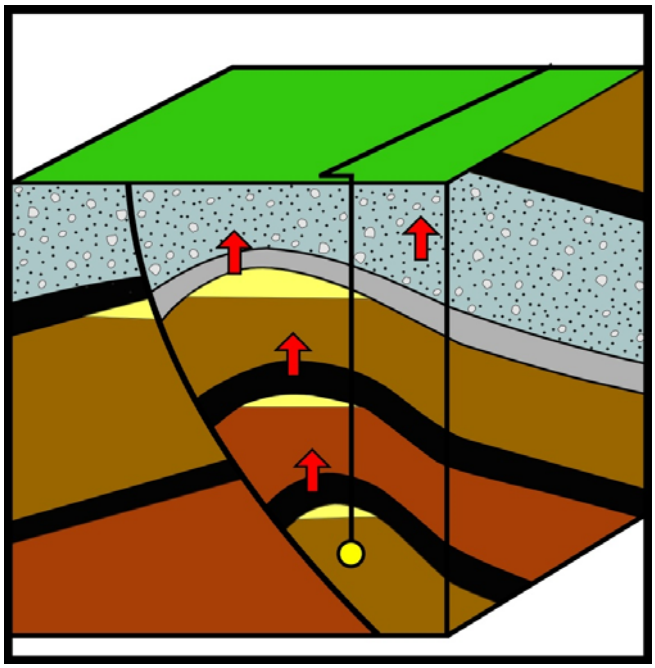
NRAP
National Risk Assessment Partnership



NSealR—A User's Guide, Third-Generation

15 May 2015

U.S. DEPARTMENT OF ENERGY

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NRAP-TRS-III-001-2015

Disclaimer

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

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NSealR—A User's Guide, Third-Generation

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Acronyms and Abbreviations

Abbreviation	Description
Acronyms/Abbreviations/Symbols	
1-D	One-dimensional
2-D	Two-dimensional
3-D	Three-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
JRC	Joint Roughness Coefficient (Barton, 1973)
LANL	Los Alamos National Laboratory
LUT	Lookup table
NaCl	Sodium chloride
NAVD88	North American Vertical Datum of 1988 (NOS, 1993)
NETL	National Energy Technology Laboratory
NIST	National Institute of Standards and Technology
NRAP	National Risk Assessment Partnership
ROM	Reduced-order model
TRS	(NRAP) Technical Report Series
Units	
^{o}C	degrees Celsius
^{o}F	degrees Fahrenheit
ft	feet
mD	millidarcy (10^{-3} D = 9.869233×10^{-16} m^2)
ηD	nanodarcy (10^{-9} D)
kg	kilograms (10^{3} g)
km	kilometers (10^{3} m)
m	meters
M, molal	molality; moles of solute/kg of solvent
mg	milligrams (10^{-3} g)
mm	millimeters (10^{-3} m)
MPa	megapascals (10^{6} Pa)
Ms	megasecond (10^{6} seconds)
Pa	pascals
ppm	parts per million, ratio of solute to solution, by weight
tonne	metric tons (10^{3} kg)
yr	years

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EXECUTIVE SUMMARY

This report provides a guide to the use of the third-generation of the NSealR computer code. The NSealR code is being developed as part of the effort to quantify the risk of geologic storage of carbon dioxide (CO_2). NSealR is constructed as a stand-alone code to describe the flow or leakage of carbon dioxide through the low permeability rock formation (or seal) overlying the storage reservoir into which carbon dioxide is injected. Eventually, the NSealR is intended to be integrated into the CO_2-PENS system as a separate module, and therefore, NSealR incorporates CO_2-PENS assumptions, parameters, formats, and definitions as appropriate for consistency (see Section 2.2).

At present, CO_2-PENS does not incorporate a seal horizon, but includes a possible description of this aspect in code documentation. NSealR is intended to address this gap and adds functionality such as allowing spatially-variable flow properties and adding complexity relative to flow through the seal. For example, to emulate CO_2-PENS flexibility, NSealR allows a number of ways to describe the seal horizon, to correspond to the user's current understanding of the barrier.

The NSealR code provides for the simulation of carbon dioxide flow through the seal barrier horizon, a rock formation that is assumed to be a thin,[1] relatively impermeable, fractured rock unit, initially saturated with saline groundwater. A two-phase, relative permeability approach and Darcy's law are used for one-dimension (1-D) flow computations of carbon dioxide through the horizon in the vertical direction.

The code is written using GoldSim's simulation software platform and is structured using seven upper-level containers (or subroutines) for the top level code logic. The logic proceeds from two containers for seal property and simulation input, followed by logic to establish the analysis basis of permeability and seal horizon thickness and fluid properties, which in turn serves as the basis for the computation container and a final container for output control.

NSealR allows definition of the fluid flow through the seal barrier using one of five options: (1) a constant defined CO_2 flux; (2) a constant (intrinsic) permeability; (3) stochastically-varying permeability; (4) an equivalent permeability across the horizon defined by fractured rock parameters; and (5) user-defined permeabilities input from a text file. The code also permits the definition of the seal barrier thickness as one of three options: (1) constant thickness 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 for the code is primarily through the use of GoldSim *Dashboards*, or graphical user interface windows, which accept numeric and logical input to specify variables and select options. The Dashboards used by the NSealR code are illustrated for the user in this guide, and the required code input variables together with proscribed ranges are also listed.

[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.

Text files are employed for input, primarily for user definition of individual properties of the 100 x 100 grid of elements describing the seal horizon. Using specialized dynamic link libraries (DLLs), the code can also generate output text files at specific time intervals for later graphics processing by other computer programs. The dynamic link libraries were written in C++ computer language and source code for these libraries is also provided in the "\source code" subdirectory and in a separate addendum to this guide.

A description of each of the external text file formats and a listing of ancillary DLLs are provided in the appendix. In addition, the variation of fluid properties with temperature, pressure, and salinity are shown.

The third-generation of the code incorporates several improvements including: 1) the ability to include random zones of decreased permeability across the seal horizon to model areas of increased fracturing or unknown wells; 2) expanded correction for in situ stress on aperture values generated by the fractured rock model, including shear stress options; and 3) inclusion of boundary pressures and saturations at the top of the seal horizon to more accurately simulate field conditions. Accordingly, several of the interface windows have been modified and a new input window has been added. Also, the structure of Dashboard controls has been modified to accommodate these improvements.

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, relatively impermeable layer of rock overlying a rock formation where carbon dioxide has been injected. The code was developed using the GoldSim simulation platform (GoldSim, 2010) 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 is envisioned as a module of an existing system 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. However, for the present development efforts, NSealR has been constructed as a stand-alone code and does not require CO_2-PENS for operation.

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 carbon dioxide, an effort that is already in the second term or generation of progress. This code version has been developed in late 2013 and in 2014 during the third-generation of the NRAP program. Subsequent versions, when completed, will add complexity by accounting for coupled flow, geochemical and geomechanical effects[3], and for multi-layer and two dimensional (2-D) aspects of flow through the seal horizon.

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

[3] 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, all defined within the CO_2-PENS integrated system analysis code to evaluate storage risk. CO_2-PENS incorporates a number of distinct components for CO_2 generation, transport, and injection into a geologic reservoir, including the potential migration out of target reservoir and impact to 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 CO_2-PENS model, taking the output from the reservoir model (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.

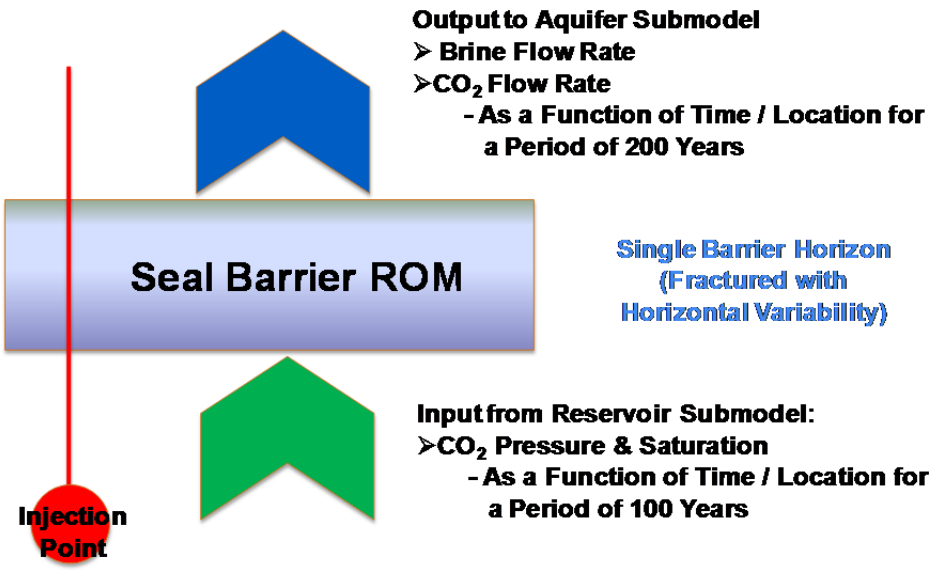

Figure 1: Seals ROM as interface between reservoir and aquifer models within CO_2-PENS.

The CO_2-PENS code 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). During 2014, NSealR predictions are expected to be baselined against detailed simulations from

the STOMP (White et al., 2012) and NFFLOW codes in order to verify the accuracy of the NSealR predictions.

There are a number of possible approaches to develop a ROM to model seal horizon response for storage. However, given the potential variability of the seal barrier properties and configuration, it was determined that the most effective approach would be to define a simple model that would include the most important aspects of flow through a seal barrier, but exclude some secondary effects based on realistic assumptions to permit rapid computations. This approach maintains flexibility in modeling a range of conditions of the seal barrier while keeping computation times short.

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.

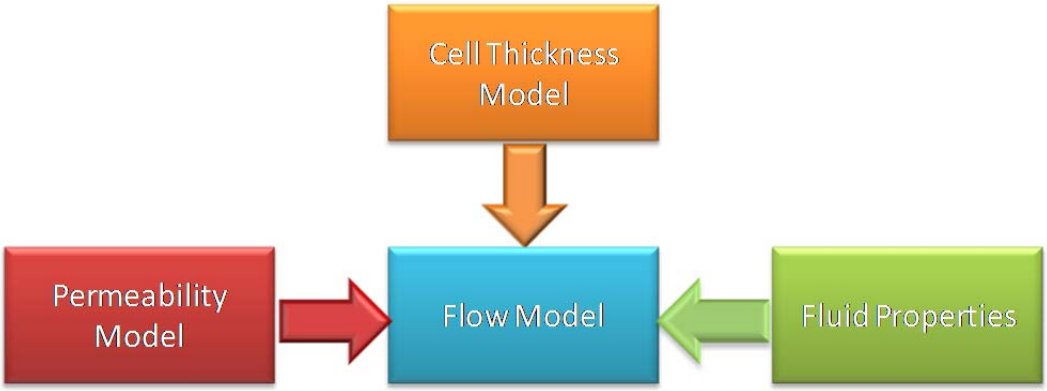

Figure 2: Task models in NSealR.

The current permeability model assumes an established vertical flow pathway through the seal horizon and does not include chemical and time-related interactions, such as dissolution 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.

2.2 PERMEABILITY MODEL/OPTIONS

2.2.1 General

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 CO_2-PENS 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.

One option is described as constant flux. This option is identified in the current CO_2-PENS code (Keating et al., 2009) under caprock properties, and essentially bypasses the entire permeability-flow model computation and allows the user to specify a carbon dioxide flux through the seal horizon. This logic has been modified in NSealR to restrict flux to those cells where there is carbon dioxide saturation at the base of the seal horizon. This option allows the user of CO_2-PENS, for example, to examine groundwater-related risk under defined boundary conditions.

A second option allows the user to define a constant (intrinsic) permeability and (connected) porosity for each cell[4]. 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.

A third option is to define 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.

A fourth option allows the user to define the 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). This option is further described in the next section.

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[4] 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.

Finally, NSealR also allows the option for the user to input a text file describing the permeability of each cell, to address site specific variability or conditions that cannot be otherwise described by the foregoing options.

2.2.2 Equivalent Permeability – Fractured Rock Description

An input option is provided which allows the user to define the equivalent permeability and porosity[4] of each cell using the fractured rock characteristics. The description is based on stochastic parameters input by the user on the extent of (connected[5]) vertical fracturing across the seal horizon, and assumes that matrix flow through the seal is small in comparison and can be ignored. One predominant set of joints/fractures is presumed in this model and the equivalent permeability is estimated based on the density of the fracture centers, the effective fracture aperture, the effective fracture length, and the average orientation in the horizontal plane.

In more detail, the number of fractures in each cell is stochastically sampled from a triangular distribution defined by the expected areal density and maximum and minimum areal densities provided by the user. The number of vertical fractures is then multiplied by the connectivity factor, allowing the user to specify that only a portion of the vertical fractures provide complete pathways through the seal barrier.

Examining each fracture within a cell, the aperture and length of the fracture are stochastically (independently) generated based on lognormal distributions defined by user-defined means and standard deviations. (In addition, if the user selects a stress-correction option, the orientation is estimated and the aperture is corrected for the in situ horizontal stress as described in Appendix A).

Using the (corrected) aperture and length of the fracture and a parallel plate concept for fracture flow (e.g., NRC, 1996; p. 120), the equivalent permeability and porosity for the single fracture is estimated. This process is then repeated for each fracture in the cell, summing the individual fracture permeability and porosity values. At the completion of processing, the summed permeability and porosity values are established as the equivalent properties for the cell. The process is then repeated for each cell of the grid.

2.3 FLOW MODEL ASSUMPTIONS

2.3.1 Theoretical 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.

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[5] As the seal barrier may in fact be composed of one or more lateral units, the "connected" vertical fracture permeability may reflect the vertical permeability of a fracture network rather than single, through-going fractures.

The development of the seal barrier theory is based on a number of assumptions on the structure and flow through the seal layer. The assumptions were made to preserve the simplicity of the code yet capture the more important aspects of flow through a seal horizon.

Specifically, the most significant assumptions are:

- The seal barrier is a relatively thin rock layer, potentially heterogeneous in properties and thickness across the horizon, but relatively homogeneous in the vertical direction.
- The fluid system consists of a two-phase flow of an aqueous sodium chloride (NaCl) solution (i.e., brine) and CO_2. The brine is considered to be the wetting fluid, and CO_2 is the nonwetting fluid. A NaCl solution is considered sufficiently representative of in situ groundwater of a storage site.
- The seal barrier is at a significant depth below the surface (i.e., at conditions of elevated pressure and temperature), and thereby CO_2 is in a supercritical state within the seal's flow domain.
- The initial state of the seal is fully saturated (with brine).
- Flow through the seal is essentially vertical, and dominated by fracturing. (The vertical axis is understood as positive in the upward direction.)
- No fluid storage is considered within the seal layer (i.e., porosity is neglected).[6]
- Flow within the seal is laminar, and Darcy's law applies to flow.
- The seal barrier is sufficiently thin so that changes in fluid density can be neglected with travel distance.
- The two fluids are assumed essentially immiscible, and therefore, there is no mass transfer between the phases within the seal barrier.
- The analysis can be described by a single drainage curve, with brine as the wetting fluid, and without saturation cycles. Therefore, a history effect (hysteresis) of the relative permeability (e.g., Lenhard and Parker, 1987) is not required for simulations and is not included in the model.
- Relative permeability and capillary pressures of the fractured rock of the seal barrier can be represented by either a Brooks-Corey relative permeability model or a van Genuchten-Mualem relative permeability model (Brooks and Corey, 1964; van Genuchten, 1980).
- Dissolved CO_2 is added to the flux computation. In the case when there is a CO_2 pressure at the base of the seal horizon, and brine flow is upward, the brine is presumed to be fully saturated with CO_2. In this case, the dissolved CO_2 is added to the total CO_2 flux through the seal.

[6] However, NSealR provides for the input for porosity as this assumption is to be removed in future versions.

2.3.2 Model Assumptions Intrinsic to CO_2-PENS

NSealR code was developed to be integrated with CO_2-PENS code, and therefore, NSealR employs a number of underlying assumptions consistent with CO_2-PENS.

For the computation of CO_2 leakage during the post-injection process, the CO_2-PENS system model assumes that the overall sequestration process can be divided into several component models. For the subsurface storage of CO_2, the components of the storage module of CO_2-PENS include: 1) sequestration reservoir, 2) caprock (seal barrier), 3) shallow formations (groundwater units), 4) boreholes, 5) faults, and 6) surface characteristics models. A basic premise of CO_2-PENS is that each component model performs an analysis of CO_2 migration independently of the other components and each model only passes a limited data set to neighboring components.

This independence requires implementing assumptions on the boundary conditions along the interface of a component with other components to calculate flow. To conduct a flow analysis through the seal layer independently of both the reservoir model and groundwater units, the flow boundary conditions along both the top and the bottom boundaries of the seal layer must be established in some fashion by NSealR. The current CO2-PENS approach provides the boundary saturations and pressures along the top of the sequestration reservoir (i.e., at the base of the seal layer), but does not define the pressures, saturations or flow along the top of the seal.

One solution to define the upper seal boundary conditions is to assume a static brine pressure condition and that the CO_2 saturation along this boundary is negligible. This allows flow computations so that the seal model can provide, in turn, CO_2 and brine volume rates at cell centers to the groundwater component model, as required by CO_2-PENS. However, this simple approach can provide overly-conservative results as the pressure and saturations can be expected to increase along the upper boundary. To address this issue, alternative methods to define the conditions along the top boundary are incorporated into this version of NSealR.

Regarding other aspects of the NSealR, the division of the seal horizon in a grid of 100 x 100 cells is based on CO_2-PENS assumptions, as are the elements, types, names, and structure in the site characteristics portion of the code. In the few cases where the design of NSealR conflicts with current CO_2-PENS operations, the difference is clearly noted in the NSealR model commentary (i.e., in the GoldSim model view of NSealR), as well as in this manual.

2.4 FLOW MODEL: TWO-PHASE FLOW THEORY

2.4.1 General

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.

In the case with laminar flow, the Darcy velocity of the wetting phase (brine) for two-phase flow can be expressed as (e.g., Silin et al., 2009):

$$u_w = \frac{k_{rw}(S_e)[k_t]}{\mu_w}\{-\nabla P_w + \rho_w g\} \quad (1)$$

where

u_w	=	Darcy velocity of wetting phase (brine) flow
k_t	=	(total or intrinsic) permeability of element
$k_{rw}(S_e)$	=	relative wetting phase permeability of element as a function of the effective wetting phase saturation of the element
μ_w	=	viscosity of the wetting phase
P_w	=	pressure of the wetting phase
ρ_w	=	density of the wetting phase
g	=	standard gravity constant
S_e	=	effective (normalized) wetting phase saturation of the element

It is understood that brine density and viscosity are functions of temperature and pressure, as well as a function of the salinity of the brine.

The effective wetting phase saturation is defined within the region defined by residual (irreducible) saturations as:

$$S_e = \left(\frac{S_w - S_{wr}}{1 - S_{wr} - S_{nr}}\right), \text{ if } S_{wr} < S_w < (1.0 - S_{nr}) \quad (2a)$$

$$S_e = 0.0, \text{ if } S_w \leq S_{wr} \quad (2b)$$

$$S_e = 1.0, \text{ if } S_w \geq (1.0 - S_{nr}) \quad (2c)$$

with the terms:

S_w	=	current wetting phase saturation of the element
S_{wr}	=	residual wetting phase saturation
S_{nr}	=	residual nonwetting phase saturation

In a similar fashion, the Darcy velocity of the *non*wetting phase (supercritical CO_2) for vertical, two-phase flow through an element can be expressed as:

$$u_n = \frac{k_{rn}(S_e)\,[k_t]}{\mu_n}\{-\nabla P_{\mathrm{n}} + \rho_n g\} \quad (3)$$

where

u_n = Darcy velocity of nonwetting phase flow (CO_2)

$k_{rn}(S_e)$ = relative nonwetting phase permeability of element as a function of the effective wetting-phase saturation of the element

μ_n = viscosity of the nonwetting phase

P_n = pressure of the nonwetting phase

ρ_n = density of nonwetting phase

Two formulations that are commonly used with these general equations to describe relative permeability are included in NSealR: 1) the Brooks-Corey model, and 2) modified van Genuchten-Mualem model. Both are described in the following sections.

2.4.2 Brooks-Corey Model

As suggested by Brooks and Corey (1966), the relative wetting phase permeability can be represented as an exponential function of the normalized saturation and a material-characteristic constant, λ:

$$k_{rw}(S_e) = S_e^{\left[\frac{2+3\lambda}{\lambda}\right]} \tag{4}$$

Note that for immiscible fluids in geologic media, the pressure within each fluid is not equal to pressures in other neighboring fluids. When two or more immiscible fluids exist within a pore space, they are separated by boundaries (interfaces), across which discontinuities in density and pressure exist (Corey, 1994). As described in more detail by Corey (1994), the force component from unbalanced cohesion at interface is called the interfacial force. The resultant of interfacial forces acting on a curved surface is balanced at equilibrium by the difference in pressure at points of contact between the fluid phases.

