ! Mol. Diff. Coef. (cm2/sec)
```

A.2.2 CHEM Input File

```
STARTDATA:
        2        4        0      ! Distance units & Flow Units used in input, X/Q option flag
        0      ! Power level (MWt)
 1727.328       ! Control room volume (m3)
        0        0        0      ! Core fractions:  Halogens (Elem., Org., Part.)
        0        0        0      ! Core fractions:  Nobles (Elem., Org., Part.)
        0        0        0      ! Core fractions:  Solids (Elem., Org., Part.)
        0        0        0      ! Core fractions:  Sodiums (Elem., Org., Part.)
        0        0        0      ! Core fractions:  Plutoniums (Elem., Org., Part.)
        0    0.008333       ! ====== Start of step 1,  StartTime (hrs), EndTime (hrs)
        0      ! Effluent Vertical velocity m/s
        0      ! Effluent flow rate (m3/s)
        0      ! Release height (m)
        0      ! Building height (m)
        0      ! Building cross sectional Area (m2)
        0      ! Horizontal Distance to receptor (m)
        0      ! Air intake height (m)
        0      ! Windspeed (m/s)
        4      ! Vertical dispersion class
        4      ! Horizontal dispersion class
 6.607264       ! Flow rate from unfiltered intake source #1 (m3/s)
        0      ! Flow rate from unfiltered intake source #2 (m3/s)
        0      ! Bottled air flow rate (m3/s)
        0      ! Flow rate from filtered intake source #1 (m3/s)
        0        0        0      ! Filter efficiencies #1, (Elem., Org., Part.)(fraction)
        0      ! Flow rate from filtered intake source #2 (feeds recirc, m3/s)
        0        0        0      ! Filter efficiencies #2, (Elem., Org., Part.)(fraction)
        0      ! Recirculation flow rate (m3/s)
        0        0        0      ! Recirc. filter efficiencies , (Elem., Org., Part.)(fraction)
        1      ! Control room occupancy factor
 0.008333   0.008333       ! ====== Start of step 2,  StartTime (hrs), EndTime (hrs)
        0      ! Effluent Vertical velocity m/s
```

```
0       ! Effluent flow rate (m3/s)
0       ! Release height (m)
0       ! Building height (m)
0       ! Building cross sectional Area (m2)
0       ! Horizontal Distance to receptor (m)
0       ! Air intake height (m)
0       ! Windspeed (m/s)
4       ! Vertical dispersion class
4       ! Horizontal dispersion class
0       ! Flow rate from unfiltered intake source #1 (m3/s)
0       ! Flow rate from unfiltered intake source #2 (m3/s)
6.607264        ! Bottled air flow rate (m3/s)
0       ! Flow rate from filtered intake source #1 (m3/s)
0         0         0       ! Filter efficiencies #1, (Elem., Org., Part.)(fraction)
0       ! Flow rate from filtered intake source #2 (feeds recirc, m3/s)
0         0         0       ! Filter efficiencies #2, (Elem., Org., Part.)(fraction)
0       ! Recirculation flow rate (m3/s)
0         0         0       ! Recirc. filter efficiencies , (Elem., Org., Part.)(fraction)
1       ! Control room occupancy factor
```

A.3 Test Case 3

Test Case 3 demonstrates a Liquid Tank Burst of hydrocloric acid.

A.3.1 EXTRAN Input File

```
STARTDATA:
          1         ! Concentration units
          1         ! ReleaseType
     13525.3          ! Initial Mass(kg or Ci)
          0         ! Release Rate (kg/s or Ci/s)
         20          ! Release Height (m)
         25          ! Storage Temperature (°C)
         30          ! Max. pool radius (m)
      912.6           ! Distance to intake (m)
         60          ! Intake height (m)
        560           ! Building Area (m2)
          0         ! Vent flow rate (m3/s)
          6         ! Wind speed (m/s)
          D         ! Atmospheric stability class
         25          ! Air temperature (°C)
```

760 ! Atmos. Pressure (mm Hg)
1116 ! Solar radiation (W/m2)
5 ! Cloud cover (tenths)
25 ! Ground temperature (°C)
HCl ! Chemical Name
36.46 ! Molecular Wt. (g/mole)
90.33 ! Boiling point (°C)
2.6 ! Liq. heat capacity (J/g/°C)
443.4 ! Heat of Vap. (J/g)
1.191 ! Specific gravity
0.1 ! Mol. Diff. Coef. (cm2/sec)

A.3.2 CHEM Input File

