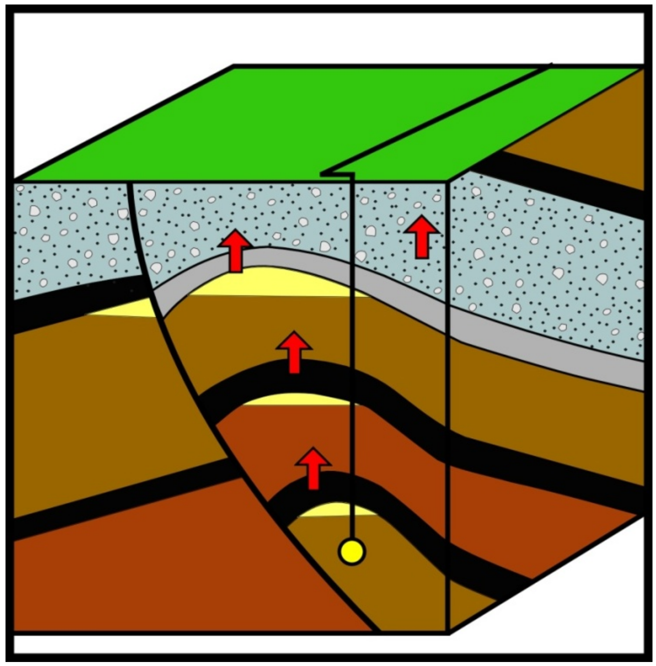

# NRAP Seal Barrier Reduced-Order Model (NSealR) Tool User's Manual, Version: 2016.11-14.1

10 November 2016


Office of Fossil Energy

NRAP-TRS-III-012-2016

# Disclaimer



**Cover Illustration:** A schematic representing the potential flow of carbon dioxide through multiple geologic aquitards (seal barriers) above the injection reservoir.

**Suggested Citation:** Lindner, E. *NRAP Seal Barrier Reduced-Order Model (NSealR) Tool User's Manual, Version: 2016.11-14.1;* NRAP-TRS-III-012-2016; NRAP Technical Report Series; U.S. Department of Energy, National Energy Technology Laboratory: Morgantown, WV, 2016; p 56.

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# NRAP Seal Barrier Reduced-Order Model (NSealR) Tool User's Manual, Version: 2016.11-14.1

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**NRAP-TRS-III-012-2016**

Level III Technical Report Series

10 November 2016

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# Table of Contents

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# Acronyms, Abbreviations, and Symbols

| Term | Description |
|---|---|
| ***Acronyms/Abbreviations*** | |
| 1-D | One-dimensional |
| 2-D | Two-dimensional |
| $CO_2$ | Carbon dioxide |
| $CO_2$-PENS | Predicting Engineered Natural Systems for $CO_2$ Storage |
| DLL | Dynamic link library |
| DOE | U.S. Department of Energy |
| EDX | Energy Data Exchange |
| LANL | Los Alamos National Laboratory |
| LUT | Lookup table |
| NaCl | Sodium chloride |
| NAVD88 | North American Vertical Datum of 1988 |
| NETL | National Energy Technology Laboratory |
| NRAP | National Risk Assessment Partnership |
| NRAP-IAM-CS | NRAP-Integrated Assessment Model-Carbon Storage |
| NSealR | NRAP Seal Barrier Reduced-order model |
| ROM | Reduced-order model |
| TRS | Technical Report Series |
| ***Units/Symbols*** | |
| µm | micrometers |
| °C | degrees Celsius |
| °F | degrees Fahrenheit |
| ft | feet |
| kg | kilograms ($10^3$ g) |
| km | kilometers ($10^3$ m) |
| m | meters |
| mD | millidarcy ($10^{-3}$ D = $9.869233\times10^{-16}$ $m^2$) |
| mg | milligrams ($10^{-3}$ g) |
| mm | millimeters ($10^{-3}$ m) |
| MPa | megapascals ($10^6$ Pa) |
| Ms | megasecond ($10^6$ seconds) |
| ηD | nanodarcy ($10^{-9}$ D) |
| Pa | pascals |
| ppm | parts per million, ratio of solute to solution, by weight |
| tonne | metric tons ($10^3$ kg) |
| s | second |
| yr | years |

# Acknowledgments

This work was completed as part of the National Risk Assessment Partnership (NRAP) project. Support for this project came from the U.S. Department of Energy's (DOE) Office of Fossil Energy's Crosscutting Research program. The author wishes to acknowledge Traci Rodosta (Carbon Storage Technology Manager), Kanwal Mahajan (Carbon Storage Division Director), M. Kylee Rice (Carbon Storage Division Project Manager), Mark Ackiewicz (Division of CCS Research Program Manager), Robert Romanosky (NETL Crosscutting Research, Office of Strategic Planning), and Regis Conrad (DOE Office of Fossil Energy) for programmatic guidance, direction, and support.

In addition, special thanks to: a) Jason Monnell, Research Assistant Professor, University of Pittsburgh, for his computations on the solubility of carbon dioxide and viscosity of brine; b) Neal Sams of AECOM for his insights on two-phase flow theory; c) Robert Dilmore of DOE NETL for his support in using GoldSim and integrating this work within NRAP; d) Gary Merrell of AECOM, for his detailed review of the original portion of the GoldSim portion of the code; and e) Dustin Crandall formerly of AECOM and now with DOE NETL for his assistance on graphics modeling. Further, the author wishes to thank Grant Bromhal, Technical Director of NRAP, within DOE NETL's Research and Innovation Center, for his management direction and support.

## **ABSTRACT**

This manual provides a brief guide to the use of the NSealR (for NRAP Seal Barrier Reduced-order model) tool developed as part of the effort to quantify the risk of geologic storage of carbon dioxide ($CO_2$) under the U.S. Department of Energy's National Risk Assessment Partnership (NRAP). This document is complementary to and abbreviated from the NRAP Technical Report, *NSealR—A User's Guide, Third-Generation* (Lindner, 2015). The NSealR code describes the flow or leakage of $CO_2$ through a low permeability rock formation (or seal) overlying the storage reservoir into which $CO_2$ is injected. A two-phase, relative permeability approach with Darcy's law is used for one-dimension (1-D) flow computations of $CO_2$ through the horizon in the vertical direction. While currently constructed to function as a stand-alone tool, NSealR is intended to characterize seal performance within a systems-level model of $CO_2$ storage performance and is structured to facilitate that application. The code is written using GoldSim's simulation software platform. This manual illustrates the program graphical user interface, describes the code inputs and provides a synopsis of the theoretical basis of NSealR.

# 1. INTRODUCTION

NSealR (for NRAP Seal Barrier Reduced-order model) was developed at the National Energy Technology Laboratory (NETL) to simulate the movement (leakage) of carbon dioxide ($CO_2$) over time through a thin[1], relatively impermeable layer of rock overlying a rock formation where $CO_2$ has been injected. The code was developed using the GoldSim simulation platform (GoldSim, 2014) and therefore, is constructed using various graphics-based software elements, which allow the user to readily trace code processes and logic. The current theoretical base considers the one-dimension (1-D), two-phase flow of $CO_2$ through brine[2]-saturated rock under $CO_2$ supercritical conditions.

The NSealR code is intended to assist in the quantitative risk assessment of geologic storage and as such, the code was originally envisioned as a module of an existing system level integrated assessment model, $CO_2$-PENS (Predicting Engineered Natural Systems for $CO_2$ Storage). $CO_2$-PENS was developed at the Los Alamos National Laboratory (LANL; Keating et al., 2009) and also uses the GoldSim software platform. For the present development effort, however, NSealR has been constructed as a stand-alone code to predict flux through a fractured sealing layer over time.

Development of NSealR began in mid-2012 as part of work of the National Risk Assessment Partnership (NRAP) program. NRAP is a multi-national-laboratory effort to develop analysis tools for evaluating risk assessment for long-term storage of $CO_2$, an effort that is already in the second term or generation of progress. This code version was developed in late 2013 and in 2014 during the third-generation of the NRAP program and is documented in Lindner (2015). A minor update was performed in 2016 and is reflected in this manual.[3] Subsequent versions, when completed, will add complexity by accounting for coupled flow, geochemical and geomechanical effects[4], and for multi-layer and two dimensional (2-D) aspects of flow through the seal horizon.

1 The "thin" assumption in NSealR reflects the treatment of fluid densities as being constant from top to bottom of the unit and flow is essentially one dimensional.

2 In this guide, the term, "brine" is used generically to describe an aqueous solution of sodium chloride (NaCl) in groundwater.

3 The Dashboards shown in the Lindner (2015) (Version 6) have been updated in this manual for current GoldSim model version (NSealR 2016.11-14.1).

4 For example, additional geomechanical effects can include aperture changes due to a varying stress field and to geochemical alteration.

## 2. DESCRIPTION AND USE OF NSealR CODE

The NSealR code was developed to simulate the flow through a thin seal formation during $CO_2$ storage as part of a larger analysis effort to evaluate storage risk. This effort is generally structured around development of an integrated assessment model (IAM) that couples models of a number of distinct system components for storage in a geologic reservoir, potential migration out of that target reservoir through leakage pathways, and impact to overlying resources such as shallow groundwater aquifers to simulate the behavior of the entire system at the site (reservoir to receptor). To simulate the storage of $CO_2$ during and after injection, distinct submodels are linked to describe the geologic storage site, including models of the reservoir, injection wells, the overlying aquifers, and potential leakage pathways from the reservoir such as existing wellbores and faults.

As such, the NSealR is conceptually a middleman for the NRAP-IAM-Carbon Storage (NRAP-IAM-CS) tool, taking the output from the reservoir models (in the form of $CO_2$ saturation and pressures at the base of the seal horizon) and providing input to the overlying aquifer models in the form of $CO_2$ and brine mass flux at the top of the seal horizon. This is illustrated in Figure 1.

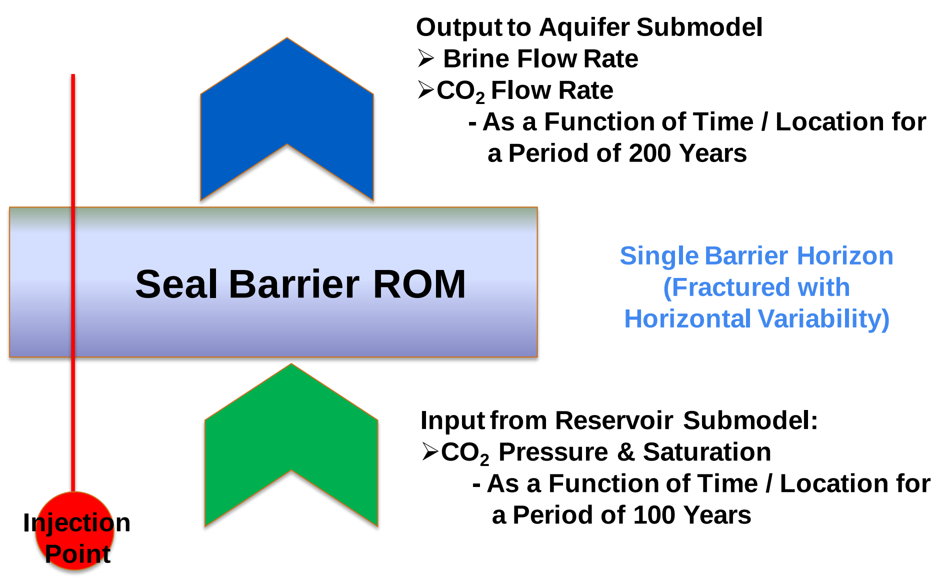


**Figure 1: Seals ROM as interface between reservoir and aquifer models within a systems-level integrated assessment model of $CO_2$ storage.**

For risk assessment, an IAM uses a Monte-Carlo approach in evaluating risk, involving a large number of possible cases (realizations) to construct a stochastic assessment of potential impacts of fluid flux outside of the reservoir. Assessment of a single scenario can require several thousands (or more) of realizations, so NRAP is developing computationally efficient modules that can predict the behavior of each component of the system. This typically involves constructing a streamlined computer code, based on (or "reduced" from) more complex computer codes. The individual component models are therefore termed in this context, "reduced-order models" or ROMs. In the case of NSealR, there is not a detailed process model from which the ROM has been developed per se; rather, NSealR represents a reduced set of physics and dimensionality from a conventional, discrete fracture flow simulator (such as NFFLOW; McKoy and Sams, 1997).

## 2.1 MODEL OVERVIEW

The structure of NSealR is relatively simplistic in concept and divides the major operations into three tasks. As illustrated in Figure 2, the basic computation tasks/models of NSealR are: (1) define the permeability of each cell; (2) define the thickness of each cell; (3) define the temperature-pressure dependent fluid properties; and (4) compute fluid flow. At the substantial depths required for sequestration, the flow computation is also strongly influenced by fluid properties that are pressure, temperature, and salinity dependent.

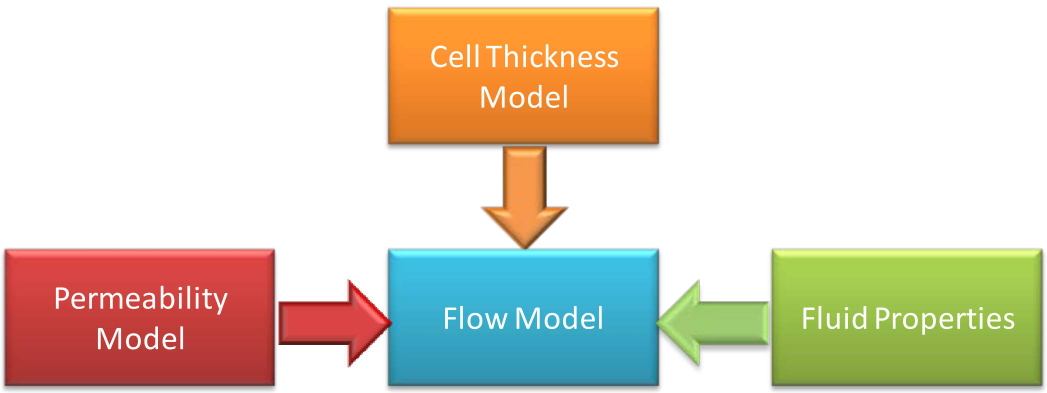


**Figure 2: Task models in NSealR.**

The current permeability model assumes established vertical flow pathways through the seal horizon and does not include chemical and time-related interactions, such as dissolution, swell and precipitation due to $CO_2$-fluid-rock interactions or erosion of preferential pathways. This model also does not include mechanical effects, such as those that could be induced by high injection pressures, such as the creation of new fractures or closure of existing fractures.

The options to define these models in NSealR are deliberately simplistic to maintain reduced computation times, but are considered sufficiently sophisticated to allow the user to capture (to a large degree) the variability of the subsurface. The model options are described in the following sections.

## 3. CODE STRUCTURE

The logic structure of NSealR is divided into seven modules or "containers", as shown in Figure 3, together with an eighth container for the user interface. Code flow in Figure 3 is from left to right, with input variables defined in the leftmost two containers, "input_seals_parameters" and "input_run_parameters."

In the center of the diagram, the "generate_seal_conditions" module defines the height (thickness) and permeability of each grid element based on the user's selections in the input containers. The average fluid parameters are defined in the "define_fluid_parameters." The results of the reservoir model are imported in the "import_reservoir_results" container and the output from this and the other central modules is employed in the computation of the two-phase flow equation. The computation itself is contained within a GoldSim External element in "compute_two_phase_flow" module, and allows the user to readily examine the coding for the analysis of flow. Finally, at the far right, control of specific output options is within the "output_results" container.