This difference in pressure, called capillary pressure, is designated by P_c, and defined in terms of the wetting phase and the nonwetting phase pressures as:

$$P_c = P_n - P_w \tag{5}$$

With the terms

P_n = nonwetting phase pressure

P_c = capillary pressure

In storage, capillary forces can act to prevent upward migration of CO_2, and can highly influence the flow process (e.g. Nielsen et al., 2012; Chalbaud et al., 2010).

Based on experimental work on various media by Brooks and Corey (1966), and omitting data for saturations above about 85%, it was found that the capillary pressure for the drainage cycle can be represented by a power-law relationship to saturation with an intercept. This relationship of capillary pressure to saturation can be expressed as (Brooks and Corey, 1966):

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

or alternatively:

$$P_c = \left[\frac{P_b}{(S_e)^{\frac{1}{\lambda}}}\right], \text{if } 0.0 < S_e \leq 1.0 \tag{6b}$$

where P_b is the bubbling pressure. The bubbling pressure is understood as the capillary pressure at 100% effective saturation from the empirical curve.

Similar to the wetting phase, the relative nonwetting phase permeability of element, k_{rn}, can be defined in terms of the wetting phase saturation and lambda as (Brooks and Corey, 1964):

$$k_{rn}(S_e) = (1 - S_e)^2 \left[1 - (S_e)^{\frac{(2+\lambda)}{\lambda}}\right] \tag{7}$$

A more extensive statement of the two-phase, Brooks-Corey model is presented in Appendix B.

2.4.3 Modified Van Genuchten-Mualem Model

Another representation for the capillary pressure-effective saturation relationship was developed by van Genuchten (1980), based on the work of Mualem (1976). This representation differs from the Brooks-Corey model as it can define capillary pressures as a continuous function, but includes additional parameters.

Based on van Genuchten (1980), the equation to solve for the capillary pressure, P_c, in terms of effective saturation, S_e, can be rewritten as:

$$P_c = \frac{1}{\alpha'}\left(S_e^{\left(-\frac{1}{m}\right)} - 1\right)^{1-m} \qquad \text{with } 0 < m < 1 \tag{8}$$

where the constant, α', is defined as:

$$\alpha' = \frac{\alpha}{g\rho_w} \tag{9}$$

and

m = characteristic parameter of the permeable medium
α = characteristic parameter of the permeable medium
ρ_w = density of the wetting phase
g = standard gravity

Extending the theoretical development of van Genuchten, Luckner et al. (1989) derived a modified form of the wetting phase relative permeability and the nonwetting phase relative permeability equations, employing two additional characteristic parameters, termed here as β and γ. These two equations (as presented by Finsterle and Pruess, 1995; Equation 9) are:

$$k_{rw}(S_e) = (\mathrm{S_e})^{\beta}\left[1-\left(1-\mathrm{S_e}^{\left(\frac{1}{\mathrm{m}}\right)}\right)^{\mathrm{m}}\right]^2 \tag{10}$$

$$k_{rn}(S_e) = (1-\mathrm{S_e})^{\gamma}\left(1-\mathrm{S_e}^{\left(\frac{1}{\mathrm{m}}\right)}\right)^{2\mathrm{m}} \tag{11}$$

In addition, Luckner et al. (1989) suggested values for the two additional parameters as:

$$\beta = \frac{1}{2} \tag{12}$$

$$\gamma = \frac{1}{3} \tag{13}$$

The modification of the van Genuchten-Mualem equation forms in Equations 10 and 11 are adopted for NSealR. The definition of parameters, β and γ, however, are left to the user. A more extensive statement of the two-phase, van Genuchten-Mualem model is presented in Appendix B.

2.5 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.[7]

[7] This differs from the current convention used in 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.

In generating a stochastic thickness for each cell, it is realized that the variability of thickness should in some fashion be autocorrelated and not be simply a stochastically-defined value independent of neighboring cells. However, as the current version of GoldSim does not incorporate an option for autocorrelation, an alternative approach was incorporated into NSealR. This approach adjusts each cell thickness by adding the average of each neighboring cell to the cell value and then adjusting the entire array of thickness values to restore the user's defined variability.

For this approach, the thickness of each cell is computed independently using a truncated normal (Gaussian) distribution defined by the mean and standard deviation specified by the user. The truncation distribution limits are defined internally by NSealR with a minimum of 0.0 m and a maximum of 1,000 m. Then each cell is subjected to a Level-2 averaging system[8], and adjusted using a correlation coefficient (ϖ) to determine a final corrected thickness (t_i'), or simply:

$$t_i' = (1 - \varpi)t_i - \varpi(\Sigma t_n) \tag{16}$$

where Σt_n represents the averaged neighbors and the correlation factor, ϖ, varies from 0.0 to 1.0 for zero to perfect correlation, respectively.

In a similar fashion, the resulting values are subjected to a second pass with a Level-1 averaging system using the same correlation coefficient. Finally, the variability of the thickness array is restored by adjusting the difference of each new averaged value from the population mean to be consistent with the original user-defined value.

While this approach is relatively unsophisticated, it is simple to apply and has been empirically demonstrated to achieve a more smooth variation in cell thickness across the seal horizon than using independently generated values alone.

2.6 UPPER BOUNDARY DEFINITION

As discussed in Section 2.3.2, given the component structure of CO_2-PENS, the seal model must assume the pressure and saturation conditions along the top of the seal boundary. This allows the seal model to perform flow computation and in turn to provide CO_2 and brine mass flow rates at cell centers to the groundwater component model of CO_2-PENS. 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 negligible.

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

[8] A "n"-level system computes the average of all cell values to a distance of "n" cells around the selected cell. For example, a Level-1 approach computes the average of the all cells in a rectangular grid up to a distance of 1 cell from the specified cell location, resulting in an average of 9 cells.

higher pressures at the top of the seal, there is a smaller pressure gradient inducing flow through the seal and resulting in lower CO_2 flow rates than NSealR would predict in the static case.

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 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 involves the use of two analytic equations to describe the top boundary conditions. This allows the user to input parametric values to relate the brine pressures and CO_2 saturations at the top of the unit to values at the base of the seal (which are input from the reservoir model). These equations presume a single injection point in the reservoir, located at a coordinate (x,y) in the horizontal plane. The general shapes of these corrections are based on an evaluation of results from the STOMP code (White et al., 2012).

As pressures along the seal base directly above the injection point will be significantly higher and the increased pressures along the top will be relatively constant, the pressure correction needs to be inverted with distance. Therefore, an increasing representation (i.e., the overall factor increases exponentially with increasing distance) is adopted to relate the base brine pressure to the top seal pressure. The distance and time terms are negative exponentials and decrease with increasing values. Specifically, the ratio of brine pressures at the top of the cell, BP_{top}, along the seal horizon are a function of the brine pressures at the cell base, BP_{bot}, the lateral distance from the injection point, r, and the time since the start of injection, t, expressed as:

$$BP_{top} = BP_{bot}\{A - Bexp(-Cr)\exp(-Dt)\} \tag{17}$$

where A, B, C and D are constants specified by the user.

Reorganizing the equation to describe a brine-pressure correction factor, F_{BP}, as

$$F_{BP} = \frac{BP_{top}}{BP_{bot}} = A - Bexp(-Cr)\exp(-Dt) \tag{18}$$

The description of CO_2 saturation requires a more complex representation than for brine pressure. The saturation at the top of the horizon is understood as not proportional to the saturation at the base of the layer. In addition, from the time injection starts, there is a significant time period until the CO_2 reaches the base of the seal layer and can flow through the seal to the top of the horizon to affect saturations there. This period is termed in NSealR as the saturation time lag, t_{lag}. Further, the saturations at the top of the seal horizon are expected to decrease with the lateral distance from the point directly above the injection location and may abruptly cease at a specific distance.

To represent this behavior, saturations at all times before the lag time are set equal to zero, as assumed by the static:

$$SC_{top} = 0.0 \qquad \text{for } t < t_{lag} \tag{19}$$

After this lag time, the saturation at the top of the horizon is considered to decay exponentially with the distance from the injection point, up to a certain characteristic distance termed *K*; saturations along the top of the seal horizon for a cell, SC_{top}, can be expressed as:

$$SC_{top} = \{G + Hexp(-Jr)\} \qquad \text{for } r \leq K \tag{20a}$$

$$SC_{top} = 0.0 \qquad \text{for } r > K \tag{20b}$$

where *G*, *H*, and *J* are constants specified by the user, and *K* is a function of time.

The saturation front spreads with time at the top of the seal horizon, which is controlled by the *K* parameter. A simple representation for *K* is taken, as a linear form with time:

$$K = at + b \tag{21}$$

where *a* and *b* are constants defined by the user. The units for these variables in NSealR assume that time is in Megaseconds (Ms) and distance in meters (m).

The brine pressure and CO_2 saturations defined along the upper seal boundary using the analytic approach are illustrated in Figures 3 and 4 for a short time frame of about 2 years (~ 63.1 Ms).

2.7 PROBABILITY DISTRIBUTIONS

To describe the potential variability of the seal barrier properties, several different distributions are employed within the code, as shown in Table 1. The selection of these distributions is based on the literature and experience with specific data sets.

For parameters defining equivalent permeability using rock fracture characteristics (i.e., for fracture aperture, length, strike, and density), distributions commonly employed to describe these forms of variability were chosen. For the current version of NSealR, the fracture aperture is described by a lognormal distribution (e.g. Snow, 1970), as is the length distribution (e.g., Baecher and Lanney, 1978). The orientation of the fractures is defined using a normal (Gaussian) distribution, truncating the deviation of the distribution at +/- 180^o from the mean. The areal density of fractures locations is described with a triangular distribution to reflect more variability than in a normal distribution.

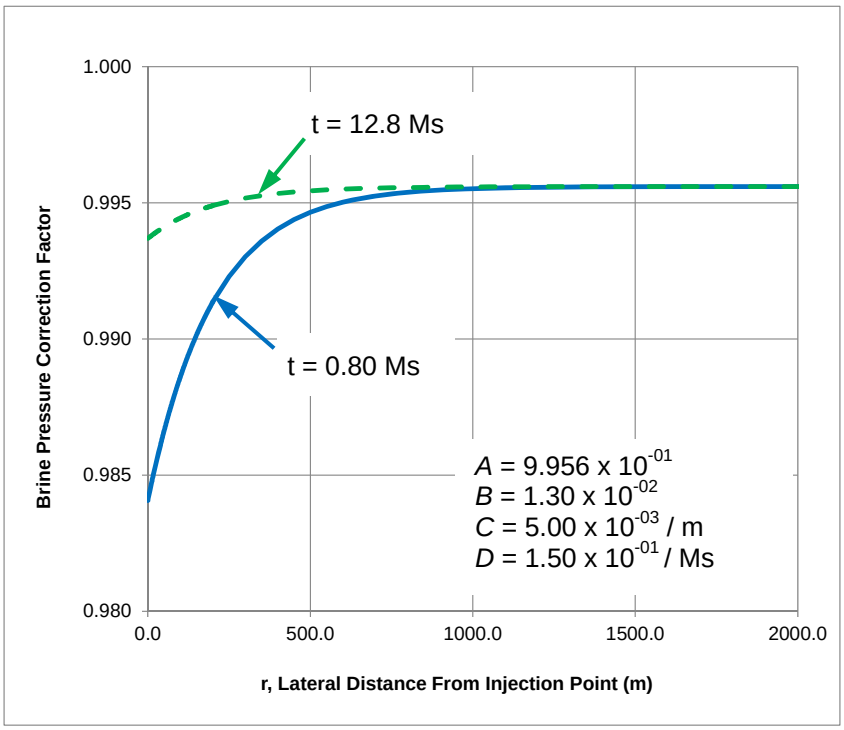

Figure 3: Example - Upper boundary brine pressure correction factor at differing times.

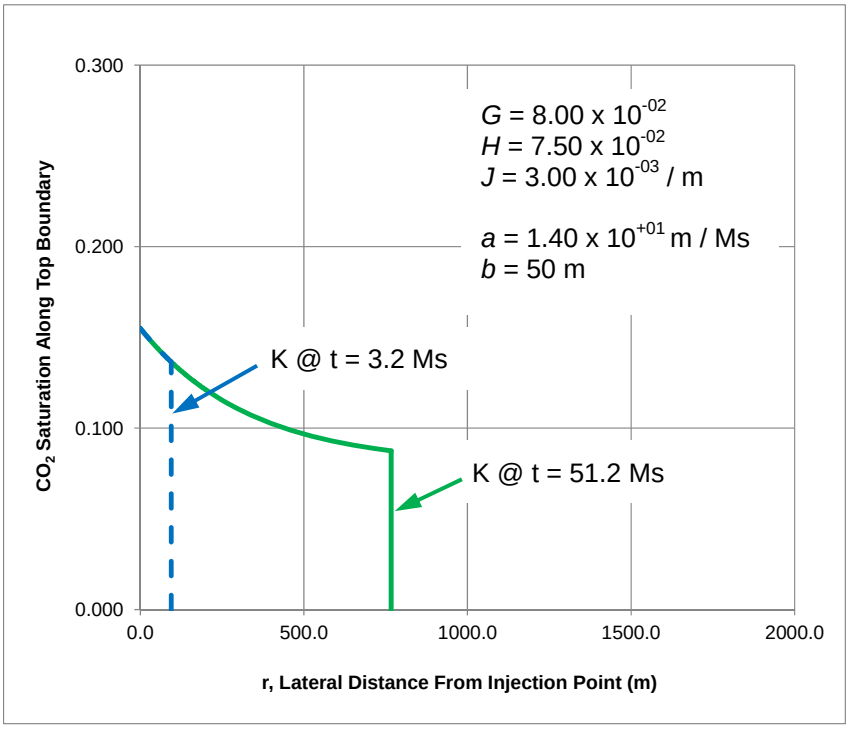

Figure 4: Example - Upper boundary CO_2 saturations at differing times.

Table 1: 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[4]	Truncated Normal	Minimum (0.0) and maximum (1.0) are defined within NSealR
Seal Barrier Height/Thickness	Truncated Normal	Minimum (0 m) and maximum (1000 m) are defined within NSealR. Adjusted with correlation factor to smooth distribution

For the two-phase parameters of residual saturations of brine and CO_2 and the lambda factor, there is little available information on the natural distribution of these values for rock fractures. To reflect this uncertainty, a uniform distribution was selected.

A truncated lognormal distribution was selected to describe stochastic permeability and a normal distribution was selected for porosity[4]. The seal thickness was chosen to be represented by a truncated normal distribution to limit unreasonable values (i.e., negative thickness values).

2.8 FLUID PROPERTIES

As noted earlier, 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 DLLs (see 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 of 0.101325[9] to 60 MPa, 0 to 180°C, and 0 to 80,000 ppm salinity[10], a target region that conservatively brackets typical temperature and pressure conditions for storage. Test cases for "cold-shallow" injection reservoirs have been simulated at 1 km depth with a temperature of 35°C and hydraulic pressure of 10 MPa and "hot-deep" reservoirs at 3 km depth at conditions of 155°C and 35 MPa (e.g., Stauffer et al., 2009a). For these two cases, a maximum injection pressure of 15 MPa for the shallow case and 45 MPa for the deep case was simulated. In summary, the stated target region for the properties data in NSealR is applicable to in situ conditions typically between 0.8 and 5.5 km below grade, depending on actual site conditions.[11]

In detail, the property data incorporated in NSealR DLLs were taken from several sources. The values for the density and viscosity of pure water and of CO_2 were generated by the software code, REFPROP, authored by Lemmon et al. (2010) of the National Institute of Standards and Technology (NIST). This code, in turn, incorporates the equation of state for the density of pure

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[9] Standard atmospheric pressure (from the website, Wikipedia).

[10] The stated range in salinity is not considered conservative. The potential range of salinity at a sequestration site is more difficult to bracket and varies with location as well as with depth. Many initial analyses on CO_2 sequestration have used pure water (salinity = 0 ppm) as a base case. In contrast, given an upper limit of 10,000 ppm of total dissolved solids in drinking water standards, and recommendations to avoid injecting into potable aquifers, it can be expected that CO_2 will be injected into formations with brine concentrations greater than the 10,000 ppm value (e.g., Tetra Tech, 2009). The salinity of typical seawater is 35,000 ppm. A range of 35,000 to 80,000 ppm was noted at one potential sequestration site (Stauffer et al., 2009b). However, groundwater salinity can be quite large at various sites, and in cases, can exceed 200,000 ppm. In more practical terms, a limit of 80,000 ppm is the upper bound of data from Sun et al. (2008) and this value was chosen in defining the target conditions for this version of NSealR.

[11] The maximum applicable depth can be estimated using general trends with depth of temperature and pressure from the literature. Assuming a geothermal gradient of 18°C per km of depth (i.e., 1°F per 100 ft) and an average surface temperature of 15°C, a value of 180°C is achieved at about 9.1 kilometers below the surface; with a geothermal gradient of 25°C per km of depth, 180°C is achieved at 6.6 km. Considering fluid pressure, using a hydrostatic pressure increase with depth of 9.8 MPa/km-depth from the surface, a limit of 60 MPa is reached at 6.1 km. Allowing for an injection pressure increase of 5 MPa over in situ conditions, a depth of 5.5 km would be a conservative maximum.

The minimum depth is dictated by the supercritical state of CO_2. CO_2 is a liquid only above 0.5 MPa at −56.6°C, and CO_2 is supercritical starting at temperature and pressure above 31°C and 7.4 MPa, respectively. Using the approximate trends noted earlier in this estimate, CO_2 is only supercritical at depths below about 0.8 km. This restricts the use of the code below this depth to maintain the assumed flow of supercritical CO_2 through the seal barrier.

water developed by Wagner and Pruss (2002), and the viscosity of water by Huber et al. (2009). The code also computes values based on the equation of state developed for CO_2 density by Span and Wagner (1996) and for CO_2 viscosity by Fenghour et al. (1998).

For salinity greater than zero, the density of brine is computed from equations and using coefficients reported by Sun et al. (2008), using pure water values from REFPROP as a starting basis (i.e., for salinity = 0). The viscosity of brine for salinities greater than zero is based on programming the equation of state as reported by Mao and Duan (2009) and computing required values. Similarly, the solubility of CO_2 is based on programming the equation of state correlations as reported by Duan et al. (2006) and computing required values.

Appendix D provides figures illustrating the variability of these parameters.

3. CODE STRUCTURE

The logic structure of NSealR is divided into seven modules or "containers", as shown in Figure 5, together with an eighth container for the user interface. Code flow in Figure 5 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

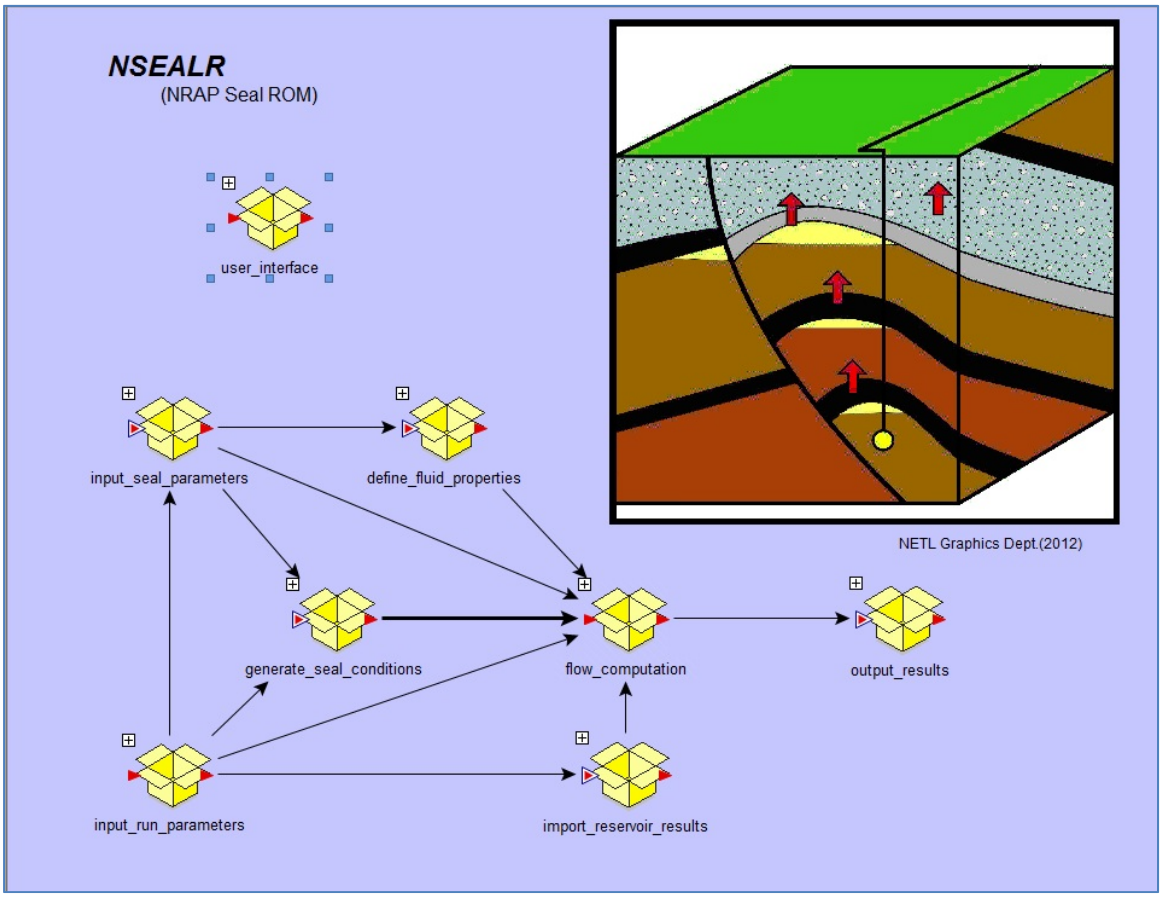

Figure 5: Top-level structure of NSealR code.