```
STARTDATA:
      2       4       0     ! Distance units & Flow Units used in input, X/Q option flag
      0    ! Power level (MWt)
1727.328     ! Control room volume (m3)
      0       0       0     ! Core fractions:  Halogens (Elem., Org., Part.)
      0       0       0     ! Core fractions:  Nobles (Elem., Org., Part.)
      0       0       0     ! Core fractions:  Solids (Elem., Org., Part.)
      0       0       0     ! Core fractions:  Sodiums (Elem., Org., Part.)
      0       0       0     ! Core fractions:  Plutoniums (Elem., Org., Part.)
      0   0.008333     ! ====== Start of step 1,  StartTime (hrs), EndTime (hrs)
      0    ! Effluent Vertical velocity m/s
      0    ! Effluent flow rate (m3/s)
      0    ! Release height (m)
      0    ! Building height (m)
      0    ! Building cross sectional Area (m2)
      0    ! Horizontal Distance to receptor (m)
      0    ! Air intake height (m)
      0    ! Windspeed (m/s)
      4    ! Vertical dispersion class
      4    ! Horizontal dispersion class
6.607264     ! Flow rate from unfiltered intake source #1 (m3/s)
      0    ! Flow rate from unfiltered intake source #2 (m3/s)
      0    ! Bottled air flow rate (m3/s)
      0    ! Flow rate from filtered intake source #1 (m3/s)
      0       0       0     ! Filter efficiencies #1, (Elem., Org., Part.)(fraction)
      0    ! Flow rate from filtered intake source #2 (feeds recirc, m3/s)
      0       0       0     ! Filter efficiencies #2, (Elem., Org., Part.)(fraction)
```

```
      0      ! Recirculation flow rate (m3/s)
      0        0        0      ! Recirc. filter efficiencies , (Elem., Org., Part.)(fraction)
      1      ! Control room occupancy factor
0.008333   0.008333      ! ====== Start of step 2,  StartTime (hrs), EndTime (hrs)
      0      ! Effluent Vertical velocity m/s
      0      ! Effluent flow rate (m3/s)
      0      ! Release height (m)
      0      ! Building height (m)
      0      ! Building cross sectional Area (m2)
      0      ! Horizontal Distance to receptor (m)
      0      ! Air intake height (m)
      0      ! Windspeed (m/s)
      4      ! Vertical dispersion class
      4      ! Horizontal dispersion class
      0      ! Flow rate from unfiltered intake source #1 (m3/s)
      0      ! Flow rate from unfiltered intake source #2 (m3/s)
6.607264      ! Bottled air flow rate (m3/s)
      0      ! Flow rate from filtered intake source #1 (m3/s)
      0        0        0      ! Filter efficiencies #1, (Elem., Org., Part.)(fraction)
      0      ! Flow rate from filtered intake source #2 (feeds recirc, m3/s)
      0        0        0      ! Filter efficiencies #2, (Elem., Org., Part.)(fraction)
      0      ! Recirculation flow rate (m3/s)
      0        0        0      ! Recirc. filter efficiencies , (Elem., Org., Part.)(fraction)
      1      ! Control room occupancy factor
```

A.4 Test Case 4

Test Case 4 demonstrates a Liquid Tank Burst of Acetic Acid.

A.4.1 EXTRAN Input File

```
STARTDATA:
          1       !Concentration units: ppm
          1       !ReleaseType: Liquid tank burst
   19853.73       !Initial mass (kg or Ci)
     -00.0        !Release rate (kg/s or Ci/s)
     -00.0        !Release height (m)
         25       !Storage temperature (øC)
        100       !Max. pool radius (m)
       4869       !Distance to intake (m)
     -00.0        !Intake height (m)
```