The module at the top of the diagram (user-interface) contains graphical user interface Dashboards, which are used for input and are described in Section 4.1.

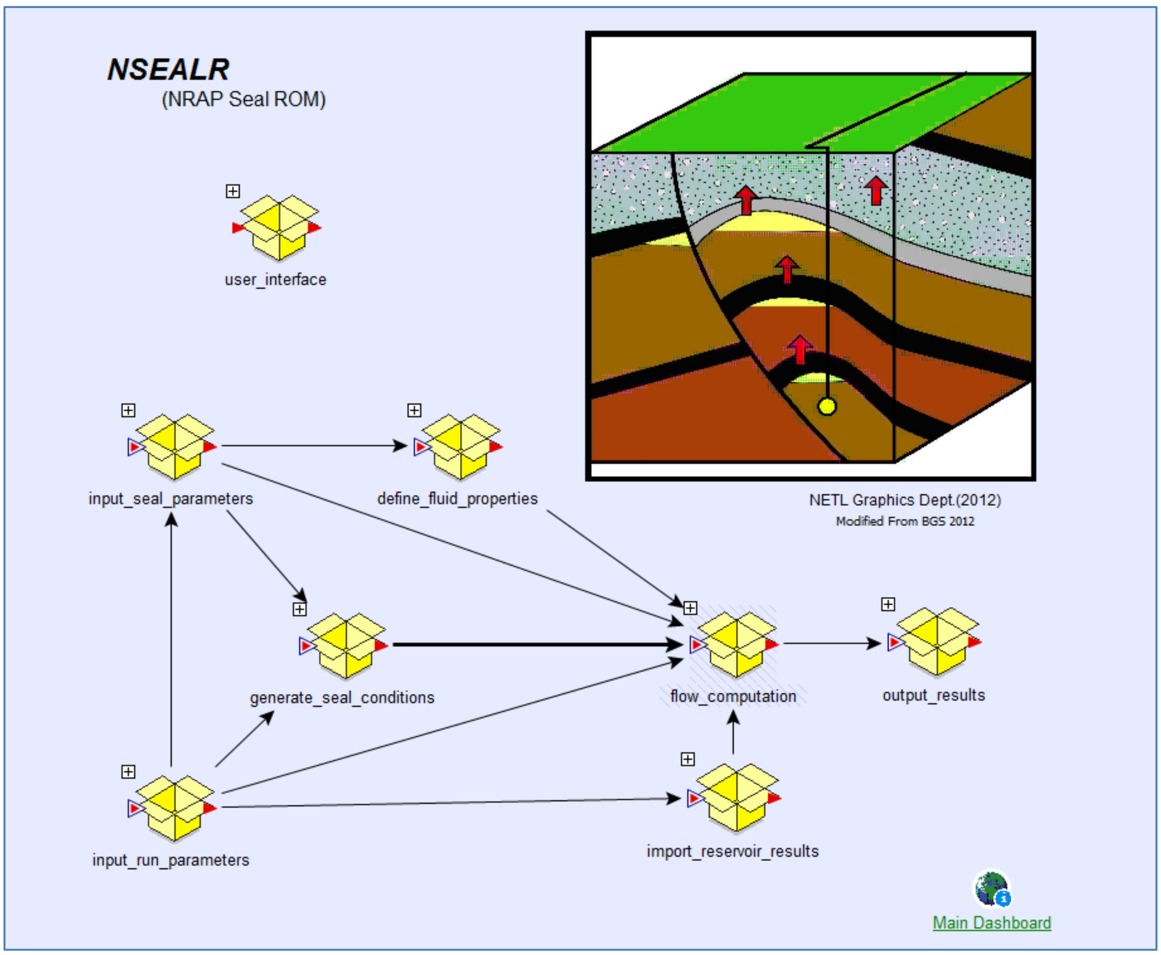


**Figure 3: Top-level structure of NSealR code.**

# 4. INPUT METHODS AND VARIABLES

## 4.1 DASHBOARDS

### 4.1.1 General

Console input for NSealR is via a series of windows in the GoldSim graphical user interface, termed *Dashboards*. The Dashboards allow for numeric and conditional input (check boxes), depending on the variable in question. In addition, in cases where the user is required to select one option from a limited number of alternatives, a list box element is provided on the Dashboard. List box elements are used for selecting the permeability model, the thickness model, the in situ stress correction method, and the top boundary conditions option.

Dashboards used for console interaction by NSealR are arranged in a menu hierarchy, as shown in Figure 4. The topmost Dashboard, *Seal_MAIN*, provides access to the input and output control Dashboards as well as to Dashboards supplying related information.

The three information Dashboards[5] are shown to the far upper right in the structure and contain information the user should review prior to code use. Specifically, the *References* Dashboard, provides a list of references used in code development. The *Contacts* Dashboard provides a list of names, phone numbers and the mailing address and for obtaining other information on the code, and the *Notices* Dashboard provides the disclaimers on code use and the applicable copyright statement.

Three output Dashboards are shown in the middle of the figure. Two Dashboards allow the user to plot results using GoldSim plotting functions (*output_plots*), or to send data periodically to file (*output_seal_control*). A third Dashboard (*property_values*) provides a listing of fluid properties at defined conditions. The GoldSim plotting options are described in more detail in the GoldSim User's Guide (GoldSim, 2014).

The input Dashboards are located at the bottom of Figure 4, and provide the user with the options to select the permeability model (*permeability*), define the two-phase parameter values *(relative_perm_input)*, define the seal thickness *(thickness_other_params)*, define active cells and heterogeneity across the seal horizon (*active_heterogeneity)*, and define the conditions along the top of the seal (*upper_boundary*). There is also a secondary Dashboard below the *Permeability* Dashboard to define stress-controlled characteristics (i.e., the *Stress-Aperture Correction* Dashboard). Two additional Dashboards are at this level which allows input of parameters that are typically related to the repository component: the simulation conditions and site characteristics, labeled as the *simulation_input* and *site_characteristics* Dashboards, respectively.

Moving between Dashboards is controlled by the Dashboard structure. To move between Dashboards, selecting one of the buttons on the current (visible) Dashboard moves to the next lower level, and each Dashboard provides a return button (blue button at bottom right) to navigate to the next upper level in the Dashboard structure.

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5 For brevity, these Dashboards are not shown here, but are shown in Lindner (2015).

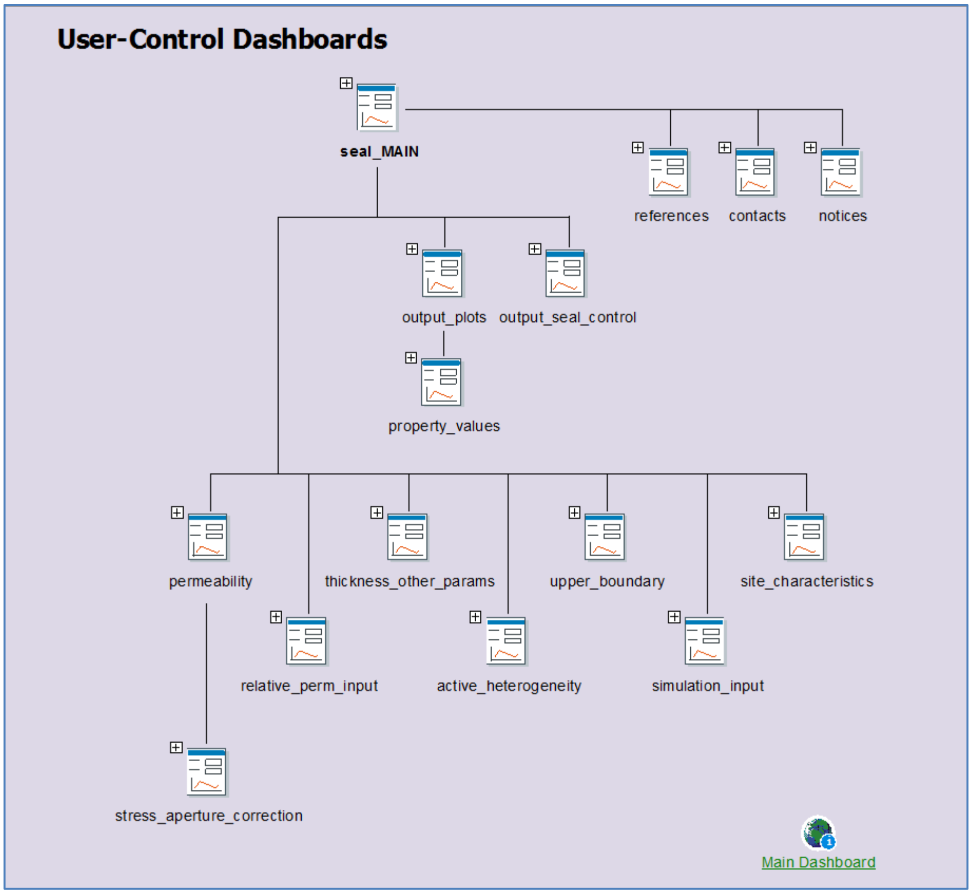



**Figure 4: NSealR structure of Dashboard controls for data input and output.**

Note that use of these Dashboards, however, does not provide all the data required for a simulation and does not check for required input files. Whenever a user-input option is selected in a Dashboard, the user must assure that the corresponding input text file is present in the file structure. Default files in the subdirectories of NSealR are provided for format guidance only and typically do not provide acceptable values for analyses.

### 4.1.2 Main Dashboard

Upon starting NSealR (using the GoldSim Player code), the topmost NSealR Dashboard (General Menu) appears as a window with three columns of buttons along the top (as shown in Figure 5). These buttons will activate the Dashboards discussed earlier. The GoldSim Player window will also appear, which is discussed later in this document.

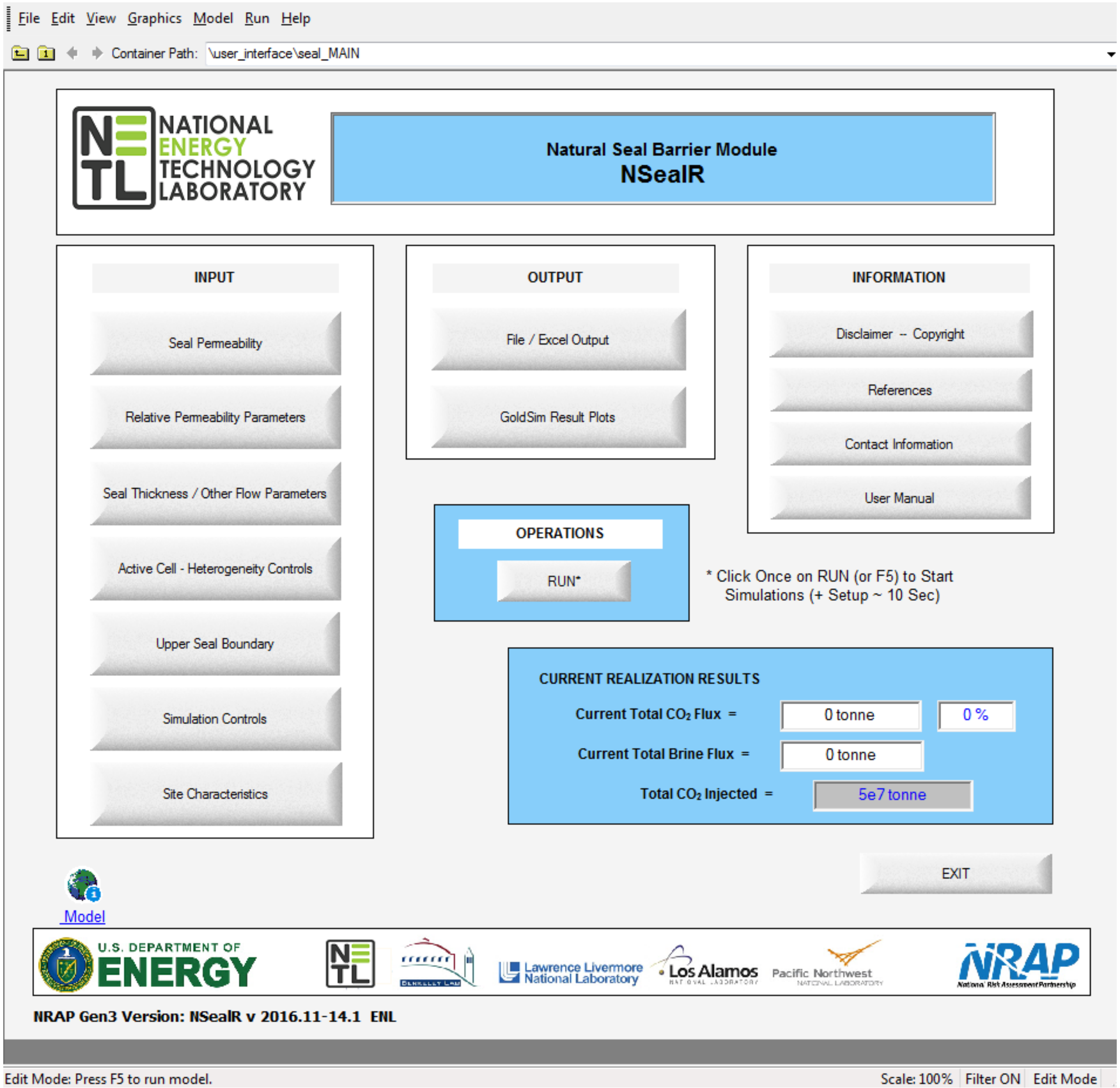



**Figure 5: Main Dashboard of NSealR.** [6]

At the left, is a column of buttons for defining various input properties; at the center are the buttons to access the output controls; and at the right is a column of buttons for information on the code. At the lower center of the Dashboard is the "Run" button for starting a simulation (after input has been defined), and at the bottom left are output boxes providing the current $CO_2$ and

6 This Dashboard has been updated from the one depicted in Lindner (2015) and the input buttons are now placed on the main Dashboard.

brine flux results for the current simulation. At the bottom right is the "Exit" button, which will close the Dashboard and terminate the program.

#### 4.1.3 Input Dashboards

As mentioned, the left column of seven buttons on the Main Dashboard provides access to other Dashboards that define input parameters. For the input column, the top five buttons provide access to Dashboards to define seal-related properties with two additional buttons to define general parameters for the reservoir and the analysis case.

***Seal Permeability***

Selection of the "Seal Permeability" button on the Main Dashboard transfers the user to the Seal Permeability Dashboard (Figure 6). This Dashboard allows the user to select one of the five options for a permeability model, and permits the input of the intrinsic permeability and porosity[7] values for the first four options (as the properties for the fifth model is defined by the user text file). The Dashboard allows definition of the permeability of the seal barrier using one of five options (described earlier):

1. Constant flux
2. User defined constant (intrinsic) permeability and (connected) porosity for each cell
3. Definition of permeability and porosity across the horizon using stochastic distributions
4. User defined equivalent permeability and porosity of each cell using the fractured rock
5. User defined input using a text file describing the permeability of each cell

Different units can be selected for some permeability options. The user can select the permeability-related units in millidarcys (mD) or nanodarcys (ηD) for permeability options (options #2 and #3). The units for fracture aperture can be in either millimeters (mm) or micrometers (µm) for the equivalent permeability defined by fractured rock parameters.

Also, when the *Stochastic Permeability* option is selected, a button labeled "Show" is revealed in the Stochastic Permeability section of the Dashboard. Clicking this button will provide a subwindow with a graphical display of the distribution.