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 6. The topmost Dashboard, *Seal_MAIN* (Figure 7), provides entry into the input system, and provides access to the input and output control Dashboards as well as to Dashboards supplying related information.

The information Dashboards 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 (Figure 8), provides a list of references used in code development. The *contacts* Dashboard (Figure 9) provides a list of names, phone numbers and the mailing address and for obtaining other information on the code, and the *notices* Dashboard (Figure 10) provides the disclaimers on code use and the applicable copyright statement.

Moving between Dashboards is controlled by the Dashboard structure. To move between Dashboards, selecting one of the option buttons on the 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.

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 do not provide (in most cases) acceptable values; these default files are provided for format guidance only.

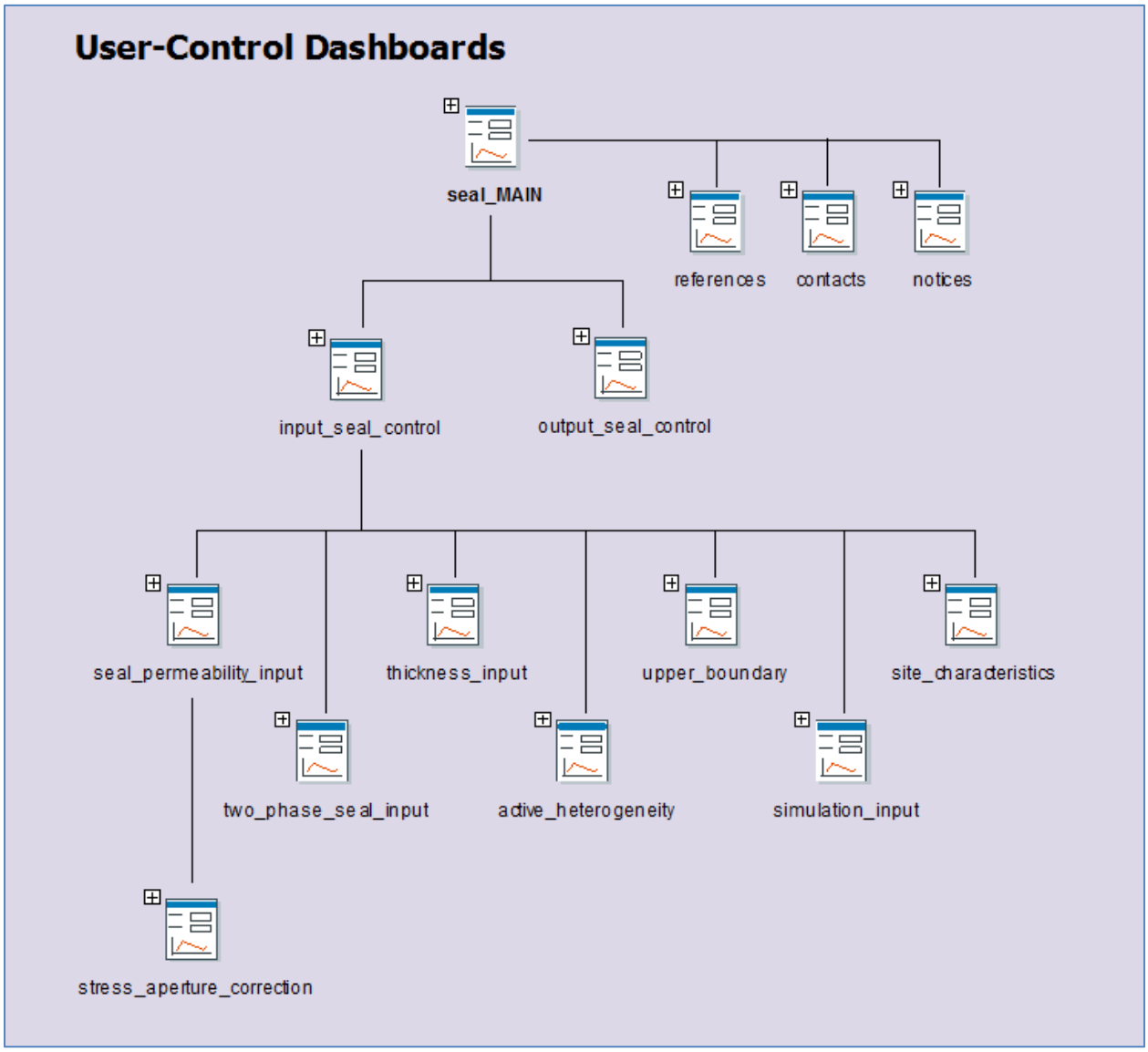

Figure 6: Structure of Dashboard controls for data input and output.

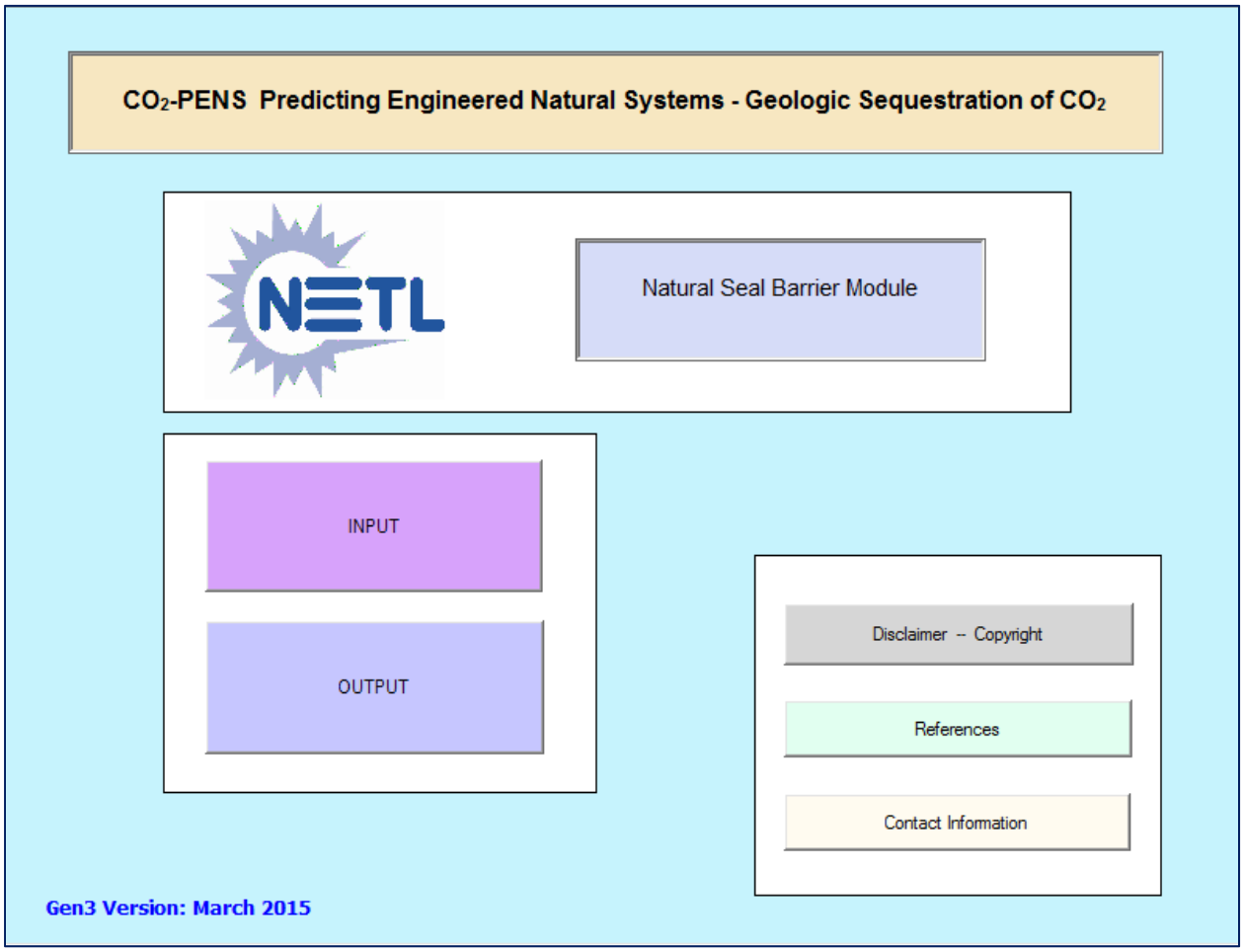

Figure 7: Main Dashboard of NSealR.

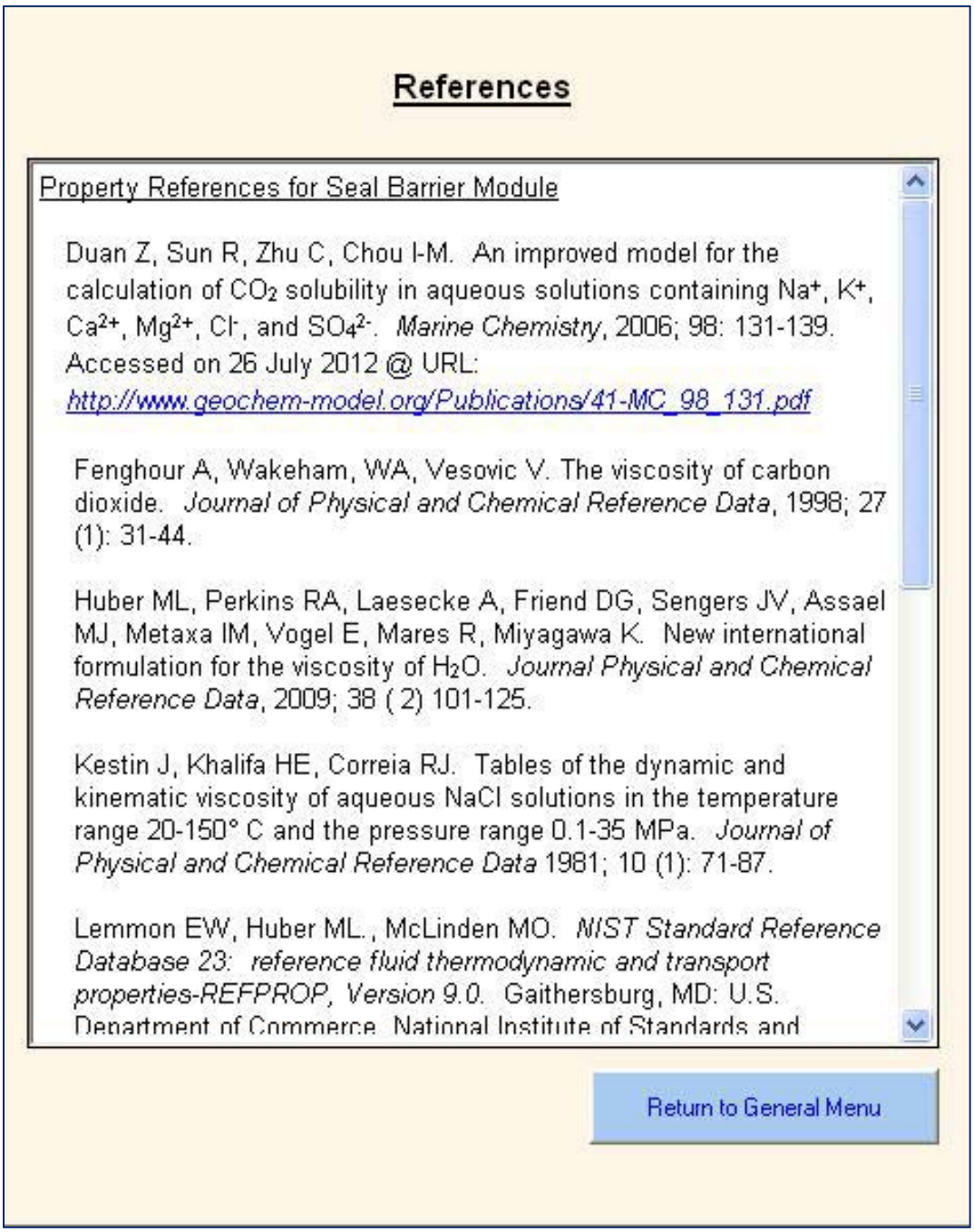

Figure 8: Reference Dashboard.

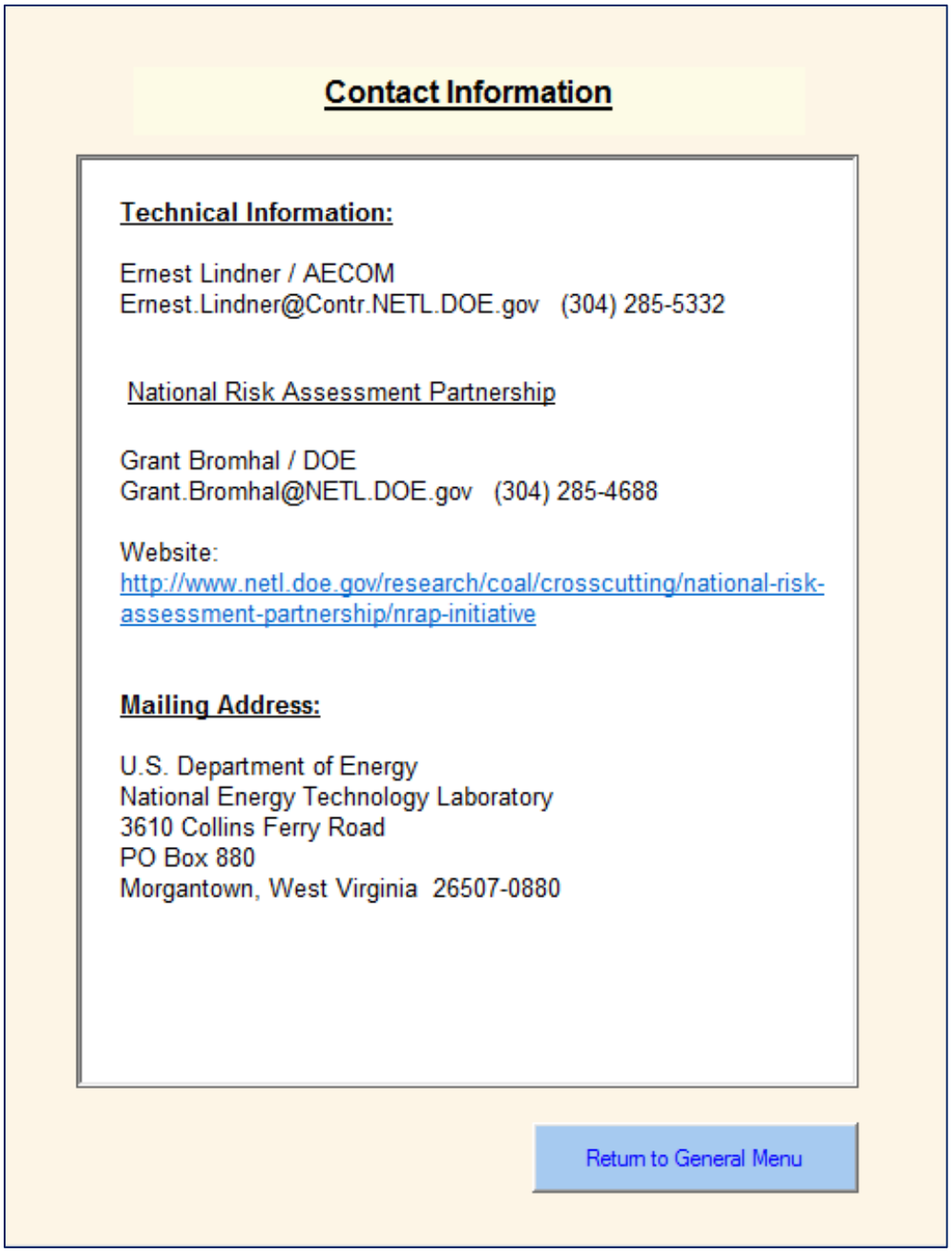

Figure 9: Contact Information Dashboard.

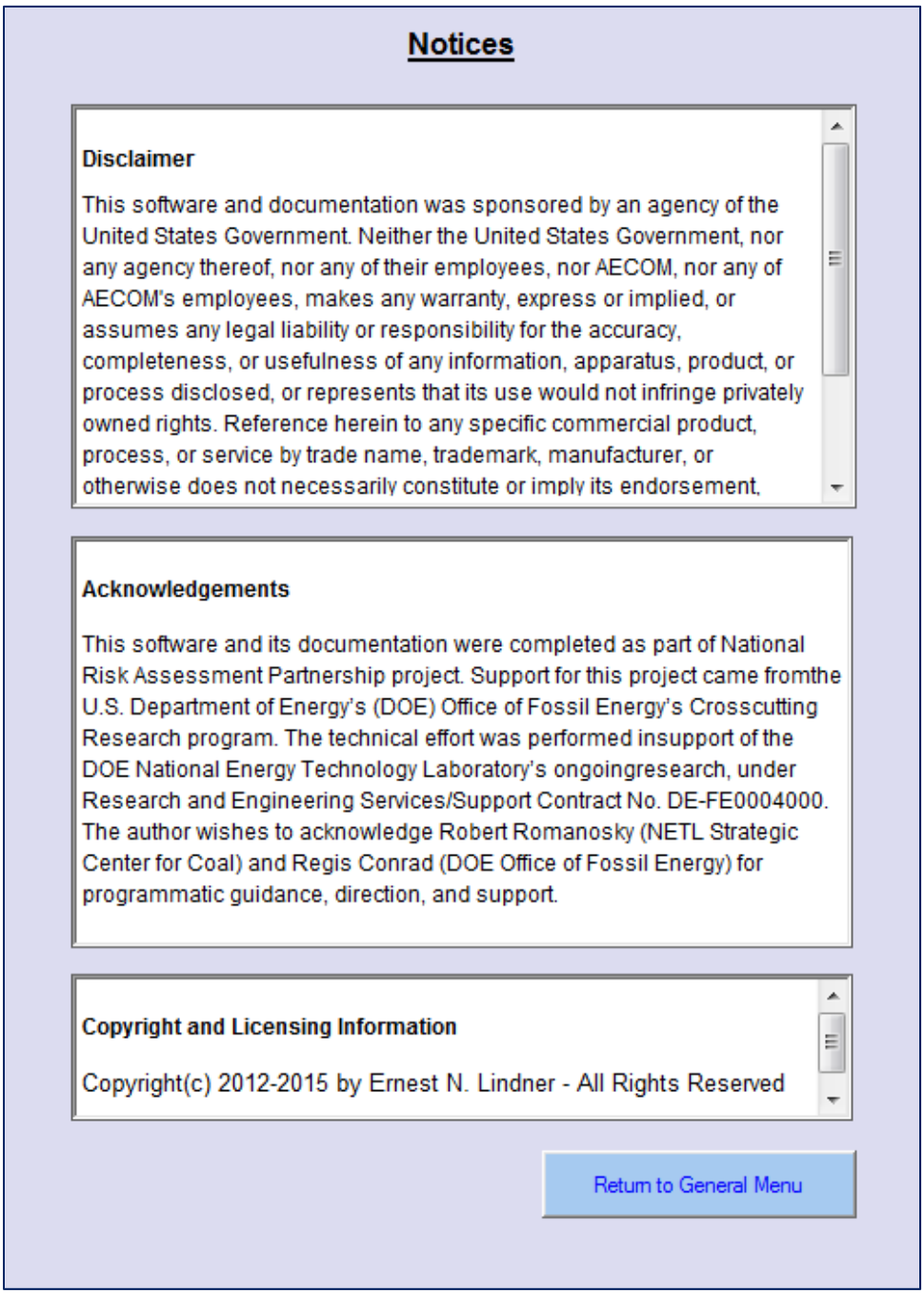

Figure 10: Notices Dashboard.

4.1.2 Input and Seal Properties Dashboards

From the main Dashboard, selecting the "Input" button places the user on the second level of the Dashboard structure. At this point, the Seal Barrier Input Dashboard (*input_seal_control*) lists a series of control buttons for the defining various input properties as shown in Figure 11. The top five buttons provide options to define seal-related properties with two additional buttons (below the horizontal line in the figure) to define general parameters for the reservoir and the analysis case.