```
-00.0          !Building area (m2)
-00.0          !Vent flow rate (m3/s)
2             !Wind speed (m/s)
F             !Atmospheric stability class
25            !Air temperature (øC)
760           !Atmos. Pressure (mm Hg)
1000          !Solar radiation (W/m2)
5             !Cloud cover (tenths)
30            !Ground temperature (øC)
Acetic Acid       !Chemical name
60.05         !Molecular Wt. (g/mole)
118.1         !Boiling point(øC)
2.18          !Liq. heat capacity (J/g/øC)
402           !Heat of Vap. (J/g)
1.05          !Specific gravity
-00.0         !Mol. Diff. Coef. (cm2/sec)
```

A.4.2 CHEM Input File

```
STARTDATA:    5   ! number of nuclide groups (HABIT 1.1 format)
      1       1       0     !Distance units & Flow Units used in input, X/Q option flag
   -00.0     !Power level (MWt)
 2208.714     !Control room volume (m3)
      0       0       0     !Core fractions:   (Elem., Org., Part.)
      0       0       0     !Core fractions:   (Elem., Org., Part.)
      0       0       0     !Core fractions:   (Elem., Org., Part.)
      0       0       0     !Core fractions:   (Elem., Org., Part.)
      0       0       0     !Core fractions:   (Elem., Org., Part.)
      0       0     !====== Start of step  1,  StartTime (hrs), EndTime (hrs)
      0    !Effluent Vertical velocity m/s
      0    !Effluent flow rate (m3/s)
      0    !Release height (m)
      4    !Building height (m)
      4    !Building cross sectional Area (m2)
     .2    !Horizontal Distance to receptor (m)
      0    !Air intake height (m)
      0    !Windspeed (m/s)
      0    !Vertical dispersion class
      0    !Horizontal dispersion class
    .25     !Flow rate from unfiltered intake source #1 (m3/s)
```

```
0     !Flow rate from unfiltered intake source #2 (m3/s)
0     !Bottled air flow rate (m3/s)
0     !Flow rate from filtered intake source #1 (m3/s)
1        0        0     !Filter efficiencies #1, (Elem., Org., Part.)(fraction)
0     !Flow rate from filtered intake source #2 (feeds recirc, m3/s)
0        0        0     !Filter efficiencies #2, (Elem., Org., Part.)(fraction)
0     !Recirculation flow rate (m3/s)
0        0        0     !Recirc. filter efficiencies , (Elem., Org., Part.)(fraction)
1     !Control room occupancy factor
```

A.5 Test Case 5

Test Case 5 demonstrates a Gas Tank Burst of Carbon Dioxide.

A.5.1 EXTRAN Input File

```
STARTDATA:
          1        !Concentration units: ppm
          3        !ReleaseType: Gas tank burst
     3336.2         !Initial mass (kg or Ci)
      -00.0         !Release rate (kg/s or Ci/s)
      -00.0         !Release height (m)
         25         !Storage temperature (øC)
      -00.0         !Max. pool radius (m)
      152.4         !Distance to intake (m)
      -00.0         !Intake height (m)
      -00.0         !Building area (m2)
      -00.0         !Vent flow rate (m3/s)
          2        !Wind speed (m/s)
          F        !Atmospheric stability class
         25         !Air temperature (øC)
     741.21         !Atmos. Pressure (mm Hg)
      -00.0         !Solar radiation (W/m2)
      -00.0         !Cloud cover (tenths)
      -00.0         !Ground temperature (øC)
Carbon Dioxide      !Chemical name
         44        !Molecular Wt. (g/mole)
      -78.5         !Boiling point(øC)
        .77        !Liq. heat capacity (J/g/øC)
        348         !Heat of Vap. (J/g)
       .468         !Specific gravity
```

```
          -00.0          !Mol. Diff. Coef. (cm2/sec)
```

A.5.2 CHEM Input File