At the bottom of this Dashboard is a check box for the option to adjust the apertures used in the *Fractured Rock Permeability* model. If the user wishes to utilize this correction, checking the option will show a green button ("Go to Stress Correction Parameters").[8] Selecting this button allows the user to access a lower level Dashboard, *stress_aperture_correction* (Figure 7).

Additional information on the Permeability model and options can be found in Appendix A.

[7] Note that porosity is not used in the flow computation in this version of NSealR.

[8] Note that the green button will only appear if the option for "Correct Aperture for In Situ Stress" is checked. Otherwise, this button is hidden.

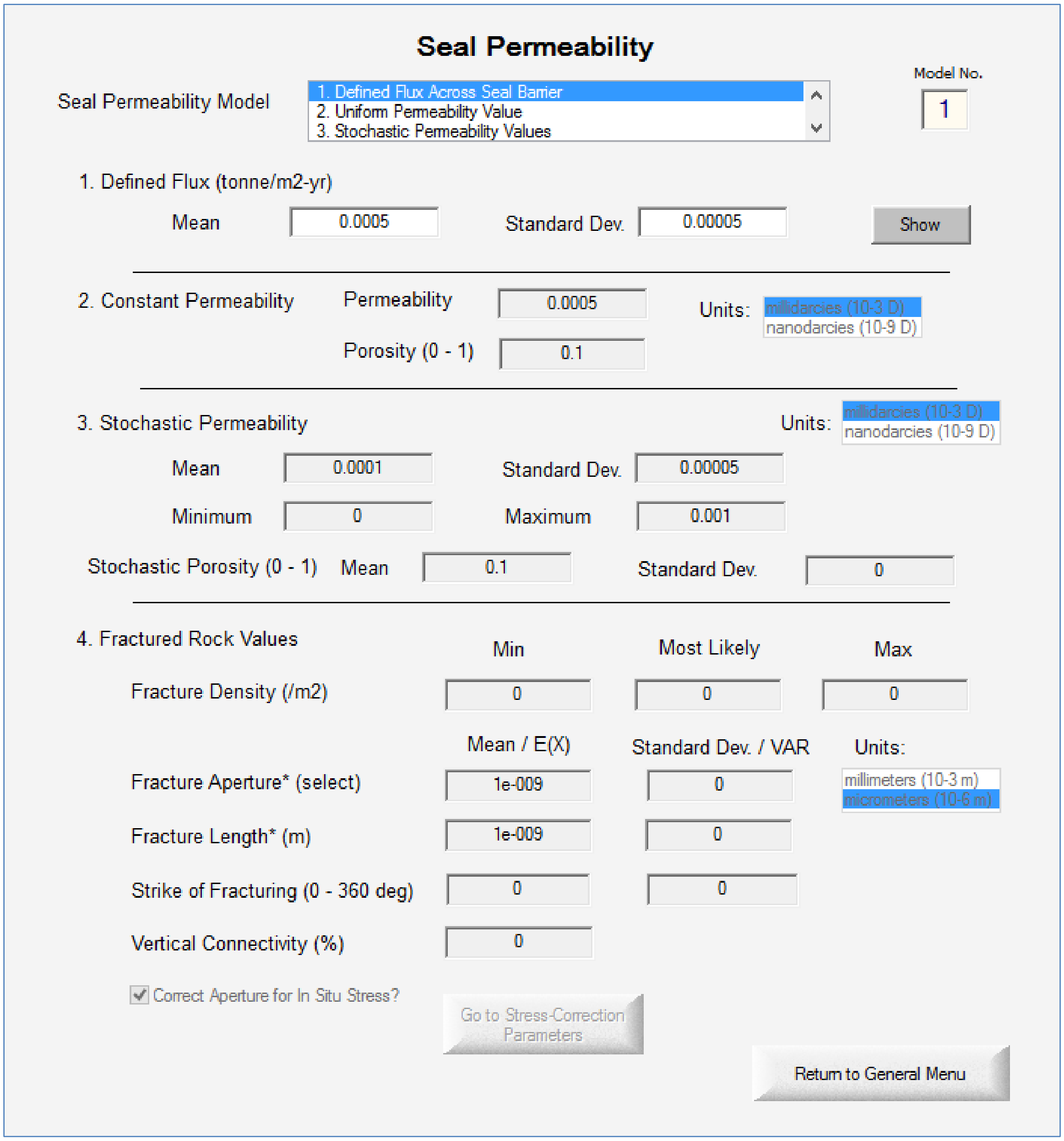



**Figure 6: Seal Permeability Dashboard.**

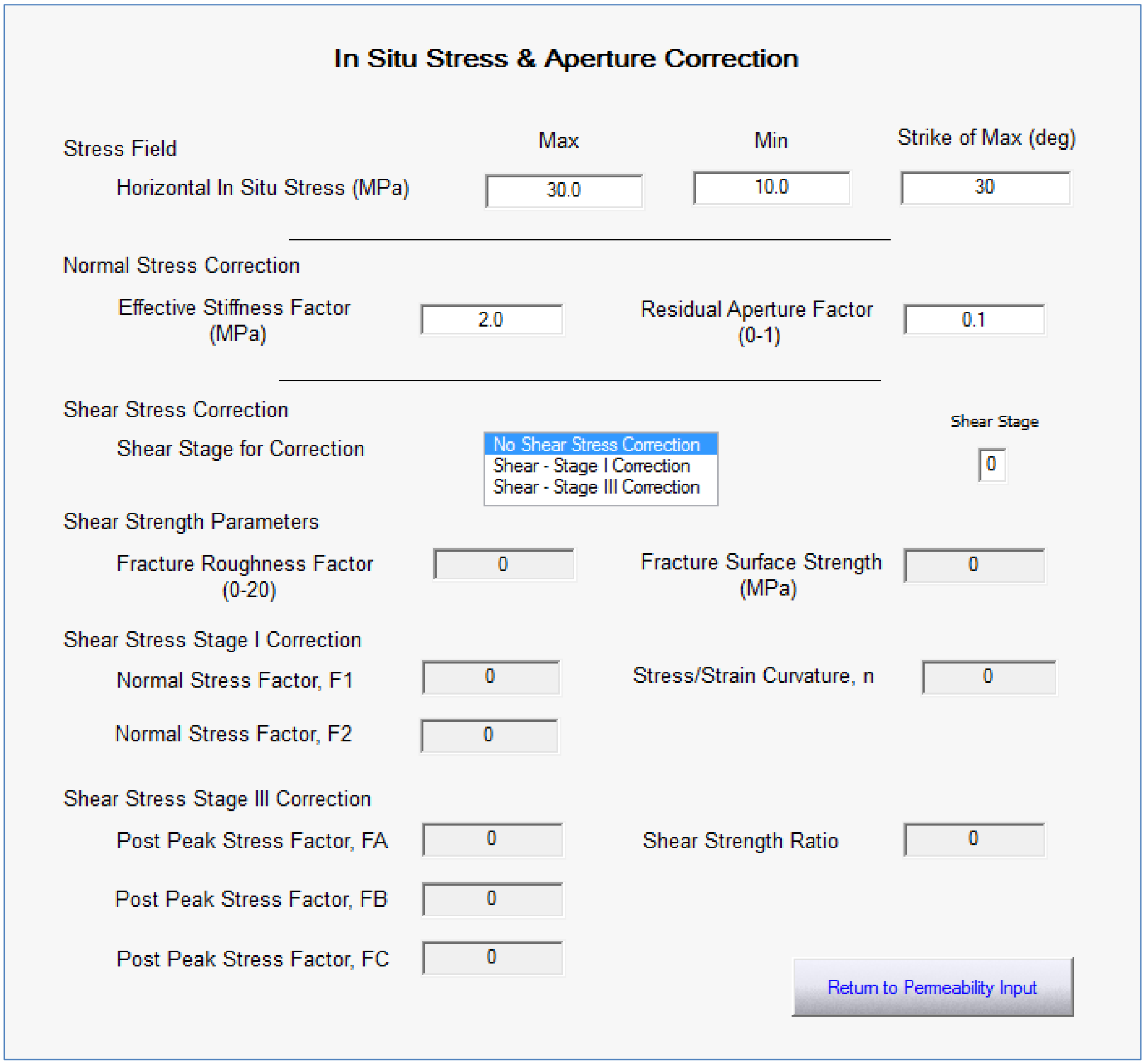
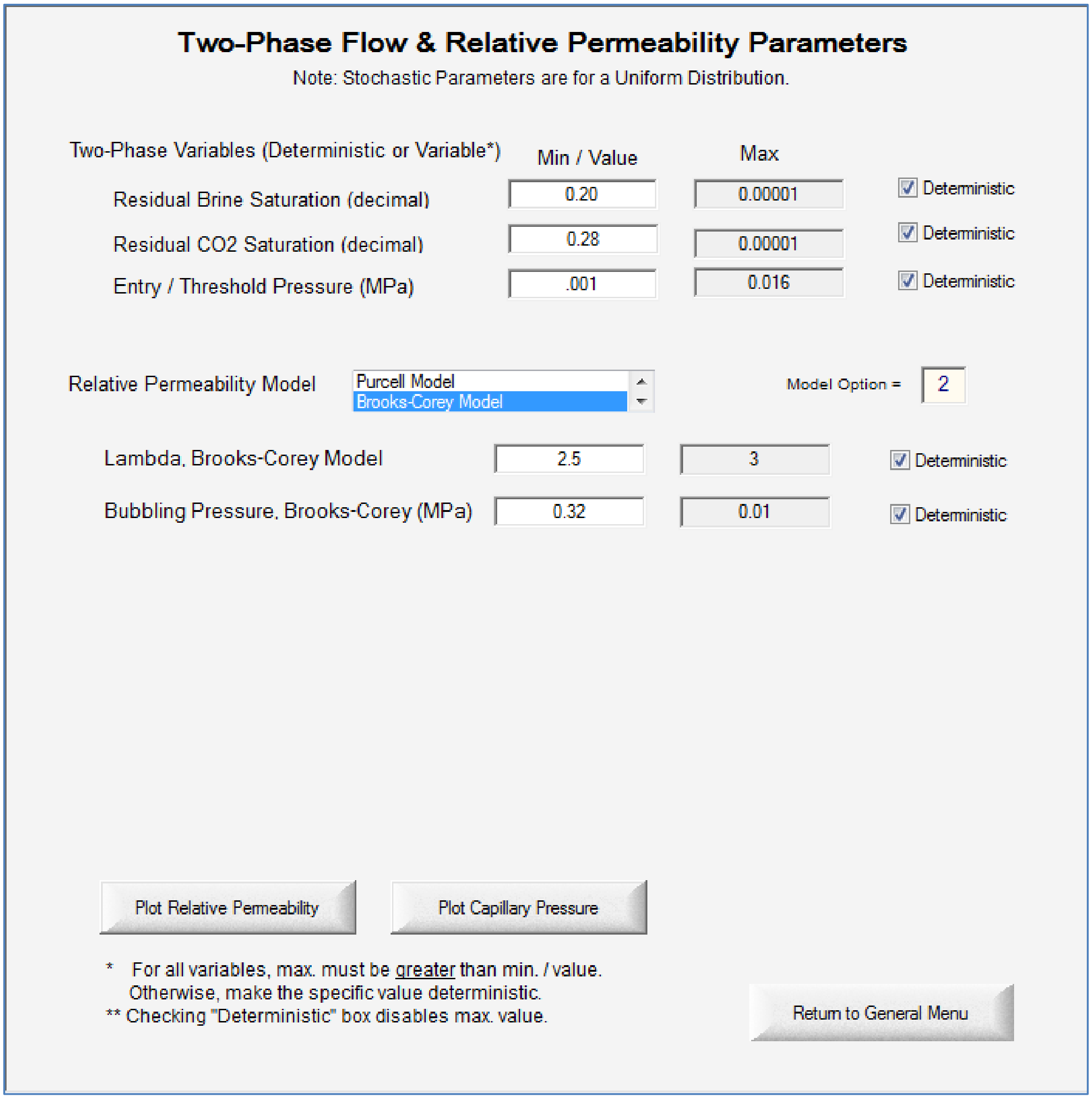



**Figure 7: In Situ Stress & Aperture Correction Dashboard.**

### *Two-Phase Flow and Relative Permeability Parameters*

Returning to the row of buttons on the Main Dashboard, the user can select the "Relative Permeability Parameters" button to obtain the *relative_perm_input* Dashboard for identifying two-phase parameters (Figure 8). This Dashboard inputs relative permeability model parameters and related two-phase variables including the residual brine saturation, the residual $CO_2$ saturation and the entry or threshold pressure for $CO_2$. Referring to relative permeability models, NSealR currently supports the selection of one of four two-phase models: (1) Purcell model, (2) Brooks-Corey model, (3) van Genuchten-Mualem model, and (4) LET General model (See Appendix C). The related parameter values shown on the Dashboard will change with the model selected from the scroll box at the center of the Dashboard. These parameters can be stochastic or deterministic in nature for the first three models, but the LET model only provides for deterministic values for computations.




Note: Two-phase model parameters can be input as a single (deterministic) value or as a variable value (defined by a minimum and a maximum, and computed using a uniform distribution). The checkbox is used to make this selection. Of importance, the maximum must be greater than the minimum in all cases for the variable option. If not, the minimum is selected as a deterministic value.

**Figure 8: Two-Phase Flow and Relative Permeability Parameters Dashboard.**

### *Seal Thickness and Reference Parameters*

The "Seal Thickness / Other Flow Parameters" button on the Main Dashboard selects the *thickness_other_params* Dashboard (Figure 9). This Dashboard allows for definition of the seal thickness model, and other related reference parameters. Four reference parameters are defined here: (1) the salinity of the brine in the seal horizon; (2) the reference brine pressure at a specified depth; (3) the reference pressure elevation (corresponding to the reference brine pressure); and (4) the reference seal temperature. The reference pressure and elevation are used to compute the static conditions at the top of the seal elements.

The seal barrier thickness or height can be defined on this Dashboard as one of three options: (1) constant across the horizon; (2) a stochastically varying barrier thickness across the horizon; and (3) an array of user-defined thickness values, input from an external text file. Input can be entered for the first two options on this Dashboard. Also, for the stochastic height option, once the user has defined parameters for a distribution, a button labeled, "Show" will be revealed. Clicking this button will provide a subwindow with a graphical display of the defined distribution.

The Dashboard also allows for definition of cell temperatures.