The five seal properties Dashboards include the options to define: (1) variables for the permeability model (*seal_permeability_input*), (2) the two-phase flow parameters and other flow conditions (*two_phase_flow_input*), (3) the thickness variation of the horizon (*thickness_input*), (4) the active/inactive cells and additional zones of heterogeneity (*active heterogeneity*), and (5) the pressure and saturation conditions assumed along the upper seal boundary (*upper_boundary*). The buttons and associated Dashboards are described in the following sections.

4.1.2.1 Seal Permeability Input Button

In more detail, upon selecting this button on the Seal Barrier Input Dashboard, the user is shown the *seal permeability* Dashboard (Figure 12). 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[12] 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) Defined constant flux

(2) Constant (intrinsic) permeability across the entire horizon

(3) Stochastically-varying permeability across the horizon

(4) A varying, equivalent permeability across the horizon, defined by fractured rock parameters

(5) An array of user-defined permeabilities

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

At the bottom of this Dashboard is a check box for the option to adjust the apertures used in the fractured rock parameter model. If the user wishes to utilize this correction, checking the option will show a green button ("Go to Stress Correction Parameters").[13] Then, depressing this button, a lower level Dashboard, *stress_aperture_correction*, is shown (Figure 13).

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

[13] 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.

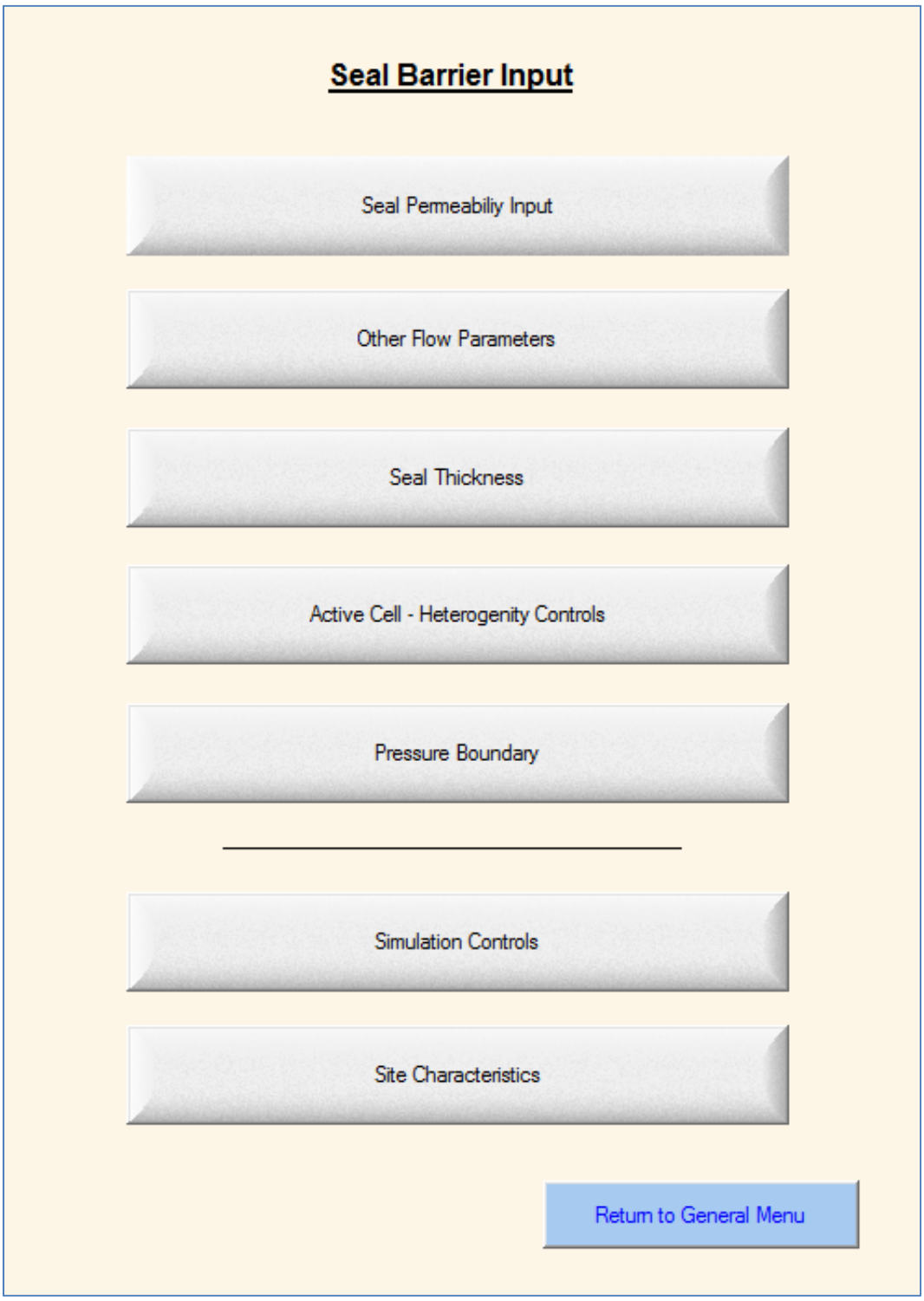
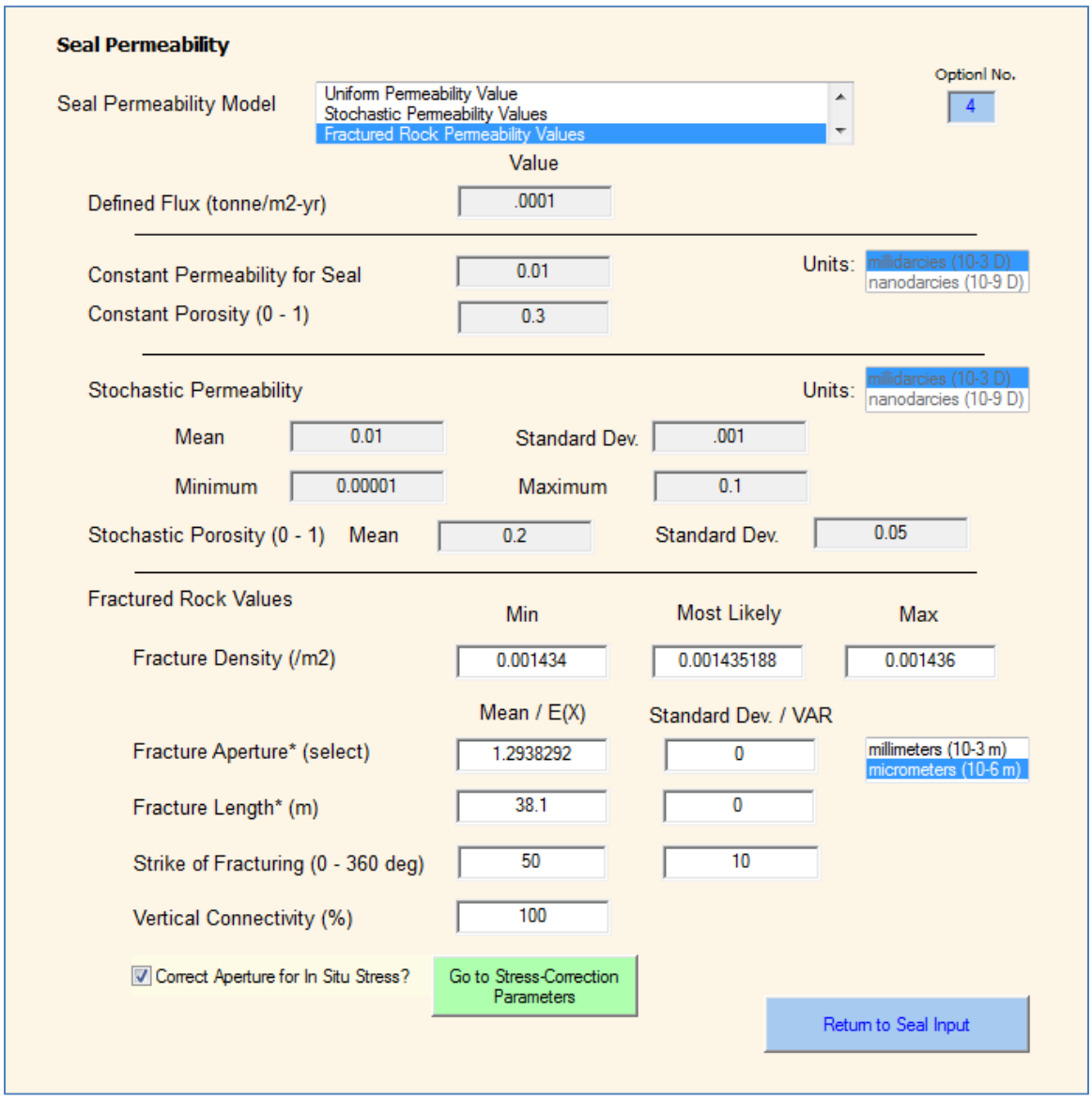


Figure 11: Seal Barrier Input Dashboard.



Notes:

[a] The white text with blue background in the "Seal Permeability Model" box indicates 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 the user.

[b] Based on the option selected, some variables are not used in the computation, as indicated by the dark backgrounds. The user cannot change values in these boxes, unless a different option is selected.

[c] By convention, upward flows are understood as positive and positive flux values represent upward flow.

Figure 12: Seal Permeability Dashboard.

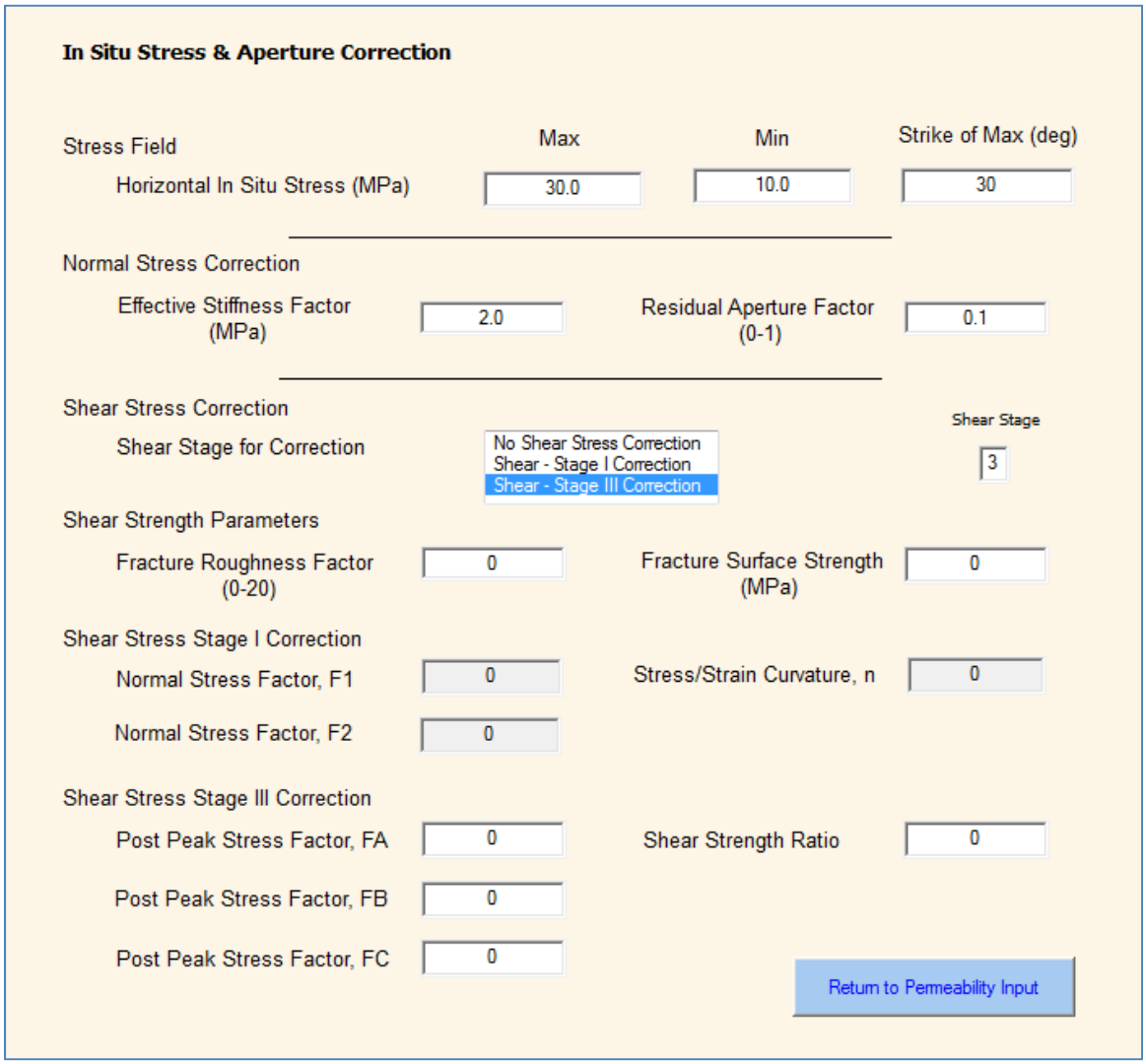


Figure 13: In Situ Stress & Aperture Correction Dashboard.

This secondary Dashboard provides for the input of all stress-related correction values for the fractured rock model. This input includes values describing the in situ, horizontal secondary principal stress ellipse (major and minor axes and the orientation of the major axis from North, i.e., the strike) representative of the regional stress.

The regional stress values and the remaining input values on the form are employed for adjusting the stochastically-generated apertures in the fractured rock permeability model, if desired, for normal and shear stresses. Adjustments for shear stresses can be defined considering either pre-peak or post-peak shear displacement. The stress-dependency options and the underlying theory of adjusting the aperture are further discussed in Appendix A.

4.1.2.2 Other Flow Parameters Button

Returning to the row of buttons on the *input_seal_control* Dashboard, the user can select the "Other Flow Parameters" button to obtain the *two_phase_flow_input* Dashboard for identifying two-phase parameters and other flow conditions (Figure 14). This Dashboard is for input of (a) the salinity of the brine in the seal, (b) the reference brine pressure at a specified depth, (c) the reference pressure elevation (corresponding to the reference brine pressure), (d) the average seal temperature, (e) the two-phase parameters of residual brine saturation and residual CO_2 saturation and (f) the entry or threshold pressure. The Dashboard also allows for the selection of the two-phase model to be used in NSealR computations, and input of the associated parameter values. If the Brooks-Corey model is selected, lambda and Bubbling Pressure are required to be input, and if the modified van Genuchten-Mulam model is chosen, the m-factor, alpha-prime, beta and gamma factors are to be defined.

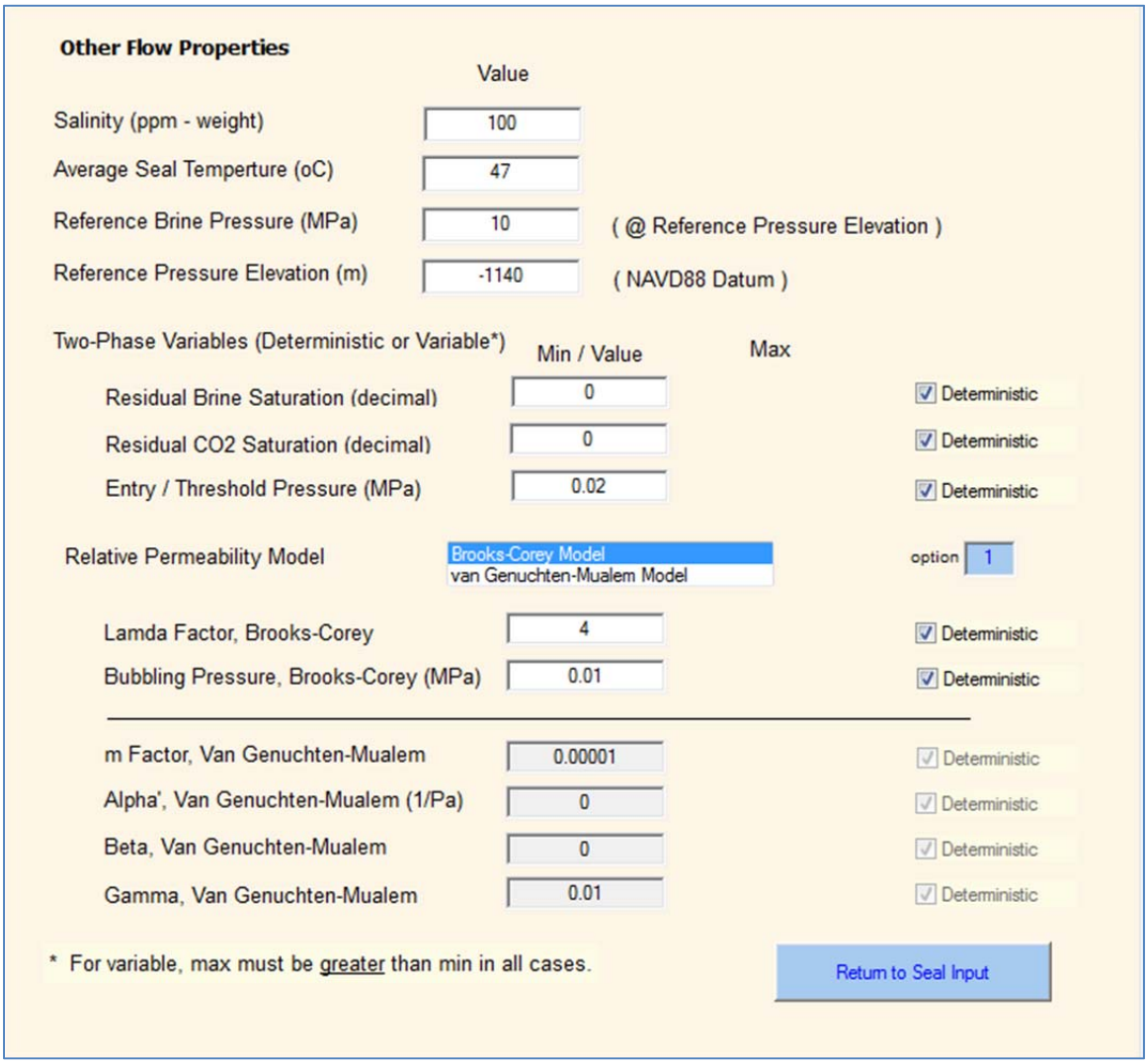
4.1.2.3 Seal Thickness Button

This button on the *input_seal_control* Dashboard selects the *thickness_input* Dashboard (Figure 15). This Dashboard allows for definition of the seal horizon model, and the input of related parameters. The seal barrier thickness or height can be defined 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.

4.1.2.4 Active Cell - Heterogeneity Controls Button

This button provides options to define active cells and random zones. The selected Dashboard (*active_heterogenity Dashboard;* Figure 16) 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).[14]

[14] 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.

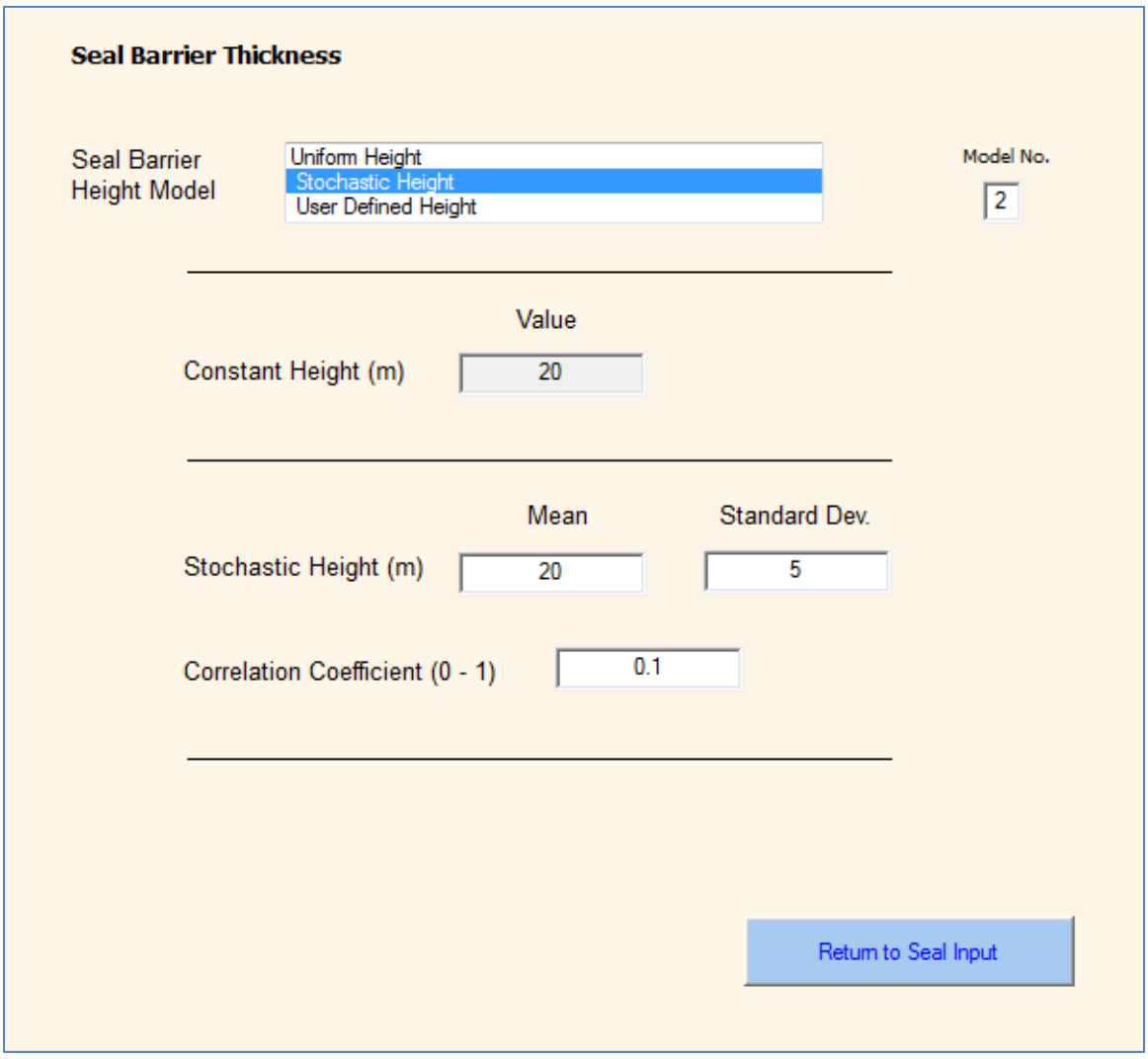


Notes:

[a] 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.