```
STARTDATA:    5   ! number of nuclide groups (HABIT 1.1 format)
        1         1         0     !Distance units & Flow Units used in input, X/Q option flag
     -00.0     !Power level (MWt)
      5509     !Control room volume (m3)
        0         0         0     !Core fractions:   (Elem., Org., Part.)
        0         0         0     !Core fractions:   (Elem., Org., Part.)
        0         0         0     !Core fractions:   (Elem., Org., Part.)
        0         0         0     !Core fractions:   (Elem., Org., Part.)
        0         0         0     !Core fractions:   (Elem., Org., Part.)
        0         0      !====== Start of step  1,  StartTime (hrs), EndTime (hrs)
        0     !Effluent Vertical velocity m/s
        0     !Effluent flow rate (m3/s)
        0     !Release height (m)
        4     !Building height (m)
        4     !Building cross sectional Area (m2)
       .2     !Horizontal Distance to receptor (m)
        0     !Air intake height (m)
        0     !Windspeed (m/s)
        0     !Vertical dispersion class
        0     !Horizontal dispersion class
     .944      !Flow rate from unfiltered intake source #1 (m3/s)
        0     !Flow rate from unfiltered intake source #2 (m3/s)
        0     !Bottled air flow rate (m3/s)
        0     !Flow rate from filtered intake source #1 (m3/s)
        1         0         0     !Filter efficiencies #1, (Elem., Org., Part.)(fraction)
        0     !Flow rate from filtered intake source #2 (feeds recirc, m3/s)
        0         0         0     !Filter efficiencies #2, (Elem., Org., Part.)(fraction)
        0     !Recirculation flow rate (m3/s)
        0         0         0     !Recirc. filter efficiencies , (Elem., Org., Part.)(fraction)
        1     !Control room occupancy factor
```

Test Case 6

Test Case 6 demonstrates a Gas Tank Burst of Acetic Acid.

A.6.1 EXTRAN Input File

```
STARTDATA:
          1        !Concentration units: ppm
          3        !ReleaseType: Gas tank burst
   453592.2         !Initial mass (kg or Ci)
     -00.0         !Release rate (kg/s or Ci/s)
     -00.0         !Release height (m)
         25        !Storage temperature (øC)
     -00.0         !Max. pool radius (m)
       6962        !Distance to intake (m)
     -00.0         !Intake height (m)
     -00.0         !Building area (m2)
     -00.0         !Vent flow rate (m3/s)
          4        !Wind speed (m/s)
          G        !Atmospheric stability class
         25        !Air temperature (øC)
        760        !Atmos. Pressure (mm Hg)
     -00.0         !Solar radiation (W/m2)
          5        !Cloud cover (tenths)
     -00.0         !Ground temperature (øC)
Acetic Acid        !Chemical name
      60.05        !Molecular Wt. (g/mole)
      118.1        !Boiling point(øC)
       2.18        !Liq. heat capacity (J/g/øC)
        402        !Heat of Vap. (J/g)
       1.05        !Specific gravity
     -00.0         !Mol. Diff. Coef. (cm2/sec)
```

A.6.2 CHEM Input File

```
STARTDATA:    5   ! number of nuclide groups (HABIT 1.1 format)
          1         1         0     !Distance units & Flow Units used in input, X/Q option flag
      -00.0     !Power level (MWt)
       1000      !Control room volume (m3)
          0         0         0     !Core fractions:   (Elem., Org., Part.)
          0         0         0     !Core fractions:   (Elem., Org., Part.)
          0         0         0     !Core fractions:   (Elem., Org., Part.)
          0         0         0     !Core fractions:   (Elem., Org., Part.)
          0         0         0     !Core fractions:   (Elem., Org., Part.)
          0         0     !====== Start of step  1,  StartTime (hrs), EndTime (hrs)
          0     !Effluent Vertical velocity m/s
```