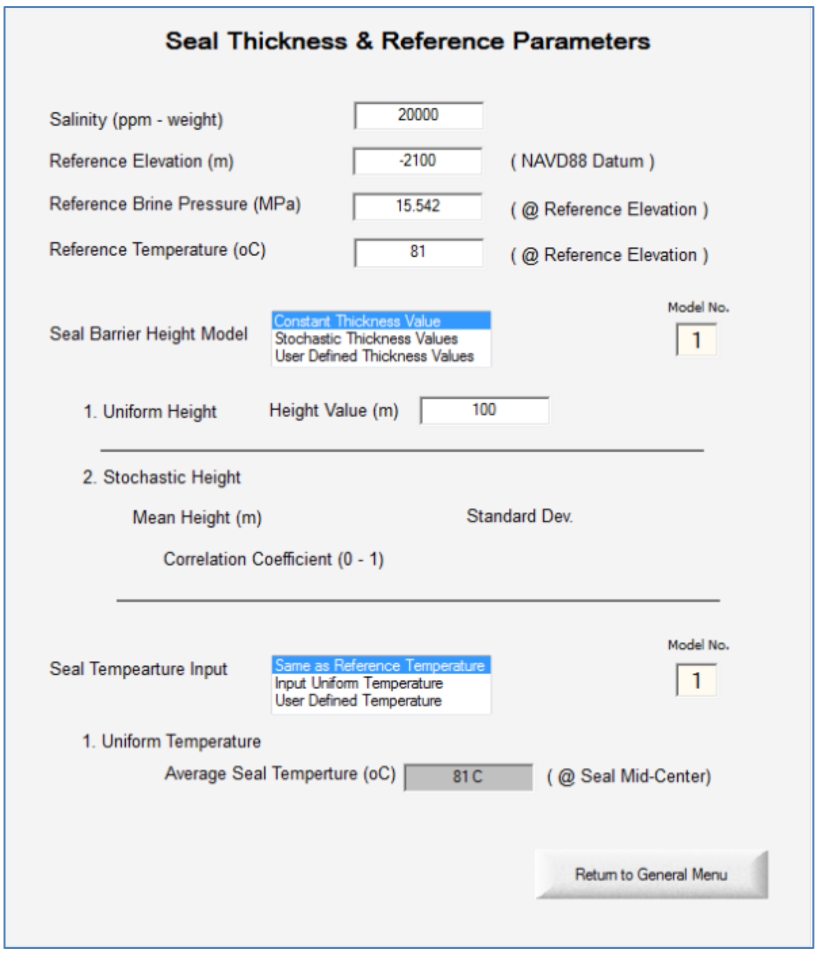



**Figure 9: Seal Thickness & Reference Parameters Dashboard.**

### *Active Cell - Heterogeneity Controls*

The *Active Cell – Heterogeneity Controls* button (Figure 5) provides options to define active cells and includes random zones. The selected Dashboard (Figure 10) allows the user to select an option to define which grid cells are active, i.e., to restrict the flow analysis to a smaller subset of cells. This allows the use of a grid area that is smaller than the full 100 x 100 cell grid as defined in $CO_2$-PENS, with active and inactive cells defined using an external text file. Inactive cells are designated in this file with an input of zero (0.0), and active cells are designated using a one (1.0).[9]

This Dashboard also permits the definition of random zones of permeability across the seal horizon. These zones can act as unknown areas of increased fracturing or the location of unknown wells. The option allows the user to define randomly selected cells with a permeability and porosity using a uniform distribution as defined by user input.

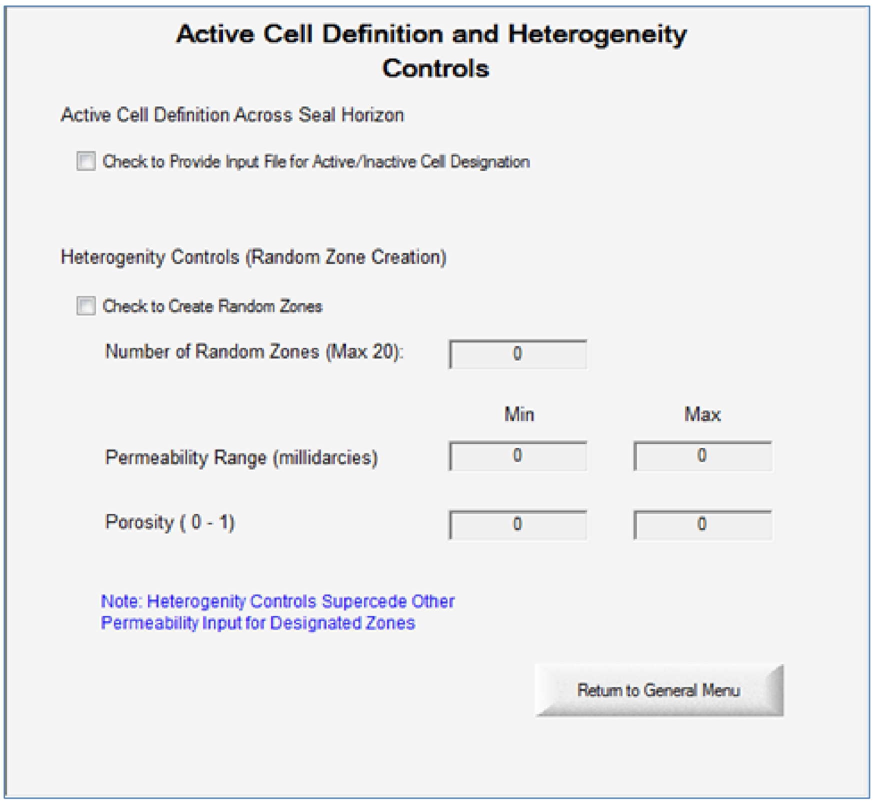



**Figure 10: Active Cell Definition and Heterogeneity Controls Dashboard.**

9 The user may use any positive value to indicate active cells in the input file for the current version of NSealR. However, in the future, higher numeric values may be used to define other variability controls in this text file, so the user is encouraged to use a value of 1.0.

The user inputs the number of zones (up to 20) and the boundary values of permeability. This definition of permeability will override the permeability values defined on the Seal Permeability Dashboard.

### *Upper Seal Boundary*

The last seal-related button on the Main Dashboard is designated as "Upper Seal Boundary". Selecting this button opens the *upper_boundary* Dashboard that defines the pressure/saturation conditions along the top of the seal horizon (Figure 11). Often it is assumed that the pressure conditions at the top of the seal horizon are static, and are computed at the top of the seal from user input (i.e., the static brine pressure is computed from the reference seal pressure and reference pressure elevation defined by the user on the Other Flow Parameters Dashboard). However, in many situations, this is not the case and can distort the computed results, and therefore, NSealR allows the user to more actively define the pressure and saturation conditions.

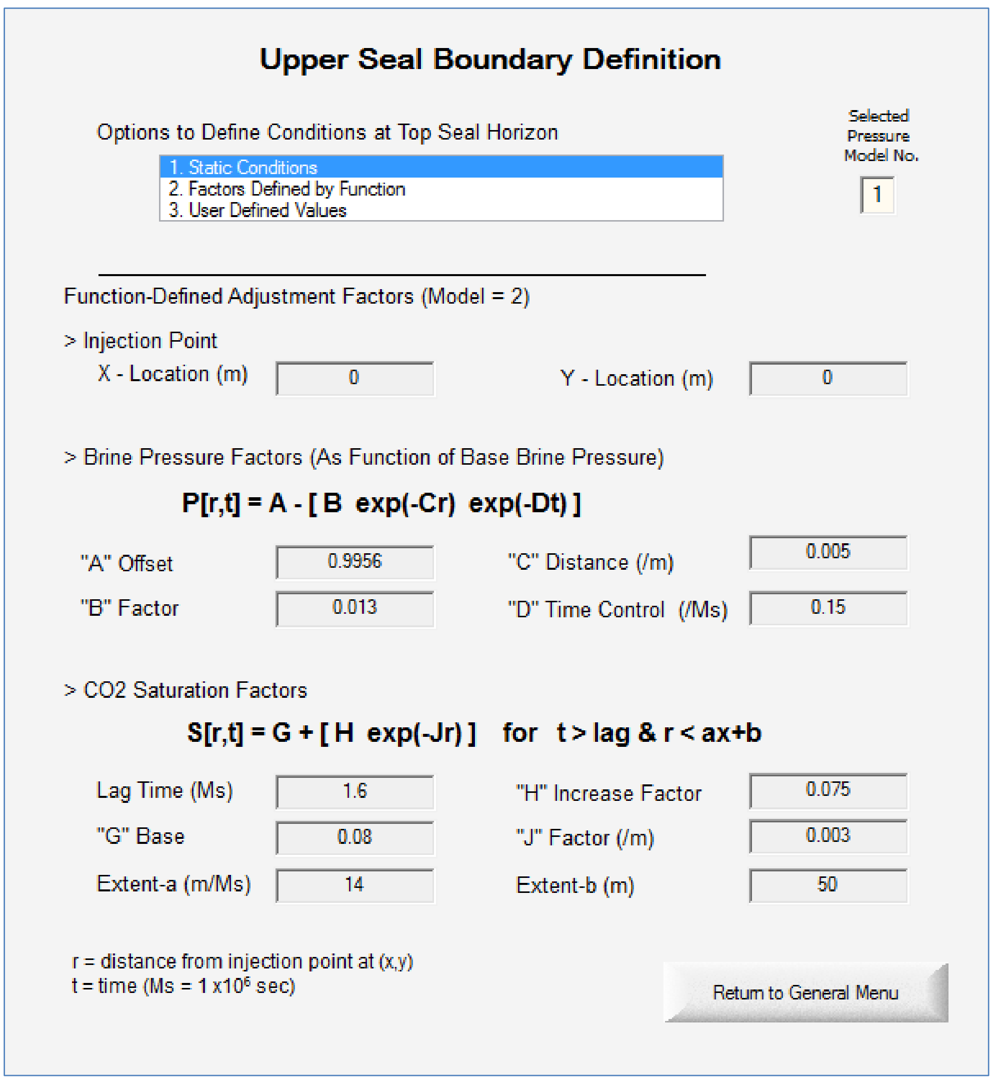



**Figure 11: Upper Seal Boundary Definition Dashboard.**

Three options for defining the upper boundary conditions are currently implemented in NSealR: 1) static conditions, 2) factors defined by function, and 3) user-defined values. The first option is the default option as mentioned, and provides static pressures and zero saturation along the top border. The second option computes the brine pressures and $CO_2$ saturations as functions of the corresponding values at the base of the seal layer. The third option allows the user to input text files with values defining the brine pressure and $CO_2$ saturation at each time step.

***Simulation Controls and Site Characteristics***

The remaining two input buttons access Dashboards to define variables that duplicate those typically set in an IAM. The Simulation Controls Dashboard (Figure 12) defines the coordinates of the model region for a uniform grid between the limits (if not, input files on grid coordinates and areas are required). The Dashboard also contains three variables which are determined internally by NSealR and are fixed for this code version. These variables include the number of grid divisions, the number of time steps, and time value, and are shown in a light font. These values are to be consistent with the NRAP-IAM-CS.

The Site Characteristics Dashboard (Figure 13) is used to define the elevation of the top of the reservoir and the surface elevation of each grid element. The user can select a simple model or employ a text file to define either of the surfaces. For the simple model options (i.e., for a constant elevation), the user is required to input a single value, otherwise a text file must be imported.

## 4.2 INPUT LIMITS

Numeric values entered by the user in all Dashboards are restricted to *reasonable* input values considering the variable in question, and each Dashboard prevents the user from attempting to assign an unreasonable value. For example, a percentage input is restricted to be within 0 to 100%, and values outside this range result in an error message. Other variables are simply limited to be positive values, and any use of negative results in an error message in this case.

Input variables are also restricted by the selection of a specific permeability or thickness model. For example, for each of the permeability options in the code shown in Figure 6, only a subset of the parameters shown on the Dashboard are used in the analysis and can be changed by the user. Upon selection of a specific option, the extraneous variables are shaded and locked, allowing input only to the boxes shown in white.

In more detail, the defined flux model has been selected in Figure 6 (shown in blue), and only the active input boxes for mean and standard deviation for the flux are shown with a white background. The remaining values (which have a darker background) cannot be changed and are not used in the analyses. The same approach applies to the selection of the Seal Barrier Height Model in Figure 9, where a constant height model is selected and the mean and standard deviation values are shaded and unchangeable.

## 4.3 INPUT VARIABLES AND UNITS

Appendix B (Table B1) provides the variables to be defined for the seal barrier, the units for input and the acceptable range of input. The units shown apply to all Dashboard input.

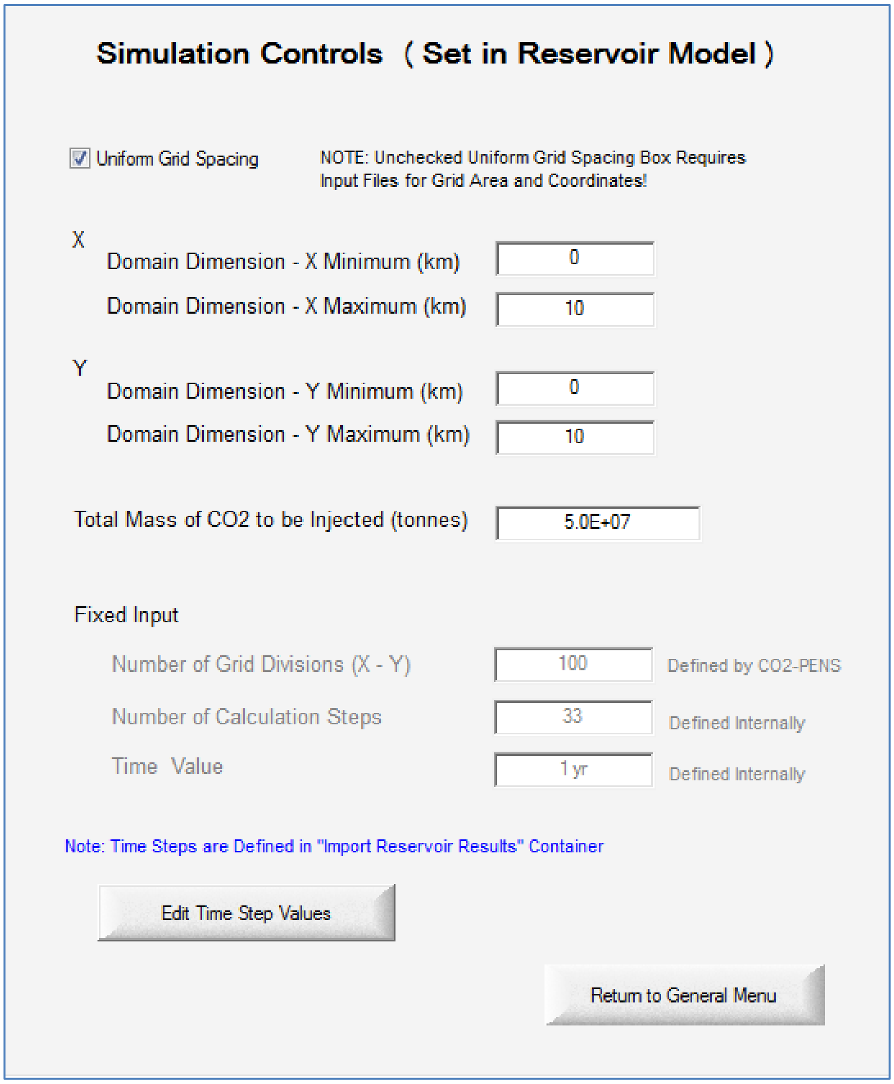
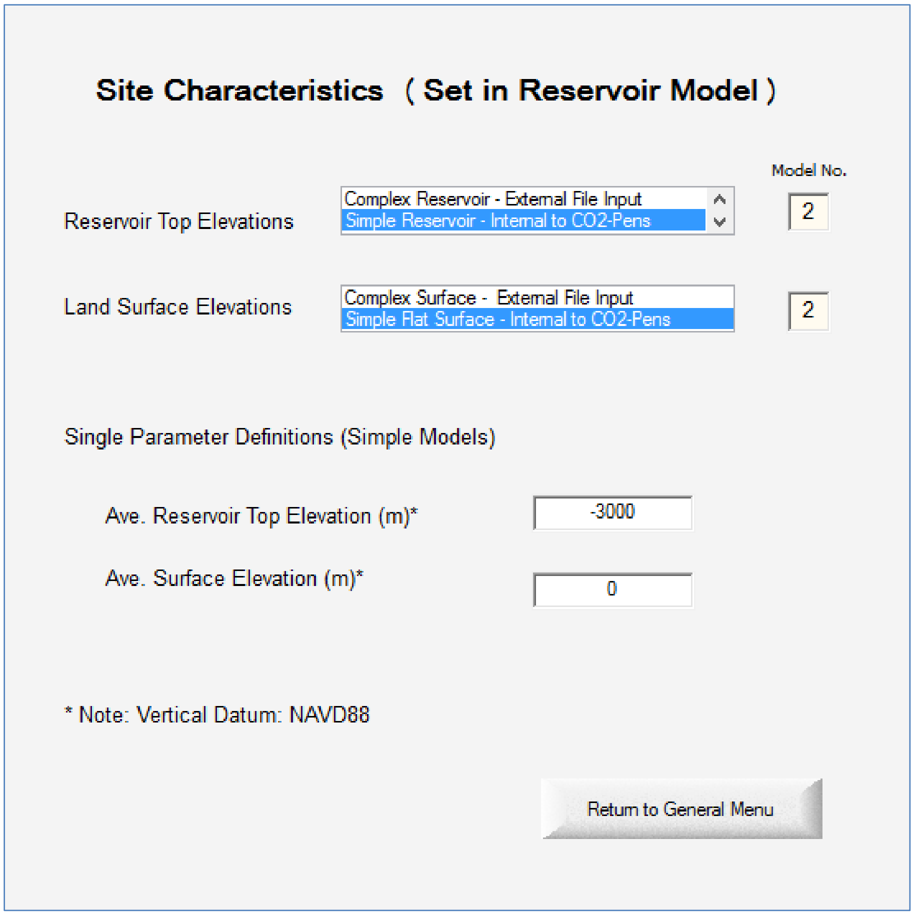



**Figure 12: Simulation Controls Dashboard.**

Note that the data units for input text files typically correspond to these values, but in some cases, the input values differ in magnitude (e.g., the data are in Pa not in MPa), as shown in the Lookup Table elements.