[b] For elevations, a vertical datum of NAVD88 (North American Vertical Datum of 1988) is specified for elevations, and at depth, negative numbers are expected.

Figure 14: Other Flow Parameters Dashboard.



Note: The blue background with white text in the "Seal Barrier Height Model" option indicates 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 15: Seal Barrier Thickness Dashboard.

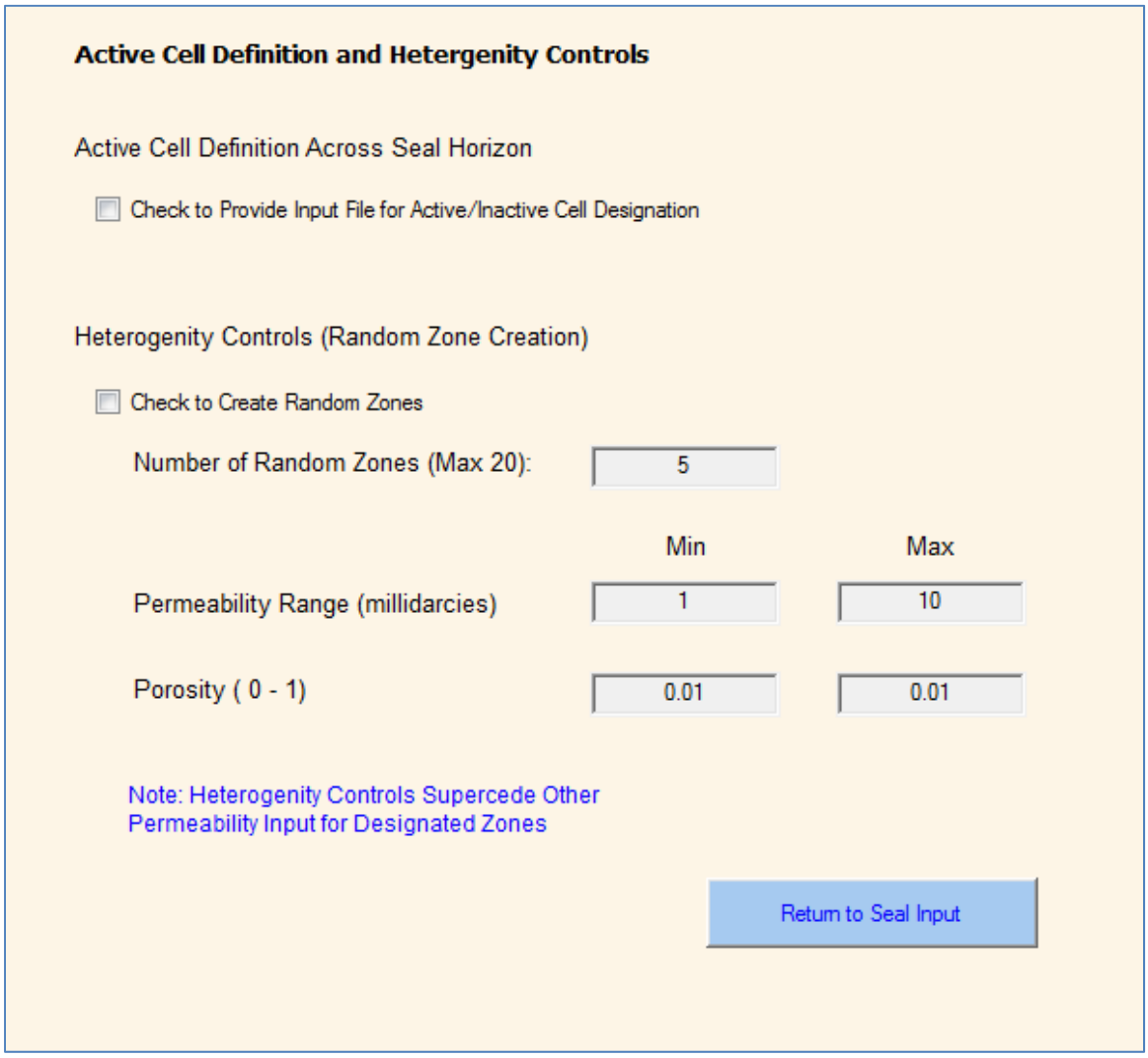


Figure 16: Active Cell Definition and Heterogeneity Dashboard.

The 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. 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.

4.1.2.5 Pressure (Upper Seal) Boundary Button

The last seal-related button is designated as "Pressure Boundary". Selecting this button opens the *upper_boundary* Dashboard that defines the pressure/saturation conditions along the top of the seal horizon (Figure 17). The current default mode for CO_2-PENS assumes 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 to more actively define the pressure and saturation conditions.

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 for CO_2-PENS as discussed, 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.

Parameters for the second option to define a function representation are also shown on this Dashboard. The equations used for the definition were described earlier in Section 2.6.

4.1.2.6 Simulation Control and Site Characteristics Buttons

The remaining two input buttons access Dashboards to define variables that are also used in CO_2-PENS. The simulation controls Dashboard (Figure 18) defines the coordinates of the model region, if the grid is uniform between the limits (if not, input files on grid coordinates and areas are required). It also defines the number of time steps. Although a box is present on this Dashboard for the number of grid divisions, this option is determined by the CO_2-PENS code and fixed for this code version.

The site characteristics Dashboard (Figure 19) 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 is required to 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 the 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 give rise to 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.

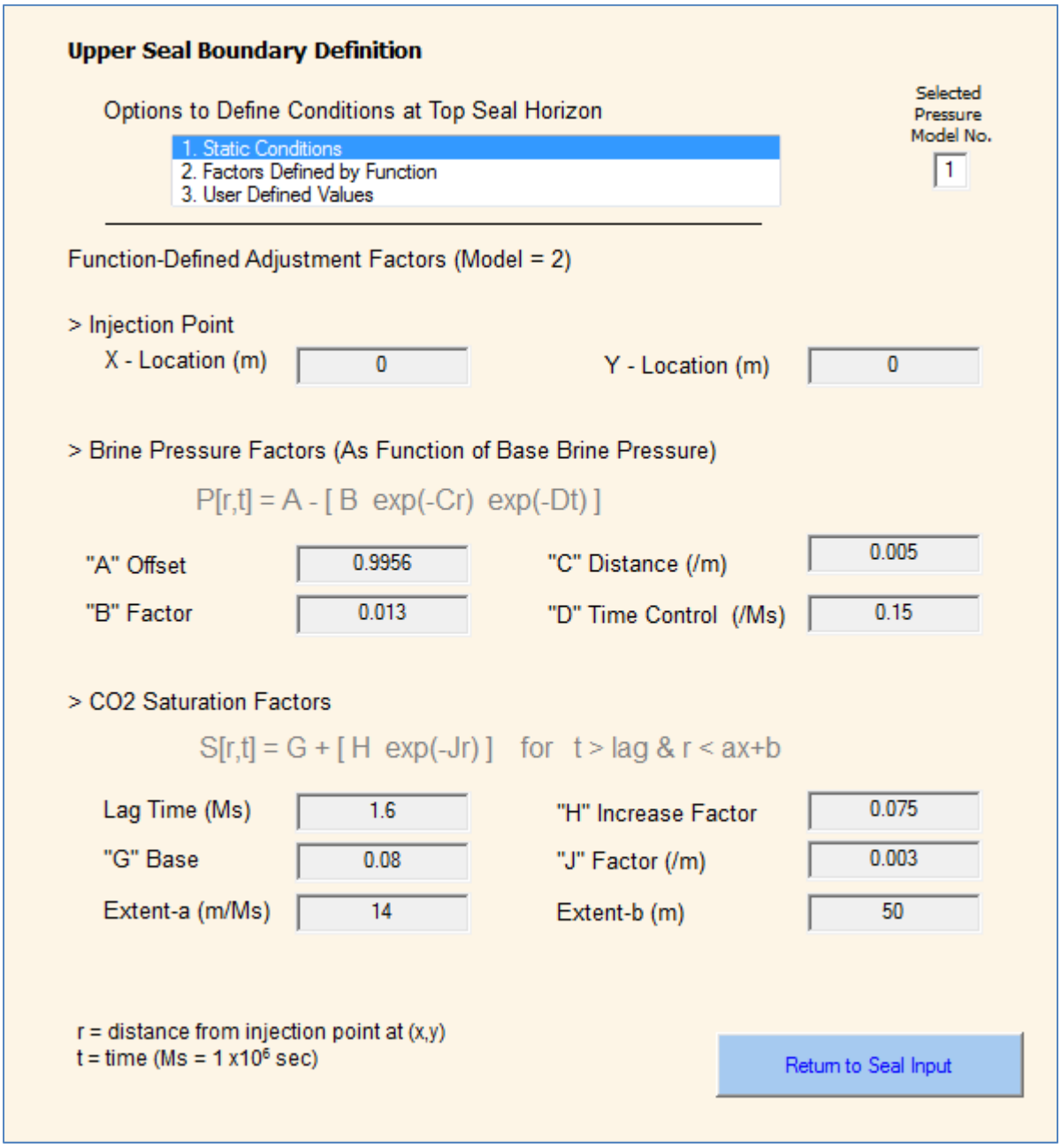


Figure 17: Upper Seal Boundary Definition Dashboard.

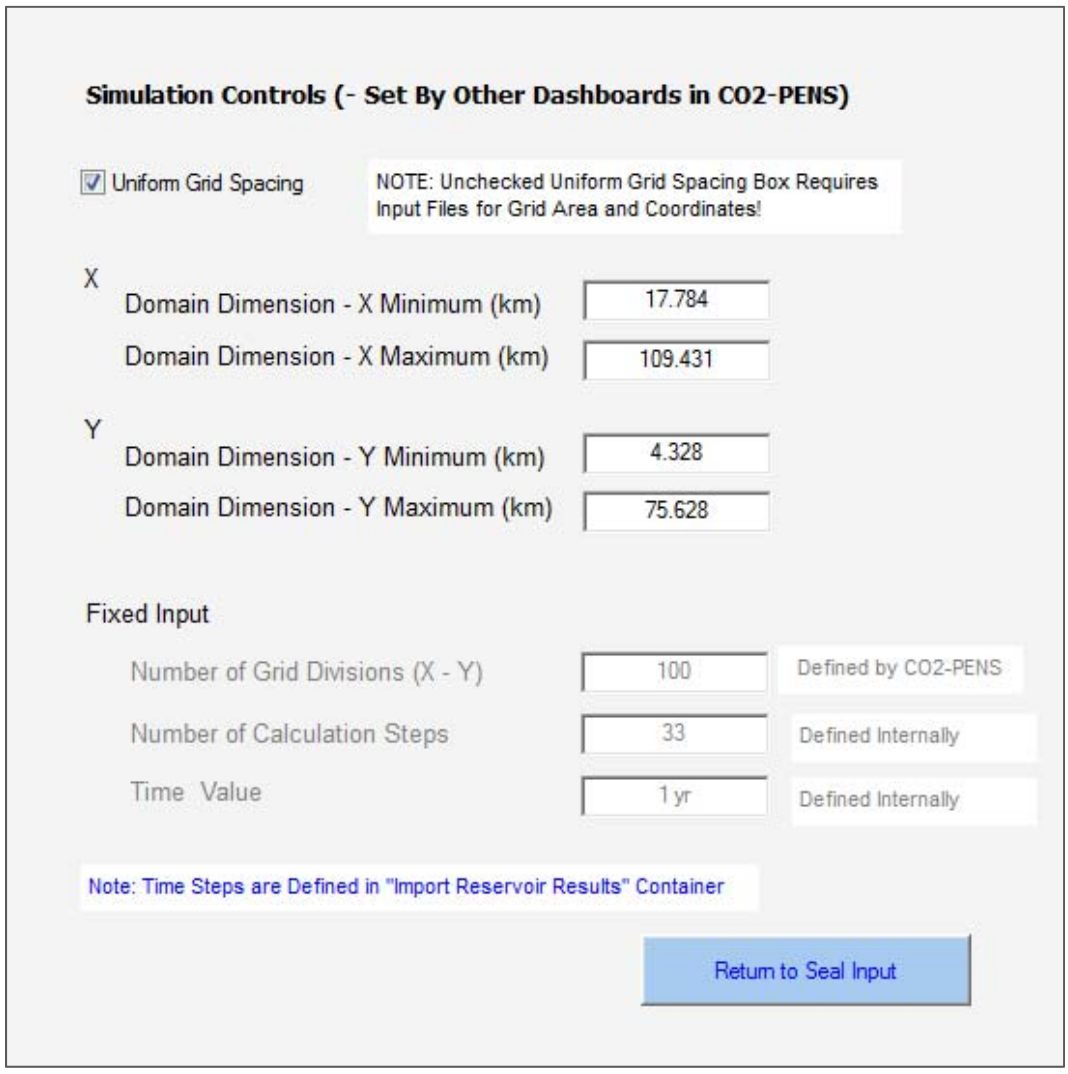
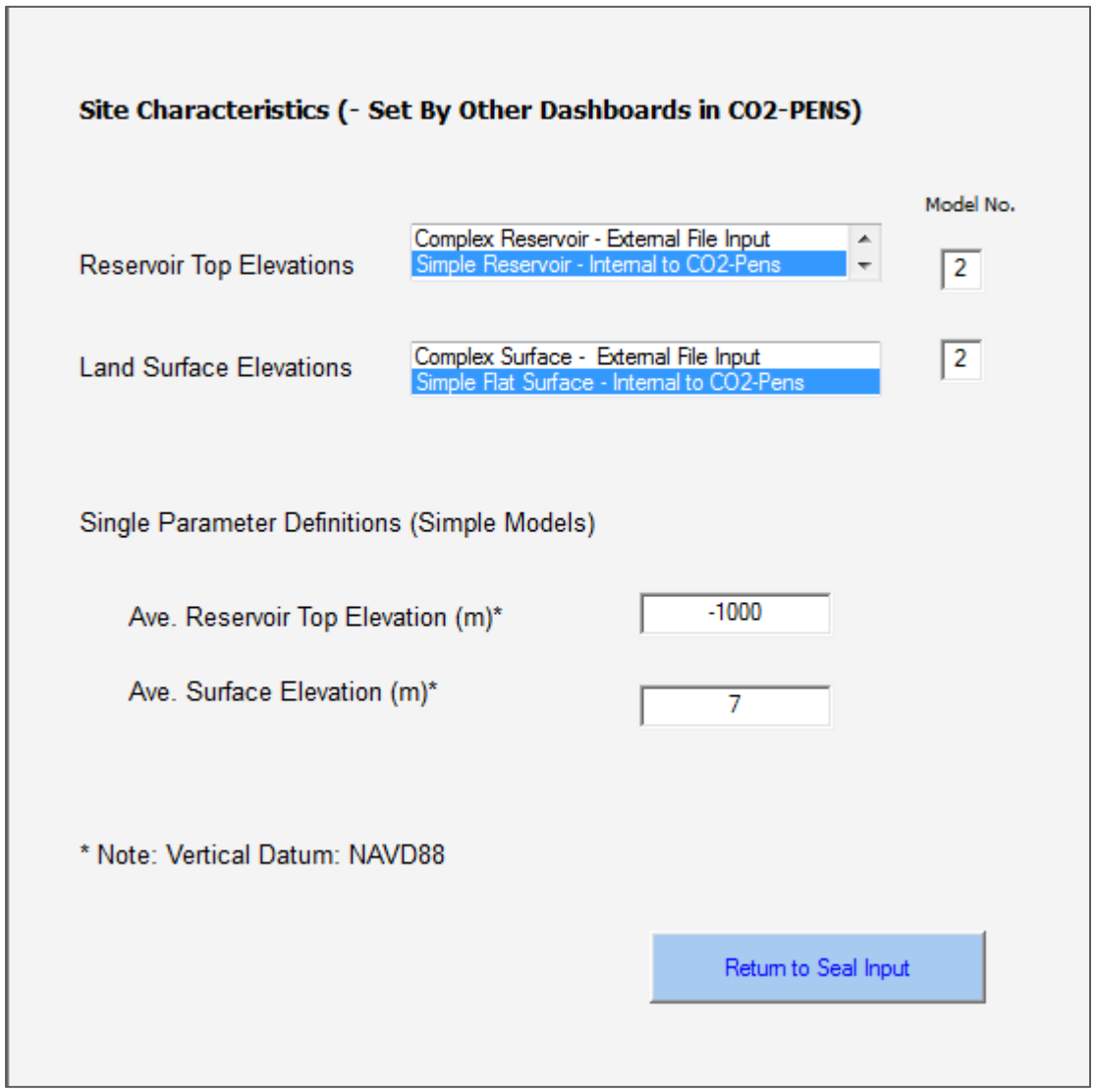


Figure 18: Simulation Controls Dashboard.



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 19: Site Characteristics Dashboard.

Input variables are also restricted by the selection of a specific permeability or thickness model. For each of the permeability options in the code shown in Figure 12, 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.

For example, in Figure 12, the stochastic model has been selected (shown in blue), and only the mean and standard deviation values for permeability and porosity together with minimum and maximum values for permeability are shown with a white background. The selected units for permeability are shown in blue (millidarcys). The remaining values (with 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 15, where a constant height model is selected and the mean and standard deviation values are shaded and unchangeable.

4.3 ACTIVE CELL DEFINITION

Computations with NSealR generally assume that each cell of the seal horizon is to be used for the specific case under consideration and computations are performed for the entire system of 10,000 cells. All cells used in the computation are labeled "active." In cases where the user wishes to use only a subset of the grid, for cells to be excluded from analysis, the user is offered two options to designate "inactive" cells.

One option (currently employed in CO_2-PENS), requires the user to designate the reservoir elevation value of the cell as the same value (or higher) than the surface elevation of the same cell. Cells with this elevation setting/condition are considered to be "inactive" and each inactive cell is excluded from flow computations. (Thickness, however, is computed for each element of the entire the grid, regardless if active or inactive.)

A second option has been added to NSealR that allows the user to designate active or inactive cells using a text file input. The option is selected by checking the appropriate box on the Active Cell Definition and Heterogeneity Dashboard (see Figure 16).

4.4 INPUT VARIABLES AND UNITS

Table 2 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.

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.