```
    0     !Effluent flow rate (m3/s)
    0     !Release height (m)
    4     !Building height (m)
    4     !Building cross sectional Area (m2)
   .2     !Horizontal Distance to receptor (m)
    0     !Air intake height (m)
    0     !Windspeed (m/s)
    0     !Vertical dispersion class
    0     !Horizontal dispersion class
.12367     !Flow rate from unfiltered intake source #1 (m3/s)
    0     !Flow rate from unfiltered intake source #2 (m3/s)
    0     !Bottled air flow rate (m3/s)
    0     !Flow rate from filtered intake source #1 (m3/s)
    1       0       0     !Filter efficiencies #1, (Elem., Org., Part.)(fraction)
    0     !Flow rate from filtered intake source #2 (feeds recirc, m3/s)
    0       0       0     !Filter efficiencies #2, (Elem., Org., Part.)(fraction)
    0     !Recirculation flow rate (m3/s)
    0       0       0     !Recirc. filter efficiencies , (Elem., Org., Part.)(fraction)
    1     !Control room occupancy factor
```

Test Case 7

Test Case 7demonstrates a Liquid Tank Burst of Chlorine.

A.7.1 EXTRAN Input File

```
STARTDATA:
      1       !Concentration units: ppm
      1       !ReleaseType: Liquid tank burst
  20000         !Initial mass (kg or Ci)
 -00.0          !Release rate (kg/s or Ci/s)
      0       !Release height (m)
     25        !Storage temperature (øC)
 -00.0          !Max. pool radius (m)
   5200         !Distance to intake (m)
     17        !Intake height (m)
 -00.0          !Building area (m2)
 -00.0          !Vent flow rate (m3/s)
      1       !Wind speed (m/s)
      G        !Atmospheric stability class
     25        !Air temperature (øC)
```

```
      760        !Atmos. Pressure (mm Hg)
        0       !Solar radiation (W/m2)
        0       !Cloud cover (tenths)
       25        !Ground temperature (øC)
 Chlorine         !Chemical name
     70.9        !Molecular Wt. (g/mole)
    -34.1        !Boiling point(øC)
     .946        !Liq. heat capacity (J/g/øC)
      288        !Heat of Vap. (J/g)
     1.57        !Specific gravity
    .0792         !Mol. Diff. Coef. (cm2/sec)
```

A.7.2 CHEM Input File

```
STARTDATA:    5   ! number of nuclide groups (HABIT 1.1 format)
        1         1         0     !Distance units & Flow Units used in input, X/Q option flag
   -00.0     !Power level (MWt)
    1011     !Control room volume (m3)
        0         0         0     !Core fractions:   (Elem., Org., Part.)
        0         0         0     !Core fractions:   (Elem., Org., Part.)
        0         0         0     !Core fractions:   (Elem., Org., Part.)
        0         0         0     !Core fractions:   (Elem., Org., Part.)
        0         0         0     !Core fractions:   (Elem., Org., Part.)
        0         0    !====== Start of step  1,  StartTime (hrs), EndTime (hrs)
        0    !Effluent Vertical velocity m/s
        0    !Effluent flow rate (m3/s)
        0    !Release height (m)
        4    !Building height (m)
        4    !Building cross sectional Area (m2)
      .31     !Horizontal Distance to receptor (m)
        0    !Air intake height (m)
        0    !Windspeed (m/s)
        0    !Vertical dispersion class
        0    !Horizontal dispersion class
      .31     !Flow rate from unfiltered intake source #1 (m3/s)
        0    !Flow rate from unfiltered intake source #2 (m3/s)
        0    !Bottled air flow rate (m3/s)
        0    !Flow rate from filtered intake source #1 (m3/s)
        1         0         0     !Filter efficiencies #1, (Elem., Org., Part.)(fraction)
        0    !Flow rate from filtered intake source #2 (feeds recirc, m3/s)
```

0 0 0 !Filter efficiencies #2, (Elem., Org., Part.)(fraction)
0 !Recirculation flow rate (m3/s)
0 0 0 !Recirc. filter efficiencies , (Elem., Org., Part.)(fraction)
1 !Control room occupancy factor