## 4.4 SOFTWARE LOADING AND EXTERNAL FILE INPUT

*The software installation requirements for NSealR development environment are detailed in Lindner (2015), Appendix F. This area also includes run notes for the software. Additionally, Appendix E of the same document includes the input file structure for user-defined input files.*




Note: The blue background with white text in the "Reservoir Top Elevations" and "Land Surface Elevations" options indicate which specific option is selected. The *number* of the selected option is displayed to the right; this numeric value is echoed by the code and cannot be directly changed by user.

**Figure 13: Site Characteristics Dashboard.**

### 4.4.1 Basic Loading Requirements

At a minimum, GoldSim requires a PC with a Windows 2003 Server, Windows XP (SP3), Windows Vista or Windows 7 operating environment. Also required is Microsoft Excel 2003 or later to be installed on the same PC. A disk space of a minimum of 200 MB is required during the installation process, 100 MB of disk space in the target directory for the installation and 40 MB of free space in Common Files folder. A 16-bit color depth is required for the console (32-bit recommended). The NSealR file structure requires an additional approximately 200 MB of disk space, and the size of the results files can be on the order of 100 MB.

### 4.4.2 Input Text Files

For complex cases, where the variable in question differs across the seal horizon in an arbitrary manner, external text files are used to define the property value for each element. The files are imported using lookup table elements in GoldSim, and are referenced as required by the input switches designated by the user on Dashboards (i.e., when the user-defined option is selected). The data structure of the text files for the NSealR is that defined by the GoldSim code, which dictates the inclusion of several header lines followed by the data array (GoldSim, 2014). The data array of 100 x 100 elements is in comma-delimited format, with each line representing a row of data, and each line (row) containing 100 columns.

Example or dummy files for each of the text file inputs are provided in the "\Lookup-Tables" directory[10]. Reservoir related input is located in the "\Lookup_Tables\reservoir" subdirectory, and includes the data files for defining the land surface elevation and the elevations of top surface of the reservoir. Seal barrier-related data files are located in the "\Lookup_Tables\seal" subdirectory for the areas, coordinates, permeability, porosity and thickness of each seal grid element.

The file formats and units are illustrated in more detail in Lindner (2015, Appendix E). Appendix B (Table B1) indicates the type of data provided by each file, when the user option is selected.

#### 4.4.3 Fluid Property Input

To define density, viscosity, and solubility parameter values that are functions of temperature, pressure and/or salinity, dynamic link libraries (DLLs) are used. The DLLs are located in the "\fluid_properties" subdirectory, and the source code incorporating tabular values is provided in a subdirectory. The files are named based on the property (e.g., viscosity for $CO_2$ based on a lookup table approach is from file, *LUT_CO2_viscosity_DLL.dll*).

#### 4.4.4 Input Files from Reservoir Module

For the current version of NSealR, the $CO_2$ pressures and saturations at each time step are provided as a text file, located in directory "\Lookup_Tables\transfer_data." The files are named for the data contained (i.e., the $CO_2$ pressures file is labeled as: *Lookup_reservoir_CO2press.txt*, and the $CO_2$ saturations file is labeled as: *Lookup_reservoir_CO2sat.txt*). The user can change these files for different cases by modifying/replacing the files or by changing the linkage of the lookup table elements in the "\import_reservoir_results" container in NSealR. (These text files are expected to be changed to DLL elements in NSealR when eventually NSealR is incorporated into NRAP-IAM-CS.) Note that data has to be provided for each time step.

Time steps (to allow control for importing reservoir saturation and pressure) are defined in the current version of NSealR in an internal component model, *calculations_steps*. Thirty three time steps are defined to cover 200 years, and these time steps control the required input of pressure and saturation data. However, GoldSim will internally subdivide these time steps for the computation which will increase the total number of time steps for a simulation. To change the time steps, the user must edit the component model data, and will need access to the GoldSim model (not the Player version). The time steps can also be changed by linking the model element to an Excel file.

[10] NSealR assumes a specific directory and file setup together with a specific file format, examples of which are distributed with the code.

# 5. RUNNING NSealR

## 5.1.1 Versions of NSealR

The NSealR tool has been released within the NRAP Phase I Tools Collaborative Workspace on the NETL Energy Data Exchange (EDX). Sign into EDX with an account that belongs to the workspace and download the NSealR tool at: https://edx.netl.doe.gov/organization/nrap-phase-i-tools.

NSealR can be implemented in one of two fashions: 1) using a GoldSim model version, or 2) using a GoldSim Player version. The model version (Version 11.1.6) (with the file extension *.gsm) requires the use of GoldSim commercially-licensed software to conduct simulations. This software will allow the user to modify NSealR computation logic and distributions except for DLLs. The GoldSim license can be obtained through the GoldSim web site at http://www.goldsim.com/Web/Products/ at various costs depending on the type of implementation.

The user can also employ the Player version of the code (Version 11.1.6) (with the file extension *.gsp). The Player version requires the user to download the GoldSim Player software, which is cost free after user registration. The Player code limits the user to implementing NSealR as constructed, but permits the user to examine the logic structure of the code (with the exception of the DLLs). The GoldSim Player can be obtained at http://www.goldsim.com/forms/playerdownload.aspx.

It is also required for the Player version that the relative directory structure, and the file names of input files and of DLLS must be maintained as distributed. The code links can be re-assigned only with the model version of the code and GoldSim. Simply, the Player version assumes the location of the support files are the same as when the Player version was created.

## 5.1.2 Player Version - Run Controller

In using the Player version, at startup a GoldSim Run Controller window will also appear together with the Main Dashboard. The Run Controller is shown in Figure 14 and will run the defined NSealR simulation(s) with the user's input. The NSealR model itself can be examined using this controller by accessing the "Navigation > Go to Model Root …" command under the Menu button.

To start NSealR, the user can depress the "Run" button on the Main Dashboard twice, use the GoldSim Run Controller, or use the shortcut, F5. The shortcut F4 or the "Reset Simulation" button on the GoldSim Run Controller will clear the model for another simulation run.


**Figure 14: GoldSim Run Controller window with annotations.**

# 6. OUTPUT CONTROLS

### 6.1.1 File / Excel Output

The GoldSim model application provides several options for the output of variables including a time history element, and the ability to examine element contents at various stages of the analysis. However, to generate specific snapshots of output for plotting after the completion of the code, several options were constructed specially within NSealR.

Selection of "File / Excel Output" button on the Main Dashboard transfers the user to the *output_seal_control* Dashboard (Figure 15) to access these options. The first control, "Text File Output - Leakage," provides text files of brine and $CO_2$ mass flux at specified time intervals for a specific realization, and written to the "\results\brine" directory and the "\results\CO2" directory, respectively. The "$CO_2$ and Brine Leakage Values to Text" option (if selected) will provide a separate text file of the mass flux for the entire 100 x 100 grid for the defined time step, with the time step number incorporated into the file name.[11]

A similar output can be selected by checking the "Output Excel File" box under the "Excel File Output - Leakage" control on the Dashboard; in this case, results will be exported to an Excel workbook[12], with each time sheet on a single spreadsheet (tab). The output can be found in the directory, "results\combined." However, this is a more time consuming output method during run time and requires data analysis within Microsoft Excel itself, which is limited by the available analysis options.

A final control on the Dashboard, "Text File Output – Input Values" permits the output of specific input data at a specified realization. The user can select three boxes: Output Permeability and Thickness Grid Values to Text file; Output Fluid Properties to Text File; and Output Reference Values to Text File. This allows the user to spot check that the input is indeed what is expected. The output can be found in directory, "results\input."

To track the selection of a specific option, a log file is also provided for each output, which logs the time when a specific file was written, and appends the data to the existing log file, providing a history of use. The log files are located in the "\results" directory.

### 6.1.2 GoldSim Result Plots

Selection of "GoldSim Result Plots" button on the Main Dashboard transfers the user to the *output_plots* Dashboard (Figure 16). This Dashboard implements several GoldSim-based plots of the simulation data. The first set of two buttons on the left side of the Dashboard provides history plots of the $CO_2$ and brine flux at the top of the seal horizon versus simulation time, respectively. Once selected, a graphic window is opened providing a display of the respective data.

[11] The user is cautioned in generating these output text files, as NSealR will replace any existing file from a prior computation. Therefore, the user must manually copy or move output files from the relevant directory at the end of an analysis run, prior to starting another run.

[12] GoldSim projects will not link to Excel workbooks without Microsoft Excel being available on the operating computer system together with GoldSim. Therefore, NSealR will not run without Microsoft Excel.

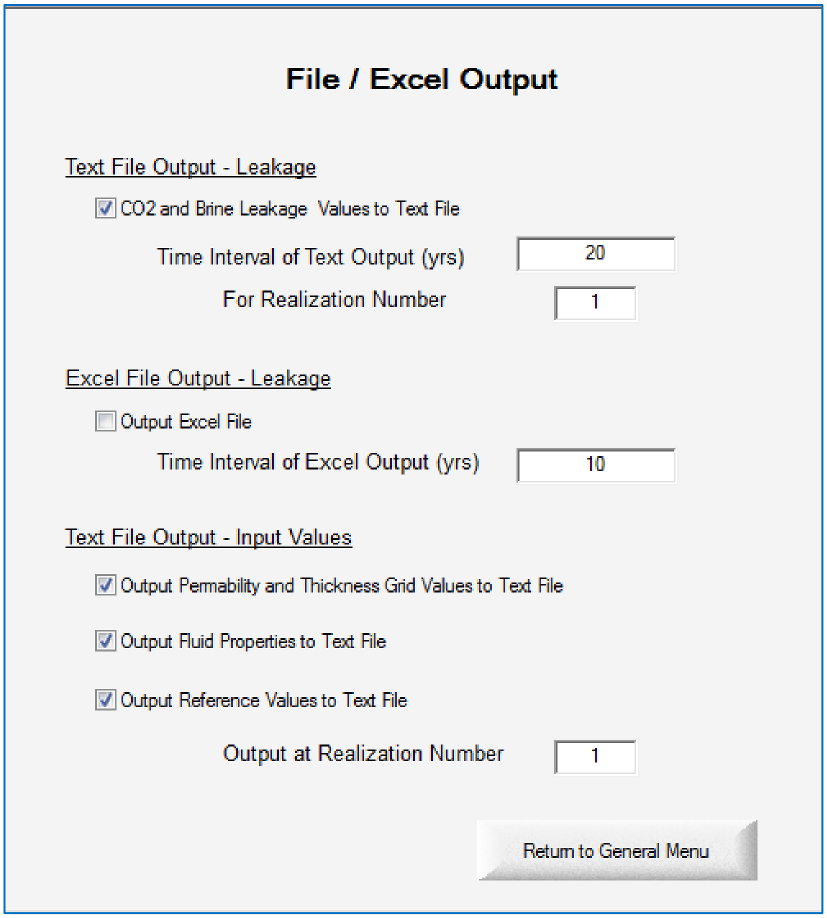



**Figure 15: Output Controls Dashboard.**

The user can modify the display by using the menu at the top of the plot menu, including plotting the current realization, plotting all realizations or showing the data in tabular form. The axes labels can also be modified.

The second set of buttons provide plots of the distribution of the total $CO_2$ and brine flux at the top of the seal horizon at the end of each simulation. Again, once selected, a graphic window is opened providing a display of the respective data, which can be modified by the user.

The last button provides a distribution of the $CO_2$ flux that exceeds the defined Flux Criterion defined in the input box below the button. The box is described as a percentage of the total injected $CO_2$ mass, which is input on the Simulations Control Dashboard. As with other plots, the user can modify the results using the graphic window menu.