Table 2: Input variables for NSealR

Input Parameter	Units	Default Value	Range	Input Source (Comment)
Seal Permeability Parameters (Dashboard: seal_permeability_input)				
Seal Permeability Model	---	2	1, 2, 3, 4, 5	1 = Uniform Flux Through Seal Barrier 2 = Uniform Permeability 3 = Stochastic Permeability 4 = Fractured Rock Permeability 5 = User Defined Permeability External File Names: *Lookup_seal_perm.txt* *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

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

Table 2: Input variables for NSealR (continued)

Input Parameter	Units	Default Value	Range	Input Source (Comment)
Stochastic Porosity - Mean[b]	---	0.1	0 to 0.9	(Active only with Option = 3 for Seal Permeability Model)
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	^{o} degrees (from North)	0	0 to 360^o	(Active only with Option = 4 for Seal Permeability Model)
Strike of Fracturing - Standard Deviation	^{o}	0	0 to 180^o	(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)

Table 2: Input variables for NSealR (continued)

Input Parameter	Units	Default Value	Range	Input Source (Comment)
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 1000	(Active only with for aperture correction)
Horizontal Stress - Minimum	MPa	0	0 to 1000	(Active only with for aperture correction)
Strike of Maximum Horizontal Stress	degrees (from North)	30 ^{o}	0 to 360^{o}	(Strike is clockwise angle from North) (Active only with for aperture)
Effective Stiffness Factor	MPa	0.2	$\geq$ 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 1 = Stage I (Pre-Peak)Shear Stress Correction 3 = Stage III (Post-Peak)Shear Stress Correction
Shear Strength – Fracture Roughness Factor	---	5	0 to 20	(Equivalent to JRC) (Active only with aperture shear stress correction option = 1 or 3)
Shear Strength – Fracture Surface Strength	MPa	100	0 to 1000	(Active only with aperture shear stress correction option = 1 or 3)
Shear Stress – Stage I Correction, Normal Stress Factor, F_1	---	0	0 to 1000	(Active only with aperture shear stress correction option = 1)
Shear Stress – Stage I Correction, Normal Stress Factor, F_2	---	0	0 to 1000	(Active only with aperture shear stress correction option = 1)

Table 2: Input variables for NSealR (continued)

Input Parameter	Units	Default Value	Range	Input Source (Comment)
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, F_A	---	0	0 to 1000	(Active only with aperture shear stress correction option = 3)
Shear Stress – Stage III Correction, Normal Stress Factor, F_B	---	0	0 to 1000	(Active only with aperture shear stress correction option = 3)
Shear Stress – Stage III Correction, Normal Stress Factor, F_C	---	0	0 to 1000	(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 1000	(Active only with aperture shear stress correction option = 3)
Other Flow Properties (Dashboard: two_phase_seal_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	^{o}C	35^{o}	10 to 180^{o}	(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, NAVD88	-1000	-10000 to -100	(Elevation for Reference Brine Pressure)

Table 2: Input variables for NSealR (continued)

Input Parameter	Units	Default Value	Range	Input Source (Comment)
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)
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: 1 = Brooks-Corey Model 2 = Modified van Genuchten-Mualem Model
Lambda Factor, Brooks-Corey - Minimum	---	2	≥ 0.01	(Active only with relative permeability model #1) (If deterministic option selected, this is value used)

Table 2: Input variables for NSealR (continued)

Input Parameter	Units	Default Value	Range	Input Source (Comment)
Lambda Factor, Brooks-Corey - Maximum	---	3	≥ 0.01	(Active only with relative permeability model #1) (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 #1) (Checking this option will hide maximum value and use minimum value without variation)
Bubbling Pressure, Brooks-Corey - Minimum	MPa	0.01	>= 0	(Must be less than the Entry Pressure) (Active only with relative permeability model #1) (If deterministic option selected, this is value used)
Bubbling Pressure, Brooks-Corey - Maximum	MPa	0.015	>= 0	(Must be less than the Entry Pressure) (Active only with relative permeability model #1) (If variable option selected, value must be greater than minimum)
Bubbling, Brooks-Corey - Deterministic	---	Un-Checked	Checked/ Unchecked	(Active only with relative permeability model #1) (Checking this option will hide maximum value and use minimum value without variation)
m Factor, Van Genuchten-Mualem - Minimum	---	0.9	1.0 E-6 to 0.999999	(Active only with relative permeability model #2) (If deterministic option selected, this is value used)

Table 2: Input variables for NSealR (continued)

Input Parameter	Units	Default Value	Range	Input Source (Comment)
m Factor, Van Genuchten-Mualem - Maximum	---	0.91	1.0 E-6 to 0.999999	(Active only with relative permeability model #2) (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 #2) (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 #2) (If deterministic option selected, this is value used)
Alpha', Van Genuchten-Mualem - Maximum	1/Pa	2.1 E-5	≥ 0	(Active only with relative permeability model #2) (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 #2) (Checking this option will hide maximum value and use minimum value without variation)
Beta, Van Genuchten-Mualem - Minimum	---	0.5	≥ 0	(Active only with relative permeability model #2) (If deterministic option selected, this is value used)
Beta, Van Genuchten-Mualem - Maximum	---	0.55	≥ 0	(Active only with relative permeability model #2) (If variable option selected, value must be greater than minimum)

Table 2: Input variables for NSealR (continued)

Input Parameter	Units	Default Value	Range	Input Source (Comment)
Beta, Van Genuchten-Mualem - Deterministic	---	Un-Checked	Checked/ Unchecked	(Active only with relative permeability model #2) (Checking this option will hide maximum value and use minimum value without variation)
Gamma, Van Genuchten-Mualem - Minimum	---	0.3333	≥ 0.01	(Active only with relative permeability model #2) (If deterministic option selected, this is value used)
Gamma Factor, Van Genuchten-Mualem - Maximum	---	0.40	≥ 0.01	(Active only with relative permeability model #2) (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 #2) (Checking this option will hide maximum value and use minimum value without variation)
Seal Thickness (Dashboard: thickness_input)				
Seal Barrier Height Options	---	1	1, 2, 3	Options: 1 = Constant Height for Seal Barrier- Internal to CO_2-PENS 2 = Stochastic Height of Seal Barrier - Variation - Internal to CO_2-PENS 3 = User Defined Variation of Seal Barrier - External File Input External File Name: Lookup_seal_thick.txt
Constant Height	m	20	0.1 to 1000	(Active only with Option = 1 for Seal Barrier Height Model)

Table 2: Input variables for NSealR (continued)

Input Parameter	Units	Default Value	Range	Input Source (Comment)
Stochastic Height - Mean	m	30	0.1 to 1000	(Active only with Option = 2 for Seal Barrier Height Model)
Stochastic Height - Standard Deviation	m	0	0 to 1000	(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)
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 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)

Table 2: Input variables for NSealR (continued)

Input Parameter	Units	Default Value	Range	Input Source (Comment)
Upper Seal Boundary Definition (Dashboard: simulation_input)				
Options to Define Conditions at Top of Seal Horizon	---	1	1, 2, 3	Option: 1 = Static Conditions 2 = Define Using Analytic Functions 3 = User Defined Values External File Names: Lookup_seal_top_ press.txt 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)
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)

Table 2: Input variables for NSealR (continued)

Input Parameter	Units	Default Value	Range	Input Source (Comment)
Simulation Controls (Dashboard: simulation_input)				
Uniform Grid Spacing	---	Checked	Checked / Unchecked	Unchecked option requires input of grid areas and coordinates External File Names: Lookup_seal_grid_area.txt; Lookup_seal_grid_coord.txt
X Domain Dimension; X Min.	km	0	0 to 1000	
X Domain Dimension; X Max.	km	10	0 to 1000	
Y Domain Dimension; Y Min.	km	0	0 to 1000	
Y Domain Dimension; Y Max.	km	10	0 to 1000	
Number of Grid Divisions	---	100	100	(Defined by CO_2-PENS)
Number of Calculation Steps	---	33	≥ 0	(Not Used)
Time Value	yr	1	---	(Not Used)
Site Characteristics (Dashboard: site_characteristics)				
Reservoir Top Elevations	---	2	1, 2, 3	Options: 1 = Complex Reservoir - External File Input 2 = Simple Reservoir - Internal to CO_2-PENS 3 = Multiple Realizations for Reservoir (Not Supported in NSealR) External File Name: Lookup_reservoir_elev.txt

Table 2: Input variables for NSealR (continued)

Input Parameter	Units	Default Value	Range	Input Source (Comment)
Land Surface Type	---	2	1, 2	Options: 1 = Complex Surface - External File Input 2 = Simple Flat Surface - Internal to CO_2-PENS External File Name: Lookup_land_surface.txt
Avg. Reservoir Top Elevation[a]	m, NAVD88	-1000	-10000 to -100	(Active only with Option = 2 for Reservoir Top Elevation)
Avg. Surface Elevation[a]	m, NAVD88	0	-1000 to +10000	(Active only with Option = 2 for Land Surface Elevation)

Note:

[a] The 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. CO_2-PENS specifies elevations in terms of above sea level.

[b] 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.

4.5 EXTERNAL FILE INPUT

4.5.1 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[16], which dictates the inclusion of several header lines followed by the data array (GoldSim, 2010). 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. 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 Appendix E. Table 2 indicates the type of data provided by each file, when the user option is selected.

4.5.2 Fluid Property Input

To define density, viscosity, and solubility parameter values that are functions of temperature, pressure and/or salinity, 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 look up table approach is from file, *LUT_CO2_viscosity_DLL.dll*).

4.5.3 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 CO_2-PENS.) Note that data has to be provided for each time step.

[16] The text file format used by CO_2-PENS differs from the text format specified by GoldSim. CO_2-PENS employs specialized DLLs for importing data, and when NSealR is incorporated into CO_2-PENS, the corresponding text file formats will need to be altered correspondingly.

Time steps (for control for importing reservoir saturation and pressure) are defined in the current version of NSealR in an Excel file, entitled "time_series.xlsx" and is also located in the directory "\Lookup_Tables\transfer_data." The specific times for each time step are entered in row format, starting in column 2, with input descriptions in column 1. Again, for different cases, this file can be modified, replaced or a new linkage established.

5. OUTPUT CONTROLS

GoldSim 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 into NSealR.

Special output controls are defined on the seals output Dashboard (Figure 20). The first control, Text File Output on 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 option (if checked) 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.[17]

A similar output can be implemented by checking the "Excel File Output on Leakage" option on the Dashboard for the run; in this case, results will be exported to an Excel workbook[18], 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 output Dashboard also permits the output of specific input data at a specified realization. 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.

[17] 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.

[18] 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 MS Excel.

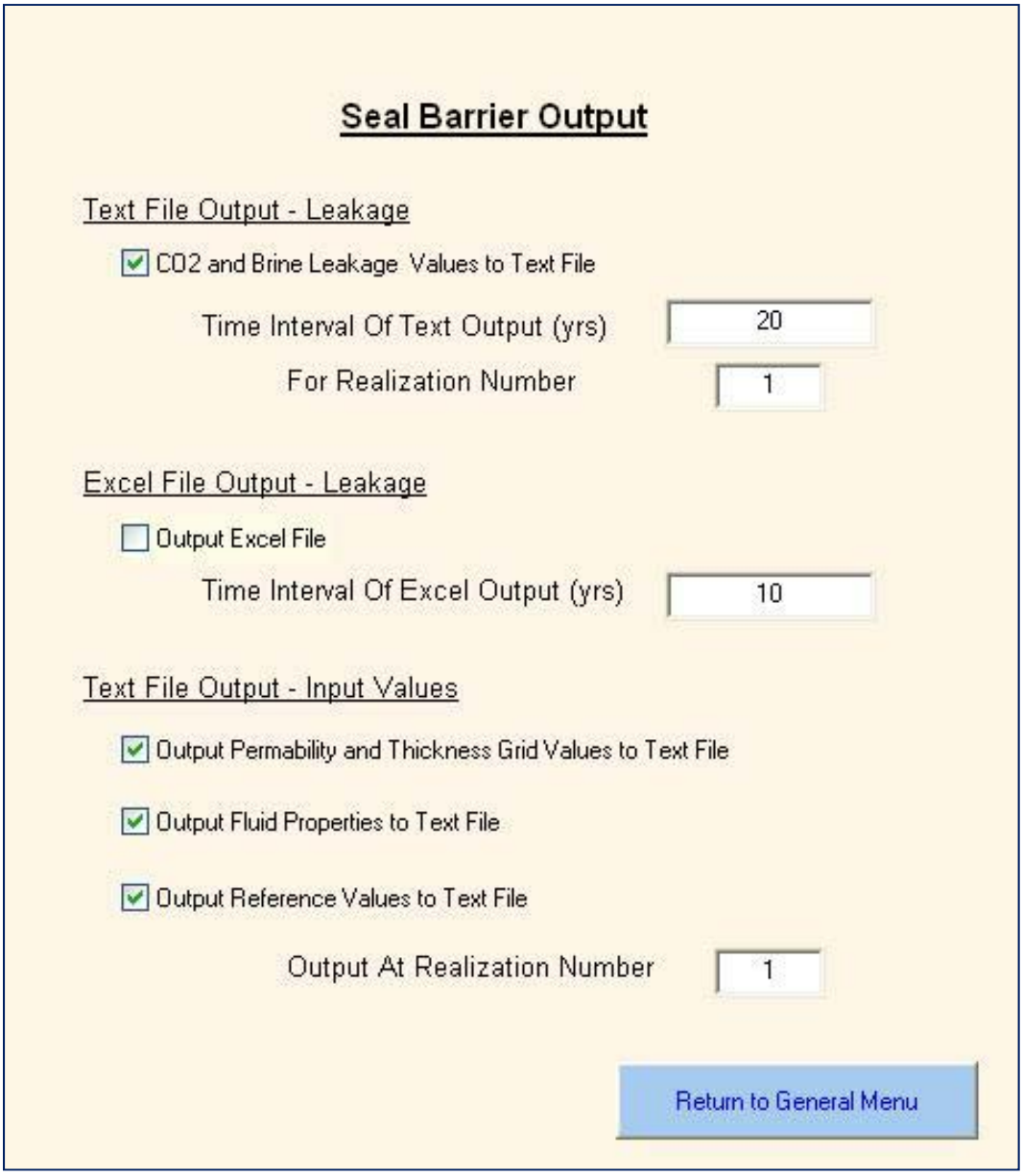


Figure 20: Output Controls Dashboard.

6. CONCLUSIONS

The NSealR code is a ROM that describes the basic response of a seal barrier for use in risk evaluations for CO_2 storage. As noted, the model makes a number of assumptions and the theory utilized at this point is somewhat constrained to describe the vertical, two-phase flow of supercritical CO_2 flowing from an injection reservoir to an overlying aquifer through a relatively-impermeable rock horizon, saturated with saline groundwater.

This user guide provides the salient details for the use of the third-generation NSealR code as a stand-alone computer code. This guide however, is not an extensive user manual and should be used together with the GoldSim User Manuals as a basis for understanding the NSealR code and its operation.

It is noted that the current version of the NSealR code has not been verified against the other flow codes to demonstrate that it can accurately simulate flow under simple conditions, nor essentially replicate the results of more complex codes within an acceptable margin of error. The code has also not been validated by comparison to a field trial or data.

Use of the code should be limited to the identified target range of conditions. The range of acceptable parameters in NSealR has been specifically targeted at in situ conditions representative of typical conditions for storage. The fluid property database in NSealR is accurate for temperatures between 0°C and 180°C, and pressures of 0.1 and 60 MPa. Use of the code outside these limits will cause code errors in the Lookup Tables elements.

This version of the code is a third-generation NRAP development code; but in the future, it is expected that the code will be verified and the underlying theory will be expanded to allow the computer model to simulate more realistic and complex processes with confidence while focused primarily on the first order processes of CO_2 storage.

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APPENDIX A: FRACTURED ROCK MODEL AND IN SITU STRESS-APERTURE CORRECTION

A.1. General

As noted earlier, NSealR allows the user to define an equivalent permeability based on rock fracture characteristics including fracture apertures (an option shown on the Seal Permeability Dashboard). In defining the aperture values for this model, the user can choose to consider the influence of in situ stress field on apertures. This option is selected using a button on the Seal Permeability Dashboard (Figure 12) which provides access to another Dashboard (Figure 13) to define the set of relevant parameters together with the horizontal, secondary in situ principal stresses. The underlying theory for the stress-related aperture corrections (and how these parameters are defined) is provided in this appendix.

In the following sections, it is understood that for fracture flow analyses, the term *aperture* represents the equivalent hydraulic aperture of a fracture using a parallel plate representation of fracture flow.[19]

A.2. Fractured Rock Model - Fracture Permeability

Fluid flow through a rock mass will occur through the intact rock material (the matrix) as well as along fractures in the rock mass. In many cases, the flow through the rock matrix can be ignored relative to the larger volume of flow through the fractures. To model the flow of fluids through a fracture, a well-known solution to the Navier-Stokes equation is adopted for the flow of a viscous fluid in a narrow gap between parallel, smooth plates (e.g., described in Zimmerman and Bodvarsson, 1996). The relationship is often termed the "cubic law" and is written describing the volumetric flow rate, Q as (modified from Gudmundsson, 2011; Eq. 15.10):

$$Q = \left(\frac{\rho_z g w a^3}{12\mu_z}\right)(-\nabla h) \qquad \text{(A-1)}$$

where g is the acceleration due to gravity, ρ_z is the fluid density, w is the width of the gap perpendicular to the flow vector, a is the aperture or the distance between the plates, μ_z is the

[19] The "aperture" in NSealR is the hydraulic aperture and represents a specific mathematical construct that is proportional to the observed effective fracture permeability. Many authors implicitly assume that the hydraulic aperture is equivalent to, or in some manner related to, the mechanical aperture. However, as observed in the laboratory, the basic flow regime along a fracture changes from a condition analogous to parallel plate flow at low stresses to flow through varying channelized across the fracture surface at higher stresses. When the later condition is achieved, a further stress increase has little effect on the flow within the channels, or simply, the effective permeability of the fracture obtains a residual value. Hence, while the mechanical aperture may continue to change with increasing applied stress, the hydraulic aperture does not. So any definition of aperture parameters for NSealR should be based on observed effective permeability changes and not directly on mechanical response.

dynamic (absolute) viscosity of the fluid, and ∇h is the gradient of hydraulic head across the flow distance. As the flow is in the opposite direction to the hydraulic head gradient, a negative sign is introduced.

For an irregular set of fractures contained in a local area, A_{cell}[20], the following approximation is used for the specific discharge across the entire area, q_{cell}:

$$q_{cell} = \frac{Q}{A_{cell}} = \left[\left(\frac{1}{A_{cell}}\right)\left(\frac{\rho_z g}{\mu_z}\right)\left(\frac{1}{12}\right)\left(\sum_{i=1}^{m} w_i a_i^3\right)\right](-\nabla h) \quad \text{(A-2)}$$

where the summation includes all fractures in the area parallel to the flow vector (m fractures).

By analogy to Darcy's law, the terms within the square brackets in Equation A-2 represent the coefficient of permeability or hydraulic conductivity, K_{cell}, across the area (e.g., Gudmundsson, 2011; Eq. 15.1). To state this explicitly, the hydraulic conductivity of the fracture set is:

$$K_{cell} = \left[\left(\frac{1}{\mathrm{A_{cell}}}\right)\left(\frac{\rho_z g}{\mu_z}\right)\left(\frac{1}{12}\right)\left(\sum_{i=1}^{m} w_i a_i^3\right)\right] \quad \text{(A-3)}$$

In turn, the hydraulic conductivity is related to the intrinsic permeability, k, as (e.g., Gudmundsson, 2011; Eq. 15.4):

$$K = \frac{k\rho_z g}{\mu_z} \quad \text{(A-4)}$$

Applying this Equation A-4 to Equation A-3, the equivalent permeability of the fracture set, k_{cell}, can be defined as:

$$k_{cell} = \frac{1}{12\mathrm{A_{cell}}}\left(\sum_{i=1}^{m} w_i a_i^3\right) \quad \text{(A-5)}$$

A.3. Fractured Rock Model - Porosity[21]

Similar to permeability, the connected porosity of the fractured rock mass can be computed by assuming the connected porosity of the rock material is small with respect to that of the porosity present in existing fractures. The porosity ratio in NSealR represents the volume of the fractures of the local area or cell.

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[20] The area of a cell in NSealR.

[21] The current flow models in NSealR do not include the storage term (porosity) in the flow equation.

Expressing the local porosity of the rock mass, ϕ_{cell}, as a ratio of the sum of the volume of all through-going fractures of the fracture set to the total local volume, the representation becomes:

$$\phi_{cell} = \left[\frac{1}{tA_{cell}}\right]\left(t\sum_{i=1}^{m} w_i a_i\right) = \left[\frac{1}{A_{cell}}\right]\left(\sum_{i=1}^{m} w_i a_i\right) \quad \text{(A-6)}$$

where the sum is conducted over each fracture *i* and for all *m* fractures in the cell area, *t* is the thickness of the seal barrier at this point (cell height), A_{cell} is the local area (cell area), w_i is the width of a fracture *i* perpendicular to the flow vector for the fracture (fracture length[22]), and a_i is the aperture of the fracture. As each fracture is assumed to penetrate the entire cell height, the porosity in this case reduces to the ratio of the sum of the fracture areas to the total area.

A.4. Fractured Rock Model - Normal Stress Correction of Aperture

Based on laboratory testing with fractures, the influence of normal stress on hydraulic conductivity or permeability of a discontinuity has been shown to be generally hyperbolic (or exponential) in nature as illustrated in Figure A-1 (e.g. NRC, 1996, p. 113).[23] Conceptually, this hydraulic response curve can be divided into three regimes: (1) a highly-nonlinear regime where a stress increase can cause a significant decrease in permeability (and therefore in the hydraulic aperture); (2) a transition regime where there is a more gradual rate of change and the aperture is approximately linearly-related to stress; and (3) a stasis regime where the aperture is relatively insensitive to stress change. These regions can be subdivided in terms of normal stress values, σ_1 and σ_2 shown in Figure A-1.

If desired, the user can implement in NSealR an aperture correction that reflects this trend with respect to the regional, in situ stress. Specifically, when the option is selected, the stochastically-generated fracture aperture values in NSealR are corrected for the in situ stress normal to the fracture, with higher normal stresses reducing the generated aperture value with a minimum aperture achieved upon reaching a defined stress limit.

The adopted correction model is empirical in nature and makes several assumptions. It considers that each fracture is *clean* (unfilled), that the surface relatively *fresh* (unweathered), and that the fracture is in a *virgin state* (the fracture has not been extensively sheared and significant stress reversals have not occurred). With these conditions and for the single loading case (i.e., no stress reversals), the response shown in Figure A-1 is considered representative.

In this model, the corrected aperture, a_n, is expressed in terms of the total effective normal stress on the fracture (i.e., the secondary stress perpendicular to the fracture) and the maximum aperture, using a hyperbolic equation. For simplicity, the relationship extends only to the limit

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[22] The fracture length in the 2-D plane, as defined by user input.

[23] Laboratory data are based on the response of mechanical aperture to normal stress. A similar relationship is understood for the equivalent hydraulic aperture, which is the focus of this discussion.

stress where residual aperture is considered to be achieved (shown as σ_2 in Figure A-1). Also, the fracture is defined as locked for negative effective normal stresses. For these conditions, the model representation is:

$$a_n = \left[1 - \beta\left(\frac{\sigma_n}{\sigma_n + \psi}\right)\right] a_{max} \quad \text{for } 0 \le \sigma_n \le \sigma_{limit} \tag{A-7a}$$

$$a_n = [\theta_{res}] a_{max} \quad \text{for } \sigma_n > \sigma_{limit} \tag{A-7b}$$

$$a_n = a_{max} \quad \text{for } \sigma_n < 0 \tag{A-7b}$$

where σ_n is the effective normal stress on the fracture, β is the fracture characteristic term, θ_{res} is the residual aperture factor, a_{max} is the maximum (uncorrected) fracture aperture and ψ is the effective fracture stiffness

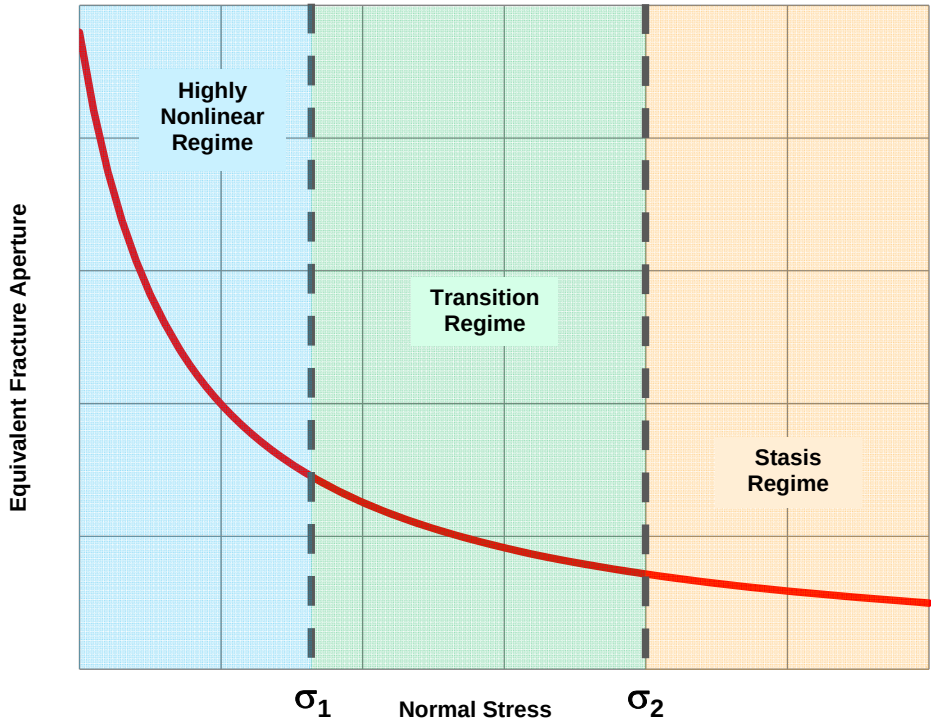


Figure A-1: Conceptual aperture-normal stress curve.

The fracture characteristic term, β is a function of the limit stress, $\sigma_{limit,}$ the residual aperture factor, θ_{res}, and the effective fracture stiffness, ψ, expressed as:

$$\beta = (1 - \theta_{res})\left[\frac{\sigma_{limit} + \psi}{\sigma_{limit}}\right] \quad \text{where } 0 \le \theta_{res} < 1.0 \tag{A-8}$$

In this model, θ_{res} is the ratio of the residual aperture to the maximum aperture (controlling the value in the status regime in Figure A-1). In addition, the effective fracture stiffness, ψ, controls the curvature of the relationship between normal stress and corrected aperture, with larger values providing a more linear decrease of aperture with increasing stress (see Figure A-2).

To complete this discussion, it is noted that the effective normal stress is understood as the difference between the total normal stress, σ_{normal}, and the fracture fluid pressure, P_{frac} or:

$$\sigma_n = \sigma_{normal} - P_{frac} \qquad \text{where } \sigma_{normal} \geq 0.0 \tag{A-9}$$

To reduce user input requirements of this model in NSealR, the stress limit is assigned an internal value of 40 MPa, and the minimum or residual aperture at this point is presumed to be 10%[24].

To implement this model, the following process is followed:

1. The maximum aperture value (a_{max}) as well as the fracture orientation is stochastically generated based on user input.
2. The total stress normal (perpendicular) to the fracture is computed from the in situ horizontal secondary principal stresses at depth (stress ellipse) considering the angle between the fracture strike and ellipse orientation.
3. The total normal stress and the fluid pressure in the fracture are used to compute the effective normal stress, σ_n on the fracture (Equation A-9)
4. A correction factor is then computed depending on the normal stress:
    a. If the normal stress is positive and less than the limit stress, the limiting closure value, β, is computed (Equation A-8) using effective fracture stiffness (ψ) defined by the user and the other parameters as assigned by NSealR. The correction factor is then computed using Equation A-7a.
    b. If the normal stress is positive and greater than the limit stress, the correction factor is assigned to the residual stress factor, θ_{res}, as shown for Equation A-7b.
    c. If the normal stress is positive, the correction factor is set equal to 1.0, as shown for Equation A-7c
5. The correction factor is then multiplied against the maximum aperture to obtain the corrected aperture, which in turn is used to compute the permeability of the cell.

[24] The limit stress value of 40 MPa was chosen based on a review of selected testing literature. It is the effective stress on the fracture and set internally as the variable, "limit_stress." The residual aperture is assumed and set internally as the variable, "residual_aperture_allowance."

To provide some guidance to the user, the stress-corrected aperture curve for NSealR is illustrated in Figure A-2 for selected values of ψ.

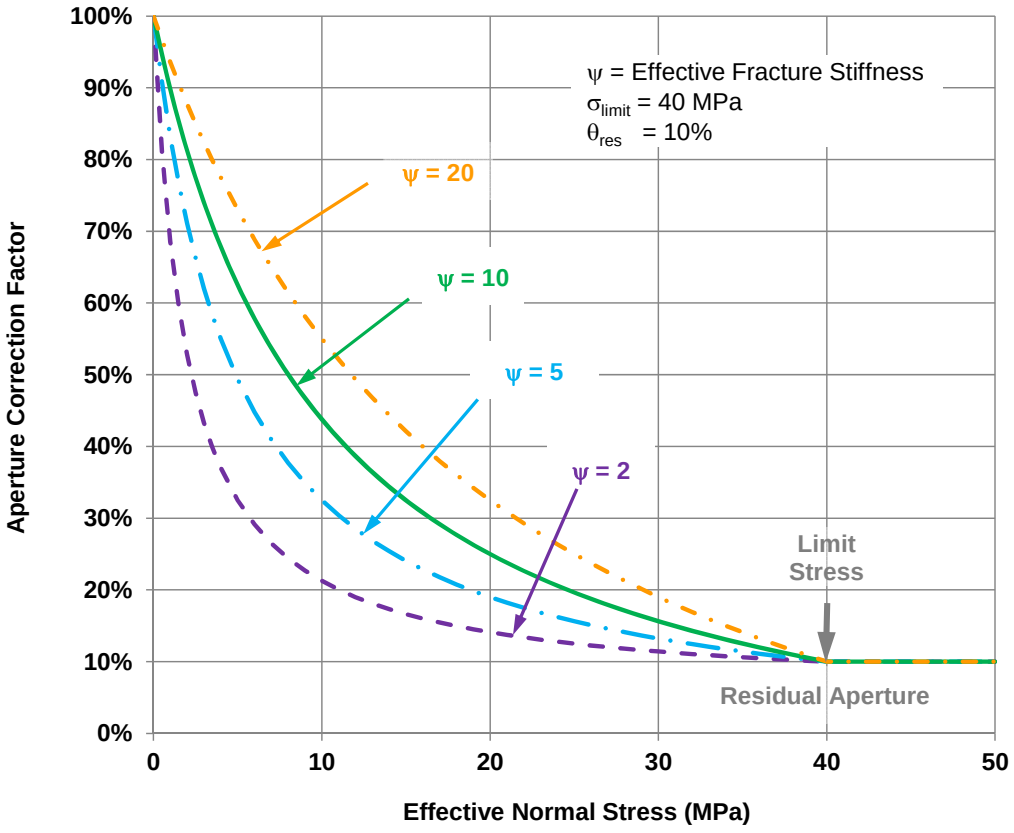


Figure A-2: Aperture correction factor as a function of normal stress.

A.5. Fractured Rock Model - Shear Stress Correction of Aperture

A.5.1. Shear Model Types

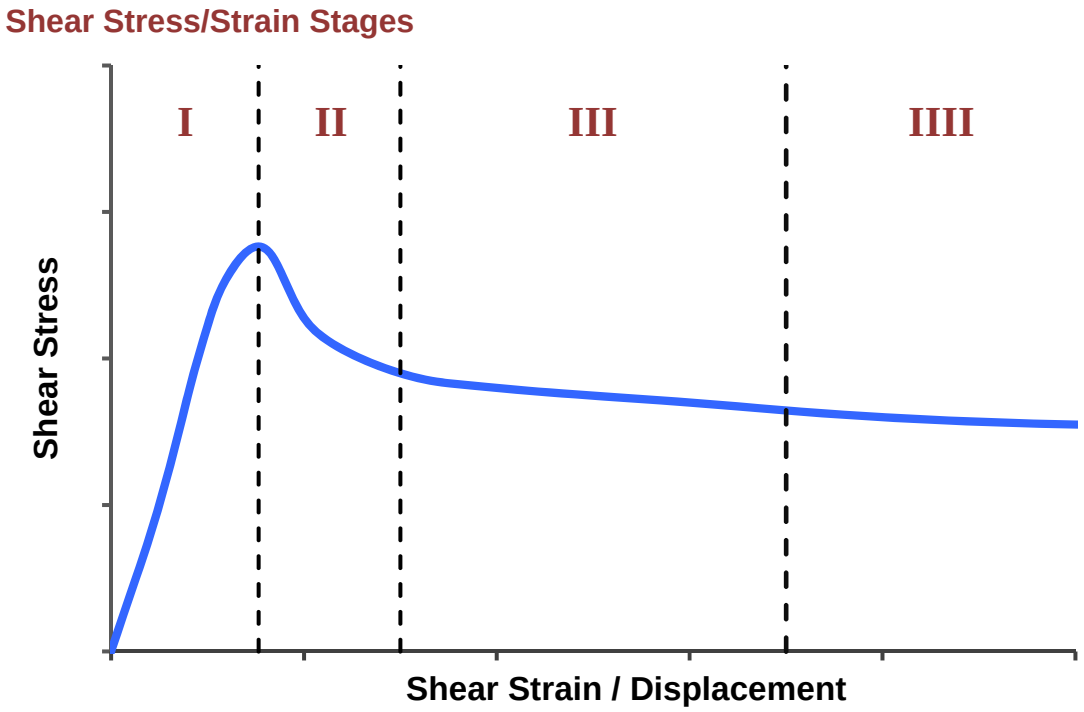
If desired, the user can also implement in NSealR an aperture correction that reflects shear stress on the fracture based on the regional, in situ stress (in addition to the normal stress correction). Specifically, when the option is selected, the stochastically-generated fracture aperture values in NSealR are corrected for the shear stress component of the in situ stress on the fracture. The shear stress correction is subdivided depending on the amount of shear strain that has occurred on the fracture, with one correction approach for pre-peak stress and the other for post-peak stress.

The typical response of a clean, fresh fracture is shown in Figure A-3 for a direct shear test (which maintains a constant rate of shear strain on a fracture subjected to a constant normal load).

Conceptually, the fracture response during shear can be subdivided into stages depending on the amount of shear strain (e.g., Barton, 1973):

1. Initial (pre-peak stress) deformation
2. Post peak stress response/deformation
3. Extended response/deformation
4. Ultimate response/deformation

As shear occurs, the characteristics of the fracture surface change, which in turn, changes fracture permeability in all directions, not just in the direction of shearing force. Depending on the normal stress and fracture roughness, the fracture may dilate (deform perpendicular to the fracture) significantly at low stresses and will not show a distinct peak stress value. At higher stresses, the asperities on the surface will fail, little dilation occurs and a strong peak shear stress is typically evident in the stress-strain curve.[25] A number of factors are required to be considered in describing the fracture permeability during this overall process.



Note: Based on Barton (1973), Figure 8.

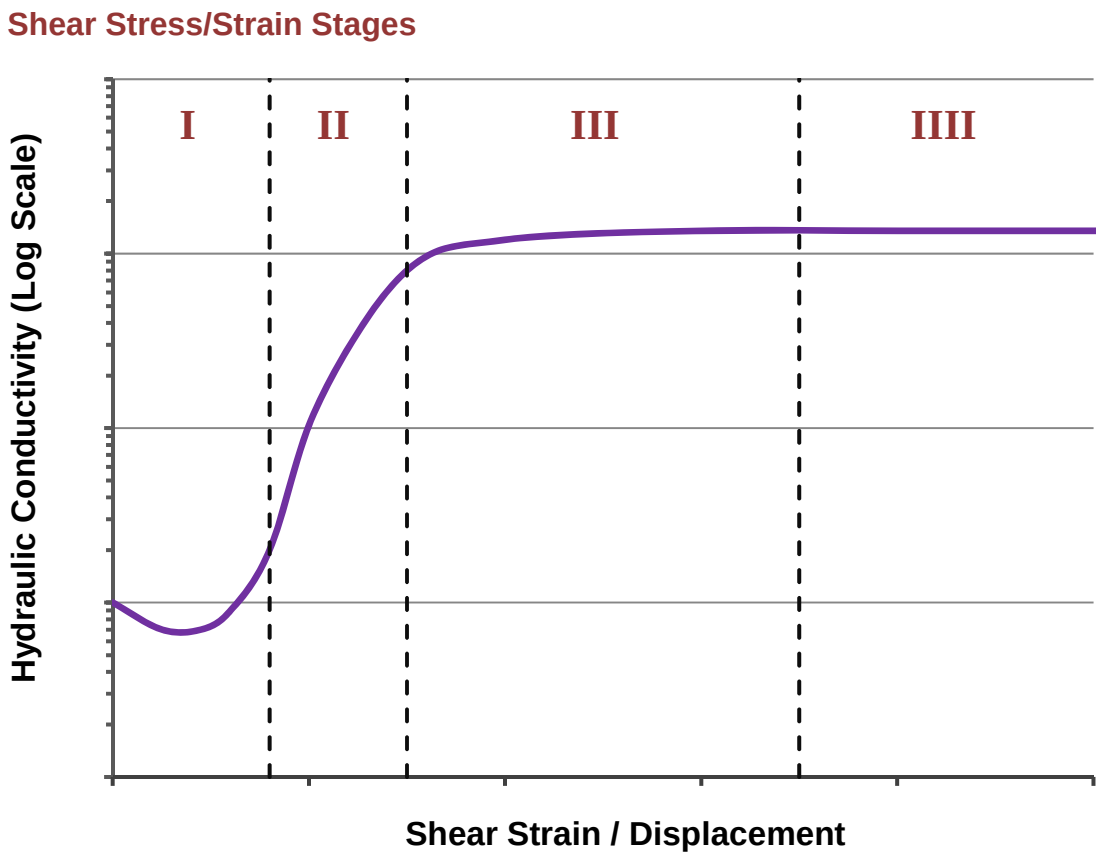
Figure A-3: Idealized stages during shear deformation of a fracture.

[25] The distinct peak in shear stress decreases with increasing smoothness/flatness of the fracture, i.e., with decreasing roughness

To capture the significant influence of the in situ shear stress on permeability, several simplifications are made to capture primary effects in an empirical model. For current purposes, NSealR provides approaches to describe permeability during only two stages, Stage I (pre-peak) and Stage III (extended).

A.5.2. Stage I Shear Model

Deformation during Stage I represents a condition of small shear strain (on the order of 1%) which precedes the peak shear stress (failure) on the fracture and subsequent large shear displacement. Based on testing and other evaluations, it is expected that the permeability of the fracture will initially decrease with shear strain (e.g., Iragorre 2010; Alejano and Alonso, 2005; Chen and Zhou, 2011) and then as the fracture surfaces fully engage during shear, the permeability will sharply increase just prior to achieving the peak shear stress, depending on the normal stress (see Figure A-4). This change in permeability is taken as essentially parabolic in nature. Further, the relationship between shear stress-strain (shear stiffness) during this stage is presumed to be largely elastic, but non-linear, and varying with the shear strain.



Note: Vertical divisions shown correspond to those shown in Figure A-3.

Figure A-4: Conceptual fracture permeability changes vs. shear strain displacement.

The Stage I empirical model employs a parabolic equation to capture the initial decrease and subsequent increase in permeability. In the model, the corrected permeability, k_s, can be represented as:

$$k_s = [A'\gamma_n^2 + \mathrm{B}'\gamma_n + C']\mathrm{k}_c \tag{A-10}$$

and adjusted to define a correction factor $F_{a\text{-}I}$:

$$F_{a-I} = \frac{k_s}{k_c} = [A'\gamma_n^2 + \mathrm{B}'^{\gamma_n} + C'] \tag{A-11}$$

In these equations, γ_n is the ratio of shear strain to the peak shear strain of the fracture, *A'* is a normal stress-dependent shear parameter, *B'* and *C'* are constant shear parameters, and k_c is the current fracture permeability.[26]

The shear parameters in the equation are defined as:

$$A' = \left[F_1\left(\frac{\sigma_n}{\sigma_c}\right)\right]^s + \mathrm{F}_2 \tag{A-12}$$

$$B' = -1 \tag{A-13}$$

$$C' = +1 \tag{A-14}$$

where F_1 and F_2 are normal-stress constants, *s* is the characteristic exponent for the shear, σ_n is the effective normal stress on the fracture and σ_c is uniaxial compressive strength of the fracture surface. For the current implementation in NSealR, *s* is set equal to -0.25.

To relate the main expression in terms of shear strain (in Equation A-10) to shear stress, the normalized shear strain, γ_n can be expressed in terms of the normalized shear stress, τ_n, using a hyperbolic representation, and reducing the form to solely a function of the curvature factor, *n* as:

$$\gamma_n = \left[\frac{(1-n)\tau_n}{1-(n\tau_n)}\right] \qquad \text{where } 0.0 \le n < 1.0 \tag{A-15}$$

[26] For the Stage I model, the aperture correction is applied after the normal stress correction; hence k_c is the corrected permeability based on the normal stress alone.

The normalized shear stress is described simply as the ratio of the current shear stress on the fracture, τ, to the peak shear stress, τ_p:

$$\tau_n = \left[\frac{\tau}{\tau_p}\right] \tag{A-16}$$

In the hyperbolic equation (A-15), the curvature factor, *n*, is allowed to vary between 0 and 1 with a value of zero producing a straight line and larger values producing a more non-linear relationship.

The peak shear stress can be described using the relationship developed by Barton (1976):

$$\tau_p = \sigma_n tan\left(\alpha log\left(\frac{\sigma_c}{\sigma_n}\right) + \phi_r\right) \tag{A-17}$$

where σ_c is taken as the uniaxial compressive strength of the fracture surface[27], α is a fracture roughness factor[28], and ϕ_r is the residual strength angle. The term α in this equation is limited to the range of 0 to 20, corresponding to the smoothest to the roughest fracture surface (per the JRC developed by Barton, 1973). Also, as noted by Barton and Choubey (1977), ϕ_r is typically within the range of 25° to 30°, and therefore, ϕ_r is set equal to 30° in the Stage I model. [29]

Finally, the permeability is considered to be proportional to the cube of the hydraulic aperture, so the final equation for this model becomes for the corrected aperture factor, F_a' is the cube root of the correction factor in Equation A-11:

$$F_{a-I}' = [A'\gamma_n^2 + \mathrm{B}'\gamma_n + C']^{\frac{1}{3}} \tag{A-18}$$

In summary, five parameters in addition to the normal and shear stresses on the fracture are required to define the response under the NSealR Stage I model:

- F_1 and F_2, shear normal-stress constants
- *n,* curvature factor on shear stress-strain
- σ_c, uniaxial compressive strength of the rock surface
- α, fracture roughness factor.

In NSealR, two of the Stage I parameters, s and ϕ_r, are set to default values.

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[27] The form of the equation presumes that the uniaxial compressive strength of the fracture surface (or wall) is equal to σ_c, the uniaxial compressive strength of rock material, which is consistent with a fresh fracture.