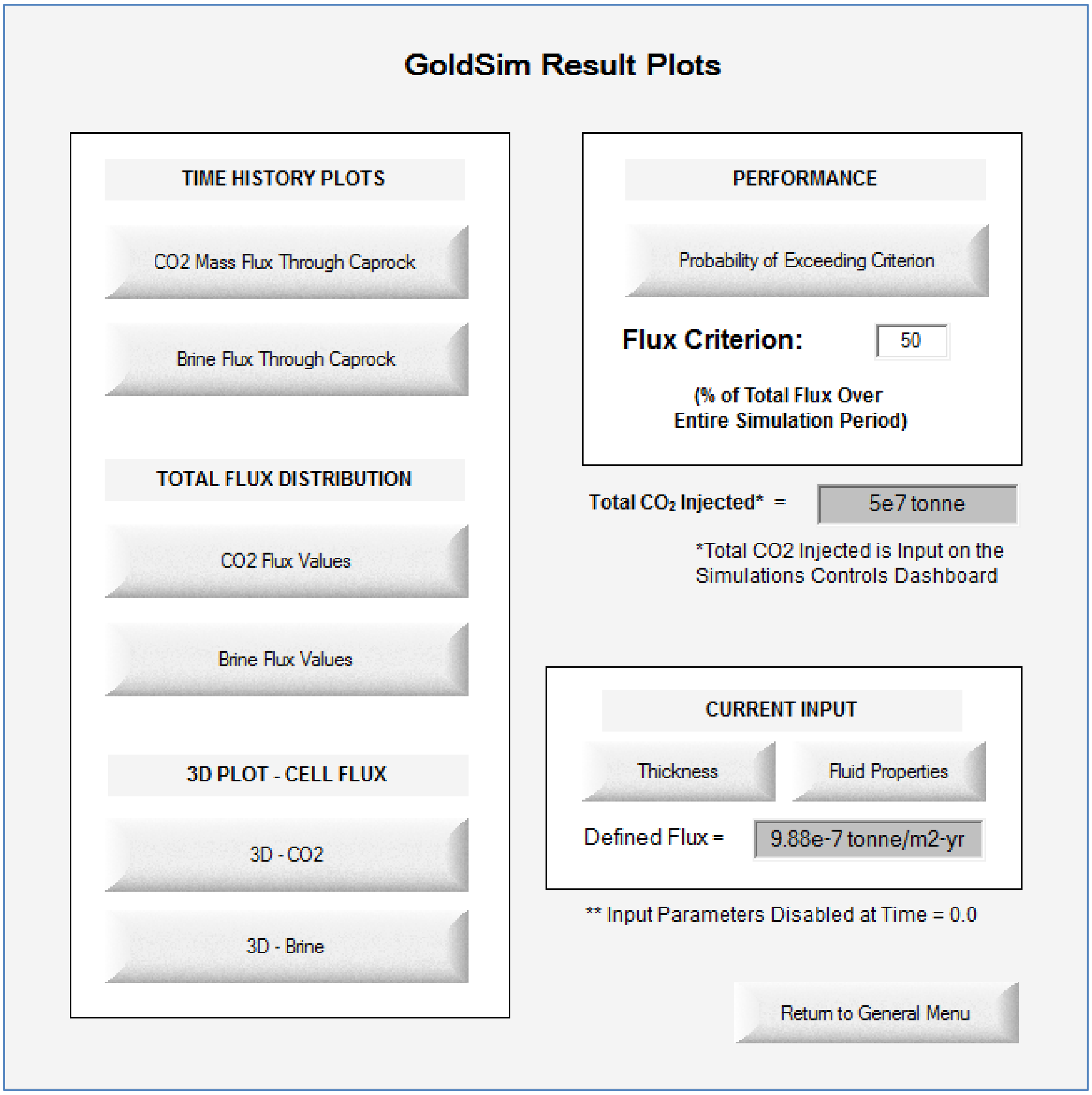



**Figure 16: GoldSim Output Plots Dashboard.**

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# APPENDIX A - PERMEABILITY MODEL/OPTIONS

## A.1 FLOW MODEL OPTIONS

The permeability model in NSealR describes the vertical permeability for each cell that is applied for each realization. If the stochastic option is selected, the permeability value for each cell will vary with each new realization. To estimate the total permeability of each cell, NSealR provides several options for the user. These options attempt to reflect a broad base of knowledge and background in those employing a geologic $CO_2$ storage IAM for varying purposes. The logic of these options was developed with basic GoldSim model elements and does not incorporate any specialized process module of GoldSim (such as the elements specific to the contaminant module). Five permeability-related options are provided in the current version of NSealR:

1. **Constant Flux** - This option was identified in $CO_2$-PENS (Keating et al., 2009) under caprock properties, and essentially bypasses the entire permeability-flow model computation and allows the user to specify a $CO_2$ flux through the seal horizon, selected using a stochastic distribution. This logic has been modified in NSealR to restrict flux to those cells where there is $CO_2$ saturation at the base of the seal horizon, and computes the brine flow as displaced by the $CO_2$ flux. This option allows the user, for example, to examine groundwater-related risk under defined boundary conditions.
2. **User Defined Constant (Intrinsic) Permeability and (Connected) Porosity for each Cell**[13] **-** This simplistic option lends itself to cases where little is known about the seal barrier except in a general fashion. NSealR permits the user to select the input units for permeability for this option (and the next) given the possible wide range of values.
3. **Definition of Permeability and Porosity across the Horizon Using Stochastic Distributions** - Specifically, a limited (truncated) lognormal probability distribution is used for permeability and a (truncated) normal (Gaussian) distribution is employed for porosity. The porosity distribution is truncated to maintain reasonable values for the ratio, i.e., within the range of 0.0 to 1.0. For permeability, the truncated distribution allows the user to specify minimum and maximum limits to explicitly define the full range of the distribution in addition to the mean and standard deviation.
4. **User Defined Equivalent Permeability and Porosity of Each Cell Using the Fractured Rock Parameters** - The model presumes that vertical fractures dominate flow through the seal horizon and that an equivalent permeability can be estimated from fracture aperture, fracture length, and fracture areal density (of fracture centers). The modeling assumptions and equations associated with this option are further described in Lindner (2015).

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[13] NSealR does not currently consider storage (i.e., porosity) in the flow through the seal horizon as fracture flow is assumed to dominate and fractures tend to have little volume, and so in practice, the user can disregard this input term. However, when more-complex models for geochemistry or multi-layer flow are introduced into NSealR, porosity will be become an active parameter and is therefore retained as input parameter in this version.

5. **User Defined Input Using a Text File Describing the Permeability of Each Cell –** This option addresses site specific variability or conditions that cannot be otherwise described by the foregoing options.

## A.2 FLOW MODEL ASSUMPTIONS

Consistent with the concept of $CO_2$ storage in a saline environment, the theoretical flow model developed for NSealR is a two-phase model employing a relationship of relative permeability as a single function of wetting-phase saturation. Currently, the model represents 1-D immiscible flow through a medium consistent with Darcy's law.

The development of the seal barrier theory is based on a number of assumptions on the structure and flow through the seal layer—assumptions made to preserve the simplicity of the code while capturing the more important aspects of flow through a seal horizon. The most significant of those assumptions include: thin seal barrier, two-phase immiscible flow (brine and $CO_2$) with brine as wetting fluid, sufficiently deep seal to maintain $CO_2$ in supercritical state, laminar vertical flow in fractures initially saturated with brine, and relative permeability described using saturation-based models. More detailed description of these theoretical modeling assumptions is provided in Lindner (2015).

Additional assumptions included in NSealR code relate to the anticipated application of this stand-alone tool as a module within a larger integrated assessment model. These assumptions relate to the assumption of independent (decoupled) behavior between different system elements, and the limited spatial resolution that is chosen to reduce the computational burden in modeling full system behavior. Again, more detailed consideration of these modeling assumptions and their implications is provided in Lindner (2015).

## A.3 FLOW MODEL: TWO-PHASE FLOW THEORY

For the vertical two-phase flow through each cell of the seal, the concept of relative permeability is adopted (Bear, 1988), allowing the description of flow of each component to be based on the effective saturation. Additional detailed information on two-phase flow can be found in Lindner (2015).

Four formulations commonly used to describe relative permeability are included in NSealR as user-defined options: 1) Purcell model (based on Purcell, 1949), (2) Brooks-Corey model (Brooks and Corey, 1964), 2) modified van Genuchten-Mualem model (van Genuchten, 1980), and (4) "LET" general model (Lomeland et al., 2005; Be, 2011). Basic theory for these models can be found in Appendix C

## A.4 CELL THICKNESS MODEL AND VARIABILITY

The thickness model in NSealR describes the thickness of the seal barrier for each cell that is applied for each realization. If the stochastic option is selected, the thickness value for each cell will vary with each realization. The thickness model is defined consistent with the concept that the layer is relatively thin (compared to the injection horizon extent and depth) and relatively planar, but may vary laterally in composition and character.

To estimate the thickness of each cell, NSealR provides three options: (1) constant thickness, (2) stochastically-varying thickness, and (3) user-defined thickness; employing a separate text file to describe the thickness of each cell. In considering the geometry of the site, the elevation of each cell is defined by subtracting the thickness of the cell from the elevation of the top of the injection horizon at the cell location to obtain the top elevation of the seal cell.[14] Stochastically generated thicknesses are then smoothed using two consecutive simple spatial averaging algorithms.

## A.5 UPPER BOUNDARY DEFINITION

During initial development, NSealR assumed that the brine pressures at the top boundary of the seal reflect a static pressure condition and that the $CO_2$ saturations along the boundary are zero. However, situations can arise where these assumed boundary assumptions are not a good representation of actual subsurface conditions. It has been noted with trial analyses with other more comprehensive flow codes that the brine pressure can increase significantly over hydrostatic conditions, and that saturations substantially exceed a zero-saturation condition for typical cases of $CO_2$ injection. This can cause issues for the computations, for example, with the higher pressures at the top of the seal, NSealR predictions would overestimate flow rates.

To allow the user to adjust the seal model for more realistic conditions, an option is included in this version of NSealR to adjust the brine pressure and $CO_2$ saturation at the top boundary. By default, the user can utilize the basic assumption of static conditions along the top boundary, or either of two additional options: 1) specific user input, or 2) use of an analytic representation. The first option allows the user to input values of brine pressure and $CO_2$ saturation for each time step. This however, can be a substantial requirement for the user, and a second option, of an analytic representation was created. The analytic representation option is described in more detail in Lindner (2015).

## A.6 PROBABILITY DISTRIBUTIONS

To describe the potential variability of the seal barrier properties, several different distributions are employed within the code, as shown in Table A1. The selection of these distributions is based on the literature and experience with specific data sets. For detailed discussion of distribution type choices, the interested reader is referred to Lindner (2015).

## A.7 FLUID PROPERTIES

The viscosity and solubility of $CO_2$ vary with temperature and pressure, and the density and viscosity of brine vary with salinity as well. Similarly, the solubility of $CO_2$ in brine varies with temperature, pressure, and salinity. These variations are incorporated into NSealR using external elements in GoldSim linked to dynamic link libraries (DLLs) (see Lindner, 2015, Appendix C). Fluid property data were obtained based on recent equation-of-state publications on pure water, saline solutions, and $CO_2$ over a range from atmospheric pressure to 60 MPa, 0 to 180°C, and 0 to 80,000 ppm salinity, a target region that conservatively brackets typical temperature and pressure conditions for carbon storage. More detailed discussion of the source of fluid property data, their application in NSealR, and figures illustrating the variability of these parameters can be found in Lindner (2015).

[14] This differs from the current convention used in the $CO_2$-PENS, which computes the thickness of the seal layer as the difference between the top of the injection horizon and the base of the first overlying aquifer.

**Table A1: Probability distributions used in NSealR**

| Input Parameter | Probability Distribution | Comment |
|---|---|---|
| Areal Density of Fracturing | Triangular | Increased spread of uncertainty |
| Entry/Threshold Pressure | Uniform | |
| Fracture Aperture | Lognormal | |
| Fracture Length | Lognormal | |
| Fracture Strike | Truncated Normal (Gaussian) | Spread truncated at +/- 180° |
| Residual Saturation - Brine | Uniform | High uncertainty in value |
| Residual Saturation - $CO_2$ | Uniform | High uncertainty in value |
| Lambda Factor (Brooks-Corey Model) | Uniform | High uncertainty in value |
| Bubbling Pressure (Brooks-Corey Model) | Uniform | High uncertainty in value |
| "m" Factor (Modified van Genuchten-Mualem Model) | Uniform | High uncertainty in value |
| Alpha-Prime (Modified van Genuchten-Mualem Model) | Uniform | High uncertainty in value |
| Beta (Modified van Genuchten-Mualem Model) | Uniform | High uncertainty in value |
| Gamma (Modified van Genuchten-Mualem Model) | Uniform | High uncertainty in value |
| Stochastic Permeability | Truncated Lognormal | |
| Stochastic Porosity[a] | Truncated Normal | Minimum (0.0) and maximum (1.0) are defined within NSealR |
| Seal Barrier Height/Thickness | Truncated Normal | Minimum (0 m) and maximum (1,000 m) are defined within NSealR. Adjusted with correlation factor to smooth distribution |

a. Although porosity is included in this table, the storage term (i.e., porosity) is not included in the flow model used in the current version of NSealR. However, porosity is expected to be incorporated in the next version of NSealR and therefore, included to minimize future changes to the interface.

## APPENDIX B - INPUT VARIABLES TABLES FOR NSealR

**Table B1: Input Variables for NSealR**

| Input Parameter | Units | Default Value | Range | Input Source (Comment) |
|---|---|---|---|---|
| ***Seal Permeability Parameters (Dashboard: permeability)*** | | | | |
| Seal Permeability Model | --- | 2 | 1, 2, 3, 4, 5 | 1 = Uniform Flux Through Seal Barrier<br>2 = Uniform Permeability<br>3 = Stochastic Permeability<br>4 = Fractured Rock Permeability<br>5 = User Defined Permeability<br>External File Names:<br>*Lookup_seal_perm.txt*<br>*Lookup_seal_porosity.txt* |
| Constant Flux | tonne/ ($m^2$-yr) | 0 | > 0 | (Active only with Option = 1 for Seal Permeability Model) |
| Constant Permeability | mD (or) ηD[15] | 3.0 E-3 | 0 to 1.0 E+6 | (Active only with Option = 2 for Seal Permeability Model) |
| Constant Porosity[b] | --- | 0.1 | 0 to 0.9 | (Active only with Option = 2 for Seal Permeability Model) |
| Stochastic Permeability – Mean | mD (or) ηD | 3.0 E-3 | 0 to 1.0 E+6 | (Active only with Option = 3 for Seal Permeability Model) Units selected by user |
| Stochastic Permeability - Standard Deviation | mD (or) ηD | 1.0 E-3 | 0 to 1.0 E+6 | (Active only with Option = 3 for Seal Permeability Model) Units selected by user |
| Stochastic Permeability - Minimum | mD (or) ηD | 0.0 | 0 to 1.0 E+6 | (Active only with Option = 3 for Seal Permeability Model) Units selected by user |
| Stochastic Permeability - Maximum | mD (or) ηD | 1.0 E+3 | 0 to 1.0 E+6 | (Active only with Option = 3 for Seal Permeability Model) Units selected by user |
| Stochastic Porosity - Mean[b] | --- | 0.1 | 0 to 0.9 | (Active only with Option = 3 for Seal Permeability Model) |

[15] The abbreviation for millidarcys in GoldSim is "md", whereas this guide uses the more common abbreviation, "mD".

**Table B1: Input Variables for NSealR**

| Input Parameter | Units | Default Value | Range | Input Source (Comment) |
|---|---|---|---|---|
| Stochastic Porosity - Standard Deviation[b] | --- | 0.05 | 0 to 0.9 | (Active only with Option = 3 for Seal Permeability Model) |
| Fracture Density - Minimum | $/m^2$ | 0.1 | ≥ 0 | (Active only with Option = 4 for Seal Permeability Model) |
| Fracture Density - Most Likely | $/m^2$ | 0.1 | ≥ 0 | (Active only with Option = 4 for Seal Permeability Model) |
| Fracture Center Density - Maximum | $/m^2$ | 0.1 | ≥ 0 | (Active only with Option = 4 for Seal Permeability Model) |
| Fracture Aperture - Mean | mm (or) µm | 1.0 | ≥ 0 | (Active only with Option = 4 for Seal Permeability Model) |
| Fracture Aperture - Standard Deviation | mm (or) µm | 0.1 | ≥ 0 | (Active only with Option = 4 for Seal Permeability Model) |
| Strike of Fracturing - Mean | ° degrees (from North) | 0 | 0 to 360° | (Active only with Option = 4 for Seal Permeability Model) |
| Strike of Fracturing - Standard Deviation | ° | 0 | 0 to 180° | (Active only with Option = 4 for Seal Permeability Model) |
| Fracture Length - Mean | m | 1.0 | > 0 | (Active only with Option = 4 for Seal Permeability Model) |
| Fracture Length - Standard Deviation | m | 0.1 | > 0 | (Active only with Option = 4 for Seal Permeability Model) |
| Vertical Connectivity | % | 100 | 0 to 100 | (Active only with Option = 4 for Seal Permeability Model) |
| Option to Correct Aperture for In Situ Stress | --- | Un-Checked | Checked/ Unchecked | (Checking this option will provide access stress-correction parameters and definition of in situ stress) |
| ***In Situ Stress & Aperture Correction (Dashboard: stress_aperture_correction)*** ***(Dashboard is only shown if Aperture Correction Option box on Seal Permeability Parameters Dashboard is checked. Parameters on Dashboard are only used with Option = 4 for Seal Permeability Model)*** | | | | |
| Horizontal Stress - Maximum | MPa | 0 | 0 to 1,000 | (Active only with for aperture correction) |
| Horizontal Stress - Minimum | MPa | 0 | 0 to 1,000 | (Active only with for aperture correction) |
| Strike of Maximum Horizontal Stress | degrees (from North) | 30° | 0 to 360° | (Strike is clockwise angle from North)<br>(Active only with for aperture) |

**Table B1: Input Variables for NSealR**

| Input Parameter | Units | Default Value | Range | Input Source (Comment) |
|---|---|---|---|---|
| Effective Stiffness Factor | MPa | 0.2 | ≥ 0.0001 | (Active only with aperture correction for in situ stress) |
| Residual Aperture Factor | --- | 0.1 | 0 to 0.9 | (Active only with aperture correction for in situ stress) |
| Shear Stress Correction Option | --- | 0 | 0, 1, 3 | 0 = No Shear Stress Correction<br>1 = Stage I (Pre-Peak)Shear Stress Correction<br>3 = Stage III (Post-Peak)Shear Stress Correction |
| Shear Strength – Fracture Roughness Factor | --- | 5 | 0 to 20 | (Equivalent to Joint Roughness Coefficient [Barton, 1973]))<br>(Active only with aperture shear stress correction option = 1 or 3) |
| Shear Strength – Fracture Surface Strength | MPa | 100 | 0 to 1,000 | (Active only with aperture shear stress correction option = 1 or 3) |
| Shear Stress – Stage I Correction, Normal Stress Factor, F1 | --- | 0 | 0 to 1,000 | (Active only with aperture shear stress correction option = 1) |
| Shear Stress – Stage I Correction, Normal Stress Factor, F2 | --- | 0 | 0 to 1,000 | (Active only with aperture shear stress correction option = 1) |
| Shear Stress – Stage I Correction, Stress/Strain Curvature, n | --- | 0 | 0 to 1 | (Active only with aperture shear stress correction option = 1) |
| Shear Stress – Stage III Correction, Normal Stress Factor, FA | --- | 0 | 0 to 1,000 | (Active only with aperture shear stress correction option = 3) |
| Shear Stress – Stage III Correction, Normal Stress Factor, FB | --- | 0 | 0 to 1,000 | (Active only with aperture shear stress correction option = 3) |
| Shear Stress – Stage III Correction, Normal Stress Factor, FC | --- | 0 | 0 to 1,000 | (Active only with aperture shear stress correction option = 3) |
| Shear Strength Ratio (Ratio of Residual Shear Strength to Peak Shear Strength at Very Low Normal Stress) | --- | 0.5 | 0 to 1,000 | (Active only with aperture shear stress correction option = 3) |

**Table B1: Input Variables for NSealR**

| Input Parameter | Units | Default Value | Range | Input Source (Comment) |
|---|---|---|---|---|
| ***Other Flow Properties (Dashboard: relative-perm_input)*** | | | | |
| Salinity | ppm | 0 | to 80,000 | (By weight (e.g., mg/kg); range reflects target conditions for storage per Section 2.5) |
| Average Seal Temperature | °C | 35° | 10 to 180° | (Range reflects target conditions for storage) |
| Reference Brine Pressure | MPa | 9.80665 | 0.1014 to 60 | (Default is the fluid pressure at 1 km depth below the phreatic surface, assuming a groundwater density of 1000 kg/m$^3$ and standard gravity; the minimum is standard atmospheric pressure, rounded up to the 4 decimal places) |
| Reference Brine Pressure Elevation | m, NAVD 88 | -1,000 | -10,000 to -100 | (Elevation for Reference Brine Pressure) |
| Residual Brine Saturation - Minimum | --- decimal | 0 | 0 to 0.5 | (If deterministic option selected, this is value used) |
| Residual Brine Saturation - Maximum | --- decimal | 0 | 0 to 0.5 | (If variable option selected, value must be greater than minimum) |
| Residual Brine Saturation - Deterministic | --- | Un-Checked | Checked/ Unchecked | (Checking this option will hide maximum value and use minimum value without variation) |
| Residual $CO_2$ Saturation - Minimum | --- decimal | 0 | 0 to 0.5 | (If deterministic option selected, this is value used) |
| Residual $CO_2$ Saturation - Maximum | --- decimal | 0 | 0 to 0.5 | (If variable option selected, value must be greater than minimum) |
| Residual $CO_2$ Saturation - Deterministic | --- | Un-Checked | Checked/ Unchecked | (Checking this option will hide maximum value and use minimum value without variation) |
| Entry/Threshold Pressure - Minimum | MPa | 0.010 | ≥ 0 | (If deterministic option selected, this is value used) |
| Entry/Threshold Pressure - Maximum | MPa | 0.015 | ≥ 0 | (If variable option selected, value must be greater than minimum) |

**Table B1: Input Variables for NSealR**

| Input Parameter | Units | Default Value | Range | Input Source (Comment) |
|---|---|---|---|---|
| Entry/Threshold Pressure | --- | Un-Checked | Checked/ Unchecked | (Checking this option will hide maximum value and use minimum value without variation) |
| Relative Permeability Model | --- | 1 | 1, 2 | Models:<br>1 = Purcell Model<br>2 = Brooks-Corey Model<br>3 = Modified van Genuchten-Mualem Model<br>4 = LET General Model |
| Lambda Factor, Purcell - Minimum | --- | 2 | ≥ 0.01 | (Active only with relative permeability model #1)<br>(If deterministic option selected, this is value used) |
| Lambda Factor, Purcell - Maximum | --- | 3 | ≥ 0.01 | (Active only with relative permeability model #1)<br>(If variable option selected, value must be greater than minimum) |
| Lambda Factor, Purcell - Deterministic | --- | Un -Checked | Checked/ Unchecked | (Active only with relative permeability model #1)<br>(Checking this option will hide maximum value and use minimum value without variation) |
| Lambda Factor, Brooks-Corey - Minimum | --- | 2 | ≥ 0.01 | (Active only with relative permeability model #2)<br>(If deterministic option selected, this is value used) |
| Lambda Factor, Brooks-Corey - Maximum | --- | 3 | ≥ 0.01 | (Active only with relative permeability model #2)<br>(If variable option selected, value must be greater than minimum) |
| Lambda Factor, Brooks-Corey - Deterministic | --- | Un -Checked | Checked/ Unchecked | (Active only with relative permeability model #2)<br>(Checking this option will hide maximum value and use minimum value without variation) |

**Table B1: Input Variables for NSealR**

| Input Parameter | Units | Default Value | Range | Input Source (Comment) |
|---|---|---|---|---|
| Bubbling Pressure, Brooks-Corey - Minimum | MPa | 0.01 | >= 0 | (Must be less than the Entry Pressure)<br>(Active only with relative permeability model #2)<br>(If deterministic option selected, this is value used) |
| Bubbling Pressure, Brooks-Corey - Maximum | MPa | 0.015 | >= 0 | (Must be less than the Entry Pressure)<br>(Active only with relative permeability model #2)<br>(If variable option selected, value must be greater than minimum) |
| Bubbling, Brooks-Corey - Deterministic | --- | Un-Checked | Checked/ Unchecked | (Active only with relative permeability model #2)<br>(Checking this option will hide maximum value and use minimum value without variation) |
| m Factor, Van Genuchten-Mualem - Minimum | --- | 0.9 | 0.0 to 1.0 | (Active only with relative permeability model #3)<br>(If deterministic option selected, this is value used) |
| m Factor, Van Genuchten-Mualem - Maximum | --- | 0.91 | 0.0 to 1.0 | (Active only with relative permeability model #3)<br>(If variable option selected, value must be greater than minimum) |
| m Factor, Van Genuchten-Mualem - Deterministic | --- | Un-Checked | Checked/ Unchecked | (Active only with relative permeability model #3)<br>(Checking this option will hide maximum value and use minimum value without variation) |
| Alpha', Van Genuchten-Mualem - Minimum | 1/Pa | 2.0 E-5 | ≥ 0 | (Active only with relative permeability model #3)<br>(If deterministic option selected, this is value used) |

**Table B1: Input Variables for NSealR**

| Input Parameter | Units | Default Value | Range | Input Source (Comment) |
|---|---|---|---|---|
| Alpha', Van Genuchten-Mualem - Maximum | 1/Pa | 2.1 E-5 | ≥ 0 | (Active only with relative permeability model #3)<br>(If variable option selected, value must be greater than minimum) |
| Alpha', Van Genuchten--Mualem Deterministic | --- | Un-Checked | Checked/ Unchecked | (Active only with relative permeability model #3)<br>(If deterministic option selected, this is value used) |
| Beta, Van Genuchten-Mualem - Minimum | --- | 0.5 | ≥ 0 | (Active only with relative permeability model #3)<br>(If variable option selected, value must be greater than minimum) |
| Beta, Van Genuchten-Mualem - Maximum | --- | 0.55 | ≥ 0 | (Active only with relative permeability model #3)<br>(Checking this option will hide maximum value and use minimum value without variation) |
| Beta, Van Genuchten-Mualem - Deterministic | --- | Un-Checked | Checked/ Unchecked | (Active only with relative permeability model #3)<br>(If deterministic option selected, this is value used) |
| Gamma, Van Genuchten-Mualem - Minimum | --- | 0.3333 | ≥ 0.01 | (Active only with relative permeability model #3)<br>(If deterministic option selected, this is value used) |
| Gamma Factor, Van Genuchten-Mualem - Maximum | --- | 0.40 | ≥ 0.01 | (Active only with relative permeability model #3)<br>(If variable option selected, value must be greater than minimum) |
| Gamma, Van Genuchten-Mualem - Deterministic | --- | Un-Checked | Checked/ Unchecked | (Active only with relative permeability model #3)<br>(Checking this option will hide maximum value and use minimum value without variation) |
| L – Wetting Parameter | --- | 1.0 | ≥ 0 | (Active only with relative permeability model #4) |

**Table B1: Input Variables for NSealR**

| Input Parameter | Units | Default Value | Range | Input Source (Comment) |
|---|---|---|---|---|
| E – Wetting Parameter | --- | 10.0 | ≥ 0 | (Active only with relative permeability model #4) |
| T – Wetting Parameter | --- | 1.25 | ≥ 0 | (Active only with relative permeability model #4) |
| L – Nonwetting Parameter | --- | 1.05 | ≥ 0 | (Active only with relative permeability model #4) |
| E – Nonwetting Parameter | --- | 10.0 | ≥ 0 | (Active only with relative permeability model #4) |
| T – Nonwetting Parameter | --- | 1.25 | ≥ 0 | (Active only with relative permeability model #4) |
| Ratio of Nonwetting to Wetting Permeability | --- | 0.6 | 0.0 to 1.0 | (Active only with relative permeability model #4) |
| "A" Exponent for Capillary Pressure | --- | 0.5 | ≥ 0 | (Active only with relative permeability model #4) |
| ***Seal Thickness (Dashboard: thickness_other_params)*** | | | | |
| Seal Barrier Height Options | --- | 1 | 1, 2, 3 | Options:<br>1 = Constant Height for Seal Barrier<br>2 = Stochastic Height of Seal Barrier<br>3 = User Defined Variation of Seal Barrier - External File Input<br>External File Name: Lookup_seal_thick.txt |
| Constant Height | m | 20 | 0.1 to 1,000 | (Active only with Option = 1 for Seal Barrier Height Model) |
| Stochastic Height - Mean | m | 30 | 0.1 to 1,000 | (Active only with Option = 2 for Seal Barrier Height Model) |
| Stochastic Height - Standard Deviation | m | 0 | 0 to 1,000 | (Active only with Option = 2 for Seal Barrier Height Model) |
| Thickness Correlation Factor | --- | 1 | 0 to 1 | (Factor controls the correlation of each stochastic cell value with adjacent neighbors, with 1.0 = total correlation, 0 = no correlation) |

**Table B1: Input Variables for NSealR**

| Input Parameter | Units | Default Value | Range | Input Source (Comment) |
|---|---|---|---|---|
| ***Active Cell Definition and Heterogeneity Controls (Dashboard: active_heterogeneity)*** | | | | |
| Provide Input File for Active/Inactive Cell Designation | --- | Un- Checked | Checked/ Unchecked | Checked option requires input of active cell designation for entire grid<br>External File Name: Lookup_seal_active.txt |
| Create Random Zones | --- | Un- Checked | Checked/ Unchecked | |
| Number of Random Zones | --- | 0 | 0 to 20 | (Active only with create random zones option is checked) |
| Stochastic Permeability - Minimum | mD | 3.0 E-3 | 0 to 1.0 E+6 | (Active only with create random zones option is checked) |
| Stochastic Permeability - Maximum | mD | 3.0 E-3 | 0 to 1.0 E+6 | (Active only with create random zones option is checked) |
| Stochastic Porosity - Minimum[b] | --- | 0.1 | 0 to 0.9 | (Active only with create random zones option is checked) |
| Stochastic Porosity - Maximum[b] | --- | 0.1 | 0 to 0.9 | (Active only with create random zones option is checked) |
| ***Upper Seal Boundary Definition (Dashboard: simulation_input)*** | | | | |
| Options to Define Conditions at Top of Seal Horizon | --- | 1 | 1, 2, 3 | Option:<br>1 = Static Conditions<br>2 = Define Using Analytic Functions<br>3 = User Defined Values<br>External File Names:<br>Lookup_seal_top_ press.txt<br>Lookup_seal_top_ sat.txt |
| Injection Point, X Coordinate | m | 0 | ≥ 0 | (Active only with Option = 2 for Conditions at Top of Seal Horizon) |
| Injection Point, Y Coordinate | m | 0 | ≥ 0 | (Active only with Option = 2 for Conditions at Top of Seal Horizon) |
| Brine Pressure Factor, A | --- | 0.9956 | 0.0 to 1.0 | (Active only with Option = 2 for Conditions at Top of Seal Horizon) |
| Brine Pressure Factor, B | --- | 0.013 | 0.0 to 1.0 | (Active only with Option = 2 for Conditions at Top of Seal Horizon) |

**Table B1: Input Variables for NSealR**

| Input Parameter | Units | Default Value | Range | Input Source (Comment) |
|---|---|---|---|---|
| Brine Pressure Factor, C | / m | 0.005 | ≥ 0 | (Active only with Option = 2 for Conditions at Top of Seal Horizon) |
| Brine Pressure Factor, D | / Ms | 0.150 | ≥ 0 | (Active only with Option = 2 for Conditions at Top of Seal Horizon) |
| $CO_2$ Saturation Factor, G | --- | 0.08 | 0.0 to 1.0 | (Active only with Option = 2 for Conditions at Top of Seal Horizon) |
| $CO_2$ Saturation Factor, H | --- | 0.075 | 0.0 to 1.0 | (Active only with Option = 2 for Conditions at Top of Seal Horizon) |
| $CO_2$ Saturation Factor, J | --- | 0.003 | ≥ 0 | (Active only with Option = 2 for Conditions at Top of Seal Horizon) |
| $CO_2$ Saturation Extent Factor, a | m / Ms | 14 | ≥ 0 | (Active only with Option = 2 for Conditions at Top of Seal Horizon) |
| $CO_2$ Saturation Extent Factor, b | m | 50 | ≥ 0 | (Active only with Option = 2 for Conditions at Top of Seal Horizon) |
| ***Simulation Controls (Dashboard: simulation_input)*** | | | | |
| Uniform Grid Spacing | --- | Checked | Checked / Unchecked | Unchecked option requires input of grid areas and coordinates<br>External File Names: Lookup_seal_grid_area.txt; Lookup_seal_grid_coord.txt |
| X Domain Dimension; X Min. | km | 0 | 0 to 1,000 | |
| X Domain Dimension; X Max. | km | 10 | 0 to 1,000 | |
| Y Domain Dimension; Y Min. | km | 0 | 0 to 1,000 | |
| Y Domain Dimension; Y Max. | km | 10 | 0 to 1,000 | |
| Number of Grid Divisions | --- | 100 | 100 | (Defined Internally) |
| Number of Calculation Steps | --- | 33 | ≥ 0 | (Defined Internally) |
| Time Value | yr | 1 | --- | (Fixed by Code) |

**Table B1: Input Variables for NSealR**

| Input Parameter | Units | Default Value | Range | Input Source (Comment) |
|---|---|---|---|---|
| ***Site Characteristics (Dashboard: site_characteristics)*** | | | | |
| Reservoir Top Elevations | --- | 2 | 1, 2, 3 | Options:<br>1 = Complex Reservoir - External File Input<br>2 = Simple Reservoir – Constant Elevation Across Top<br>3 = Multiple Realizations for Reservoir (Not Supported in NSealR)<br>External File Name: Lookup_reservoir_elev.txt |
| Land Surface Type | --- | 2 | 1, 2 | Options:<br>1 = Complex Surface - External File Input<br>2 = Simple Flat Surface<br>External File Name: Lookup_land_surface.txt |
| Avg. Reservoir Top Elevation[a] | m, NAVD 88 | -1,000 | -10,000 to -100 | (Active only with Option = 2 for Reservoir Top Elevation) |
| Avg. Surface Elevation[a] | m, NAVD 88 | 0 | -1,000 to +10,000 | (Active only with Option = 2 for Land Surface Elevation) |

Notes:

b. The reference vertical datum of NAVD88 (North American Vertical Datum of 1988) is specified for elevations, as it is the official datum for the continental United States (NOS, 1993), but any elevation system can be used for NSealR computations, if used consistently.

c. Although porosity is included in this table, the storage term (i.e., porosity) is not included in the flow model used in the current version of NSealR. However, porosity is expected to be incorporated in the next version of NSealR and therefore, included to minimize future changes to the interface.

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# APPENDIX C – TWO-PHASE RELATIVE PERMEABILITY MODELS

## C.1 GENERAL

Four two-phase relative permeability models are implemented in the current model of NSealR. The theoretical description of the models are provided in this appendix to assist the user in defining input values.

### C.1.1 Purcell Model

The Purcell model (based on Purcell, 1949) is described by employing a single characteristic parameter, λ, which provides for a symmetric description of the wetting and the nonwetting relative permeability expressions as a function of the effective saturation, $S_e$. The equations for relative permeability are modified from Li and Horne (2006)[16].

The wetting relative permeability is expressed as:

$$k_{rw} = S_e^{\frac{2+\lambda}{\lambda}} \tag{C-1}$$

and the nonwetting relative permeability as:

$$k_{rw} = (1 - S_e)^{\frac{2+\lambda}{\lambda}} \tag{C-2}$$

Note that as λ increases, the expression becomes highly linear, and appears similar to what has been termed the "X" model (e.g., Chen, 2005). For this application, the capillary pressure for the Purcell model is defined similar to the Brooks Corey model, except that the entry (or threshold) pressure is assumed as the basis.

The capillary pressure relationship is taken as:

$$P_c = \left\{ \frac{P_e}{S_e^{\frac{1}{\lambda}}} \right\} \tag{C-3}$$

Where $P_e$ is the entry pressure, and $P_c$ is the capillary pressure.

### C.1.2 Brooks-Cory Model

Based on empirical observations, Brooks and Corey (1966) developed a set of equations to describe the nonhysteretic flow of two immiscible fluids in a functional manner in a porous medium. The equations relate the relative permeability to effective saturation using two characteristic parameters, termed lambda (**λ**) and bubbling pressure ($P_b$). The equations were originally developed for a liquid-gas system, but are considered applicable for a fluid-fluid

16 The placement of the parenthesis has been changed from the source for the nonwetting phase.

system (Brooks and Corey, 1964). The equations are also understood as adequate to describe the equivalent-fracture flow in NSealR.

In describing the two-phase system, one fluid is designated the wetting (phase) fluid and the other as the nonwetting (phase) fluid. As defined by Brooks and Corey (1966), the curvature is always concave toward the wetting fluid at the interface of the two fluids. For a system of an aqueous sodium chloride solution (brine) and a supercritical carbon dioxide (as defined for NSealR), the brine is understood to be the wetting fluid.

The equations were developed for the drainage case (where the wetting fluid is displaced by the nonwetting fluid), but the equations can also be used to represent the imbibition case, (the nonwetting fluid is displaced by the wetting fluid), although the specific parameter values of the curve may differ (Brooks and Corey, 1966). It is also noted that the relationships are path-dependent in nature (i.e. hysteresis is exhibited during cycles in saturation), but this effect is not included in the model.

As two distinct phases are present, there is a tension or pressure differential at the interface between the fluids and the pressures in each phase differ. The capillary pressure, $P_c$, is defined as the difference between the pressure of the nonwetting fluid, $P_n$, and the pressure of the wetting fluid, $P_w$ (Brooks and Corey, 1966):

$$P_c \equiv P_n - P_w \tag{C-4}$$

The effective saturation is related to the capillary pressure though a simple power-relationship (Brooks and Corey, 1966):

$$S_e = \left[\frac{P_b}{P_c}\right]^{\lambda} \qquad \text{if } \mathrm{P}_c \geq \mathrm{P}_b \tag{C-5a}$$

and the saturation remains essentially constant at lower capillary pressure (defined as the zone of residual or irreducible nonwetting saturation) that can be defined explicitly:

$$S_e = 1.0 \qquad \text{if } \mathrm{P_c} < P_b \tag{C-5b}$$

where $P_b$ is a material constant, termed the bubbling pressure. The bubbling pressure represents the extrapolation of the log-log curve with the ordinate, $S_w = 1.0$, and essentially is a curve-fitting parameter for the model.

Introducing the concept of an entry pressure (i.e., the pressure needed to initially force the wetting fluid through a wetting fluid saturated sample) will further restrict the capillary-saturation relationship, as no flow occurs at pressures less than the entry pressure. Introducing the entry pressure term, $P_e$, the equation becomes:

$$S_e = \left[\frac{P_b}{P_c}\right]^{\lambda} \qquad \text{if } \mathrm{P_c} \geq \mathrm{P_e} \tag{C-6a}$$

$$S_e = 1.0 \qquad \text{if } P_c < P_e \tag{C-6b}$$

This revised form is shown, e.g., in Corey and Brooks (1999), and serves as a basis to describe the flow of each phase.

The Brooks-Corey model defines each of the relative permeabilities in terms of lambda and effective saturation.

For the wetting phase, the relative permeability is defined as (Brooks and Corey, 1966,):

$$k_{rw} = S_e^{\left[\frac{2+3\lambda}{\lambda}\right]} \tag{C-7}$$

Similarly, the relative permeability is defined for the nonwetting phase as (Brooks and Corey, 1966):

$$k_{rn} = (1 - S_e)^2 \left\{1 - S_e^{\left[\frac{2+\lambda}{\lambda}\right]}\right\} \tag{C-8}$$

### C.1.3 Modified van Genuchten -Mualem Model

To better describe the nonhysteretic flow of two immiscible fluids in a functional manner in a porous medium, van Genuchten (1980) selected an alternative form for the relationship and developed a relationship based on concepts identified by Mualem (1976). Mualem (1976) described a relationship to predict relative permeability based on the soil retention curve.

The van Genuchten-Mualem model relates the hydraulic pressure to the effective saturation using a more complex form than the Corey-Brooks model with three characteristic parameters. The relationship was originally developed for a liquid-gas system but again is considered adequate to describe the equivalent-fracture flow in NSealR.

Employing an effective (wetting phase) saturation defined earlier (for the specific case where the residual nonwetting saturation = 0), the author adopts a general class of equations which relates equivalent saturation, $S_e$, to the pressure head, *h*, (van Genuchten, 1980):

$$S_e = \left\{\frac{1}{1 + (\alpha h)^n}\right\}^m \tag{C-9a}$$

or alternately,

$$S_e = \{1 + (\alpha h)^n\}^{-m} \tag{C-9b}$$

where $\alpha$, *m*, and *n* are characteristic parameters of the permeable medium.

The equation (a particular form of the Incomplete Beta Function) can be solved for the case where *h* is positive and *m* is defined in terms of *n* as:

$$m \equiv \left(1 - \frac{1}{n}\right) \qquad \text{for } 0 < m < 1 \qquad \text{(C-10)}$$

Introducing a capillary pressure term to replace pressure head in the equation, the form becomes (e.g., White and Oostrom, 2000):

$$S_e = \left\{1 + \left(\alpha \left[\frac{P_c}{\rho_w g}\right]\right)^n\right\}^{-m} \qquad \text{if } \mathrm{P}_c \geq 0 \qquad \text{(C-11)}$$

where

| | | |
|---|---|---|
| $P_c$ | = | capillary pressure |
| $\rho_w$ | = | density of the wetting phase |
| $g$ | = | standard gravity |

For the drainage case, capillary pressures below the entry pressure, $P_e$, it is understood that no entry of the nonwetting fluid occurs and the saturation remains constant. This applies an additional restriction (e.g., Ippisch et al., 2006):

$$S_e = \left\{1 + \left(\alpha \left[\frac{P_c}{\rho_w g}\right]\right)^n\right\}^{-m} \qquad \text{if } \mathrm{P}_c \geq \mathrm{P}_e \qquad \text{(C-12a)}$$

$$S_e = 1 \qquad \text{if } 0 < P_c < \mathrm{P}_e \qquad \text{(C-12b)}$$

Replacing the *n* term in this equation with its equivalent *m* value, the *n* term can be eliminated:

$$S_e = \left\{1 + \left(\alpha \left[\frac{P_c}{\rho_w g}\right]\right)^{\left[\frac{1}{1-m}\right]}\right\}^{-m} \qquad \text{if } \mathrm{P}_c \geq \mathrm{P}_e \qquad \text{(C-13)}$$

The equation can then be rewritten to solve for the capillary pressure in terms of effective saturation as:

$$P_c = \frac{1}{\alpha'}\left\{S_e^{\left(-\frac{1}{m}\right)} - 1\right\}^{1-m} \qquad \text{for } 0 < m < 1 \qquad \text{(C-14)}$$

and the constants are merged into a single term, $\alpha'$:

$$\alpha' = \frac{\alpha}{g\rho_w} \quad \text{(C-15)}$$

Extending the theoretical development represented by Equation C-9, van Genuchten developed a relationship for wetting phase permeability, $k_{rw}$, in terms of effective saturation (van Genuchten, 1980):

$$k_{rw} = (S_e)^{\frac{1}{2}}\left[1 - \left(1 - (S_e)^{\frac{1}{m}}\right)^m\right]^2 \quad \text{(C-16)}$$

Luckner et al. (1989) derived a modified form of this wetting equation, replacing the square root on the first effective saturation term with a characteristic parameter (termed here) β (Luckner et al., 1989). Luckner et al. (1989) also provided an expression for the nonwetting phase relative permeability using a second characteristic parameter, γ (Luckner et al., 1989).

These two equations (as presented by Finsterle and Pruess, 1995) are:

$$k_{rw} = (S_e)^{\beta}\left[1 - \left(1 - S_e^{\left(\frac{1}{m}\right)}\right)^m\right]^2 \quad \text{(C-17)}$$

$$k_{rn} = (1 - S_e)^{\gamma}\left[1 - S_e^{\left(\frac{1}{m}\right)}\right]^{2m} \quad \text{(C-18)}$$

This modification of the van Genuchten-Mualem equational form is adopted for NSealR. These relative permeability equations can then be used to assess carbon dioxide flow similar to the Brooks-Corey model.

To implement the modified van Genuchten-Mualem model as described, four characteristic parameters are required: $\alpha', \beta, \gamma$ and *m*. The remaining term, *n*, mentioned earlier is defined in terms of m (per Equation C-10). Referring to Equation C-14, some authors redefine the inverse of $\alpha'$ as the entry pressure (i.e., specifically as the air entry pressure or capillary air pressure) (e.g., Finsterle, 2007; Cinar, 2006), but this approach is considered inappropriate for describing an accurate relationship (see Ippisch et al., 2006) and is not adopted here.

### C.1.4 LET General Model

In order to provide a more representative model to simulate relative permeability laboratory results, a number of recent models have been developed. The LET model (Lomeland et al., 2005; Be, 2011) is similar to the Brooks Corey model but adds more degrees of freedom in order to accommodate the more-complex shape of some measured relative permeability curves.

The LET relative permeability model is described by 3 parameters for both the wetting phase and the nonwetting phases, as represented by the letters L, E, T, together with an additional ratio parameter for a total of seven parameters.

The equation for wetting relative permeability is represented as a function of the effective saturation, $S_e$, as (modified from Lomeland et al., 2012)[17]:

$$k_{rw} = \frac{{S_e}^{Lw}}{{S_e}^{Lw} + E_w(1-S_e)^{Tw}} \tag{C-19}$$

and uses three characteristic parameters, $L_w$, $E_w$ and $T_w$.

The equation for nonowetting relative permeability is similar (modified from Lomeland et al., 2012[18]):

$$k_{rw} = \frac{R_n(1-S_e)^{Ln}}{(1-S_e)^{Ln} + E_n {S_e}^{Tn}} \tag{C-20}$$

which uses three additional characteristic parameters, $L_n$, $E_n$ and $T_n$ together with a parameter equal to the ratio of the nonwetting relative permeability at maximum to the wetting phase relative permeability at maximum, expressed as *Rn*.

The capillary pressure relationship is taken similar to Brooks-Corey model:

$$P_c = \left\{\frac{P_e}{{S_e}^A}\right\} \tag{C-21}$$

Where $P_e$ is the entry pressure, and $A$ is an exponent value.

A more general formulation would be:

$$P_c = B\left\{\frac{P_e}{{S_e}^A}\right\} \tag{C-22}$$

which will be adopted in the future.

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[17] The term $k_{rw}$ is omitted so the wetting phase permeability at maximum is equal to the total permeability, and this equation has a value of 1.00 at that point. This deletion reflects the conditions of the sequestration case, where the wetting fluid is brine, and the nonwetting fluid is $CO_2$, expressed as a function of the normalized wetting fluid saturation.

[18] The ratio term, $R_n$, is introduced to achieve the nonsymmetric curve such as illustrated by Be (2011).

NRAP is an initiative within DOE's Office of Fossil Energy and is led by the National Energy Technology Laboratory (NETL). It is a multi-national-lab effort that leverages broad technical capabilities across the DOE complex to develop an integrated science base that can be applied to risk assessment for long-term storage of carbon dioxide ($CO_2$). NRAP involves five DOE national laboratories: NETL, Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), and Pacific Northwest National Laboratory (PNNL).

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