[28] This term is identical to the joint roughness coefficient (JRC) that was developed by Barton (1973) for describing and estimating the surface roughness of a fracture.

[29] This simplification is to reduce the required input for NSealR. Note that Barton and Choubey (1977) also set ϕ_r to 30° for their analyses.

Figure A-5 illustrates the use of the shear aperture correction for permeability. While complex, the equation form clearly simulates the desired response as discussed.

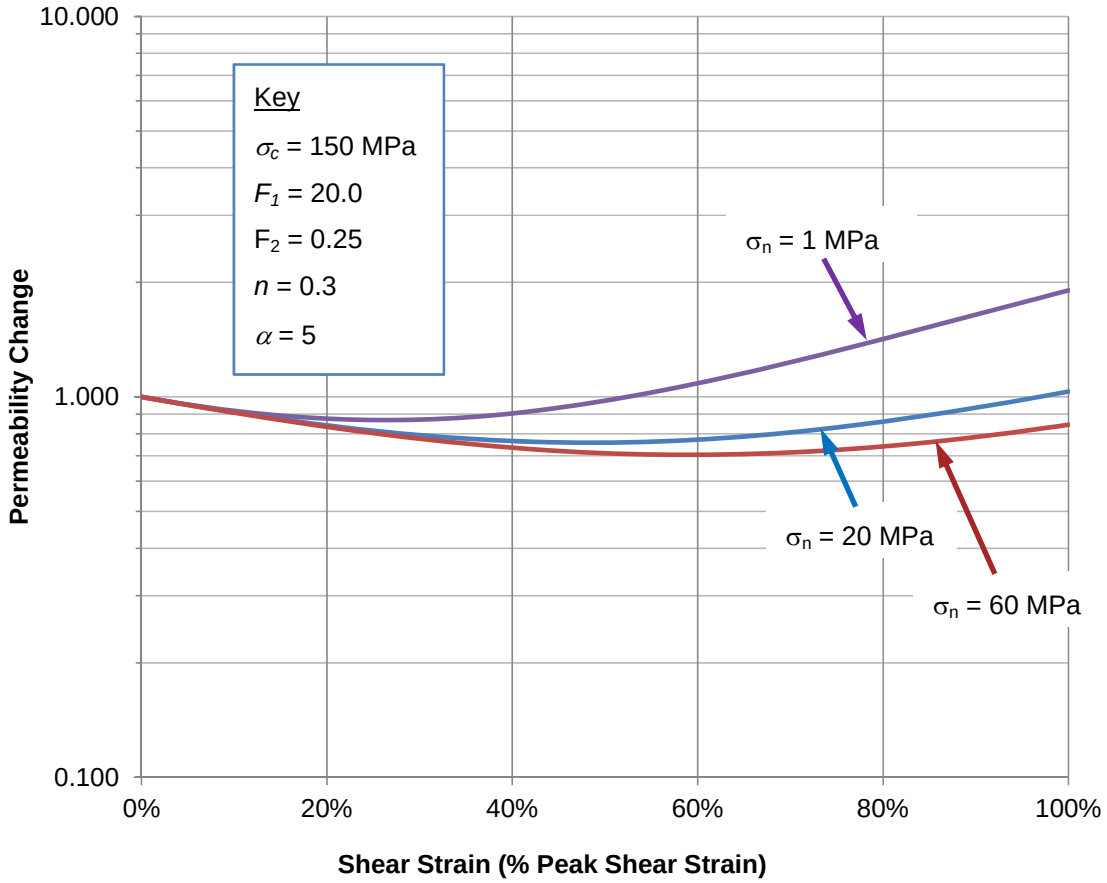

Figure A-5: Example of Stage I shear model correction for permeability.

A.5.3. Stage III Shear Model

Following Stage I deformation, the permeability of the fracture can increase rapidly as well as significantly during Stage II, and then asymptote to a limit value during Stage III (see Figure A-4). Given the rapid change in permeability in Stage II, and the inability to determine the amount of shear strain that a fracture may have experienced (there is no unique stress-strain relationship post-peak), a Stage II model is not developed in NSealR, and all post-peak response is described by a Stage III model.

As noted, Stage III is a region where the permeability increases significantly but has attained a relatively constant value (e.g., Esaki et al., 1999)[30]. Again, there is no direct method to estimate shear strain from the current shear stress, and the secant modulus is unknown. From experimental work, this permeability is dependent on normal stress and the fracture roughness. In many cases, the Stage III permeability is expected to be significantly larger than the starting permeability of the virgin fracture, on the order of a magnitude larger or more (e.g., Barton et al., 1985). However, this permeability value may be reduced by gouge/detritus created during the shearing process.

For the Stage III model, the normal stress dependence is represented by a general exponential equation, which asymptotes to a constant value at a critical stress, σ_{crit}. The permeability correction factor for Stage III, $F_{a\text{-}III}$, is expressed as:

$$F_{a-III} = \frac{k_s}{k_c} = \left\{F_x \exp\left[F_y \left(\frac{\sigma_n}{\sigma_{crit}}\right)\right] + F_z\right\} \qquad \text{for } 0<\sigma_n \leq \sigma_{crit} \qquad \text{(A-19a)}$$

$$F_{a-III} = \left\{F_x \exp\left[F_y\right] + F_z\right\} \qquad \text{for } \sigma_n > \sigma_{crit} \qquad \text{(A-19b)}$$

where F_x, F_y and F_z are model constants, σ_n is the effective normal stress on the fracture and σ_{crit} is critical stress value. For NSealR, the critical value is set equal to the uniaxial compressive strength, σ_c.

Finally, the permeability is considered to be proportional to the cube of the hydraulic aperture, so the final equation for this model becomes for the corrected aperture factor, $F_{a\text{-}III}'$ is the cube root of the correction factor in Equation A-19:

$$F_{a-III}' = [F_{a-III}]^{\frac{1}{3}} \qquad \text{(A-20)}$$

In utilizing the Stage III model, NSealR also checks that the shear stress on the fracture computed from the nominal in situ stress does not exceed the computed residual shear strength of the fracture, τ_r. Explicitly, the following requirement is checked internally:

$$\tau \leq \tau_r \qquad \text{(A-21)}$$

The residual strength can be computed from the peak strength using a simple ratio concept with the understanding that at very high normal stresses, the peak and residual strength are equal[31].

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[30] While fracture dilatancy is related to a large part of this increase, the permeability does not always directly vary with the value of the mechanical aperture. For example, as seen in data presented by Esaki et al. (1999), the permeability is relatively constant while the mechanical aperture continues to increase/dilate.

[31] Conceptually, at very high normal stresses, shear deformation will remove all asperities, achieving a smooth surface, and at this point, the observed shear strength will be equal to the basic material strength, which is stress independent. In this discussion, a very high normal stress is defined as the uniaxial compressive strength. Note that this concept neglects the effects of any detritus on the surface created during shear.

Using the peak shear strength value τ_p as shown in Equation A-17, a correction can be applied to obtain the residual strength as a function of the normal stress (modified from Goodman, 1976, Equation 60):

$$\tau_r = \left\{R_o + [1 - R_o]\left(\frac{\sigma_n}{\sigma_c}\right)\right\}\tau_p \qquad \text{for } 0 < \sigma_n < \sigma_c \qquad \text{(A-22a)}$$

$$\tau_r = \tau_p \qquad \text{for } \sigma_n \geq \sigma_c \qquad \text{(A-22a)}$$

where R_o is the strength ratio (i.e., the ratio of the peak strength to the residual strength at very low normal stress values for the fracture), σ_n is normal stress on the fracture, and σ_c is uniaxial compressive strength of the fracture surface.

In summary, six parameters (in addition to the normal stress on the fracture) are used to define the response under the NSealR Stage III model:

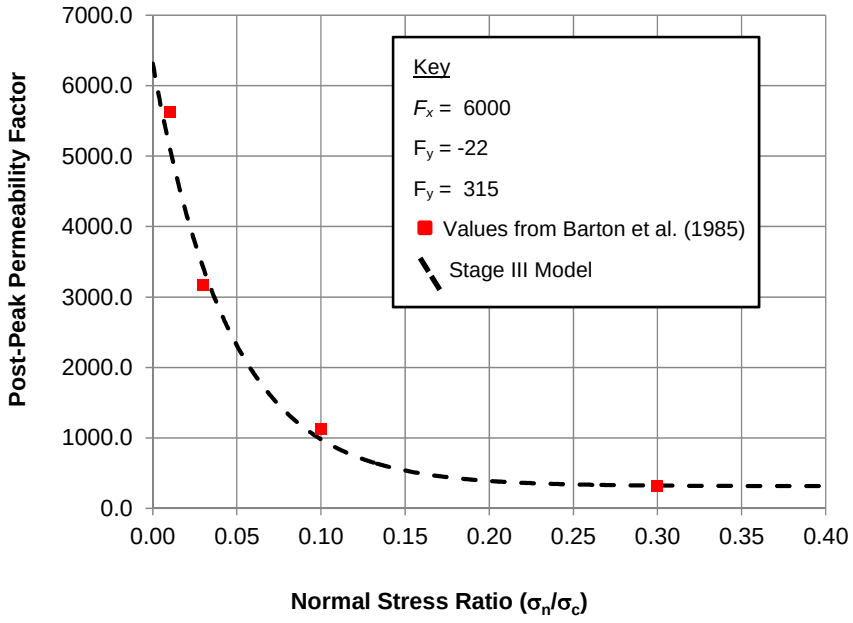
- F_X, F_Y and F_Z, the model constants
- R_o, shear strength ratio
- σ_c, uniaxial compressive strength of the rock surface
- α, fracture roughness factor

In addition, one Stage III parameter, ϕ_r, is set to a default value.

As shown in Figure A-6, the developed Stage III equations can be fit to exiting evaluations; in this case, the Stage III model is used to represent values for softer rock (tuff with σ_c = 100 MPa) evaluated by Barton et al. (1985; Figure 22)[32]. In addition, a data fit to stronger granitic samples (σ_c = 165 MPa) are shown in Figure A-7. In this case, the data do not correspond to the expected trend of higher conductivity at lower normal stress levels.

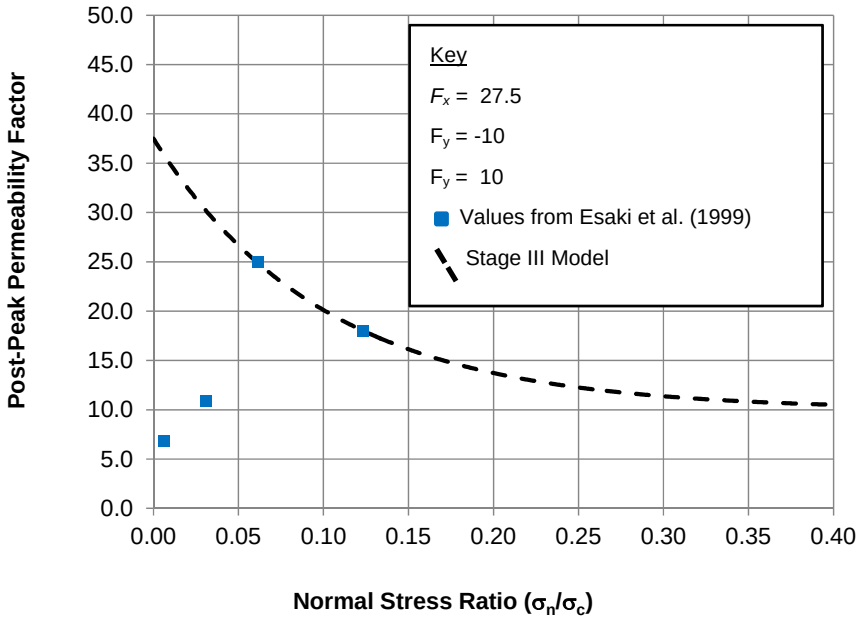
Note in curve fitting the Stage III model to data, the terms, F_x and F_z, define the limits of the empirical curve fit, where F_x is equal to the correction value at very high normal stress, and the sum of the these values, ($F_x + F_z$), is equal to the correction value at zero normal stress. The third term, F_y, controls the curvature of the representation is always negative.

[32] Values are not testing data, rather values are understood to be resulting design values from an evaluation of laboratory data.



Note: Ratios computed from permeability evaluation values shown by Barton et al. (1985), Figure 22; results are for potential conductivity variation for welded tuff with σ_c = 100 MPa.

Figure A-6: Example of a Stage III shear model correction fit to Barton et al. (1985).



Note: Ratios computed from laboratory testing shown by Esaki et al. (1999) in Figures 5 to 6; hydraulic conductivity data are for granite samples with σ_c = 165 MPa, and evaluated at a shear displacement of 10 mm.

Figure A-7: Example of a Stage III model correction fit to Esaki et al. (1999).

APPENDIX B: TWO-PHASE THEORY

B.1 Effective Saturation

In describing the relationships between capillary pressure and fracture saturation for two-phase flow, the total saturation of the fully saturated system is understood as the sum of the wetting phase saturation. S_w, and the nonwetting phase saturation, S_n, for the case of thermodynamic equilibrium, or simply:

$$S_w + S_n = 1 \tag{B-1}$$

The wetting phase saturation, S_w, is often employed as a key parameter in describing these relationships. However, as the fracture (or matrix) system tends to retain phase components, the developed relationships are applicable only within a range of the wetting phase saturation, termed the effective wetting phase saturation, S_e, or simply the *effective saturation*.

The effective saturation is the normalized wetting phase saturation adjusted to fit the range of interest or applicability. Three general regions or zones for consideration are illustrated in Figure B-1 (Luckner et al., 1989). For low wetting phase saturations, a zone where the flow of the wetting phase may no longer be coherent (Zone A, Figure B-1) is defined by the residual wetting phase saturation, S_{rw}. Conversely at low nonwetting phase saturations (i.e., at high wetting phase saturations) a zone defined by the residual nonwetting phase saturation, S_{rn}, can exist where the flow of the nonwetting phase may no longer be coherent (Zone C, Figure B-1).

The effective saturation has been defined by some authors across both Zones B and C. For the present context, analyses are limited to the conditions where both fluids exhibit coherent flow (i.e. in only Zone B in Figure B-1), and the effective saturation is thus defined as:

$$S_e = \left(\frac{S_w - S_{rw}}{1 - S_{rw} - S_{rn}}\right) \qquad \text{if } S_{rw} < S_w < (1.0 - S_{rn}) \tag{B-2a}$$

$$S_e = 0.0 \qquad \text{if } S_w \leq S_{rw} \tag{B-2b}$$

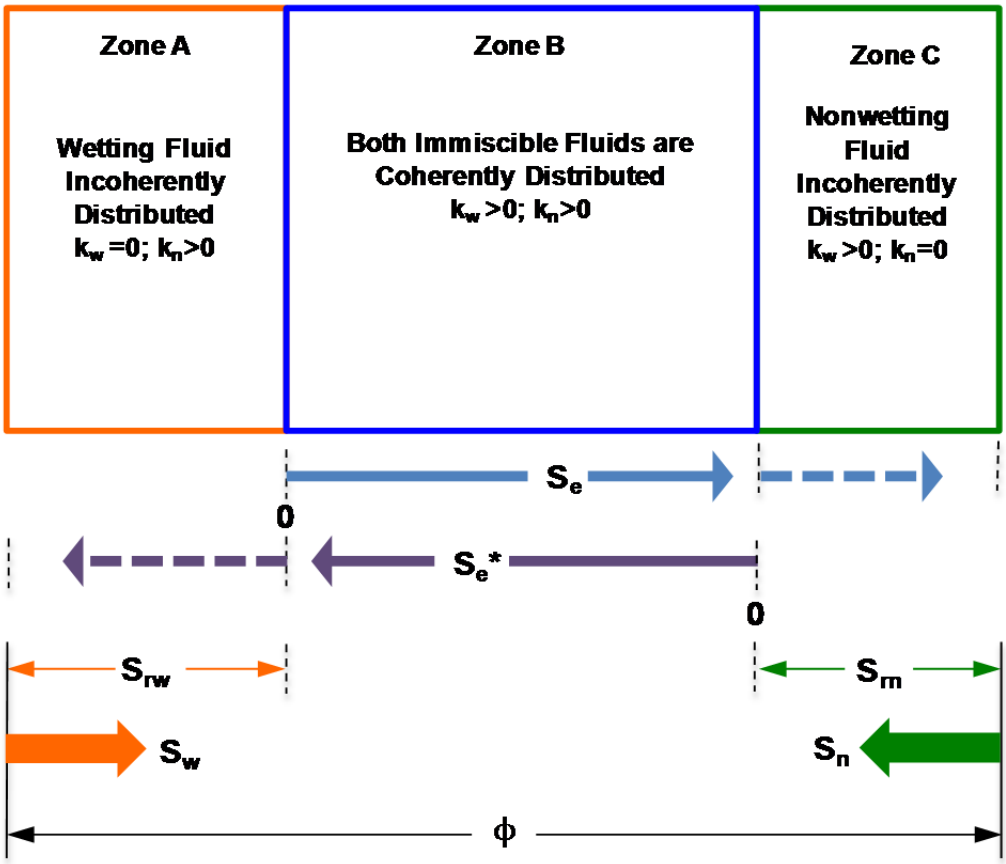
$$S_e = 1.0 \qquad \text{if } S_w \geq (1.0 - S_{rn}) \tag{B-2c}$$

The relative permeability as a function of effective saturation is illustrated for an ideal case in Figure B-2.

It is noted that if the nonwetting residual saturation is taken as negligible or not considered in the model description (e.g., in water-air systems), the normalized saturation equation reduces to the form as shown in many papers (e.g., as in Brooks and Corey, 1964, Definitions):

$$S_e = \left(\frac{S_w - S_{rw}}{1 - S_{rw}}\right) \qquad \text{for } S_{rw} < S_w < 1.0 \tag{B-3}$$

For the present context, the more general form in Equation B-2 is used in NSealR for effective saturation.



Key:

k_w = permeability of wetting phase fluid

k_n = permeability of nonwetting phase fluid

S_e = effective (wetting) saturation

S_e* = effective (nonwetting) saturation

S_w = wetting phase saturation

S_n = nonwetting phase saturation

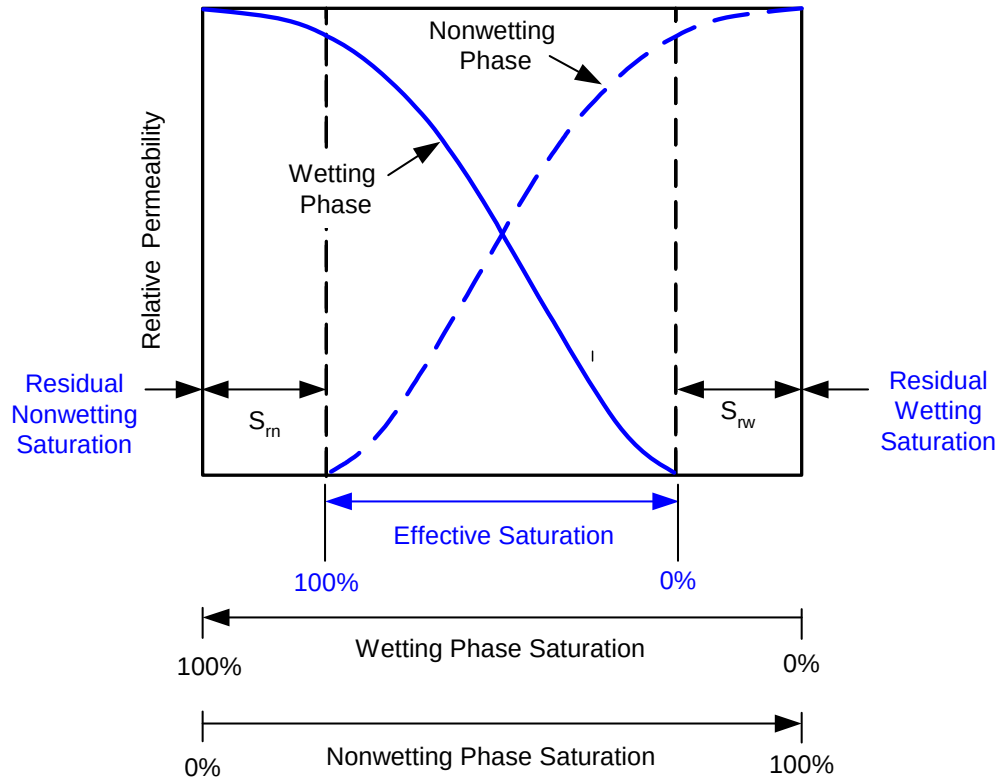
S_{rw} = residual wetting phase saturation

S_{rn} = residual nonwetting phase saturation

ϕ = entire range of wetting/nonwetting saturations

Note: Modified from Luckner et al., 1987.

Figure B-1: Conceptual zones of two-phase flow with immiscible fluids.



Note:

[a] The axes have been reversed in this figure from the previous figure to illustrate the drainage case, i.e., where the saturation of the wetting fluid decreases as the eye proceeds from left to right.

Figure B-2: Idealized relative permeabilities versus effective saturation used in NSealR for drainage case.

B.2 Relative Permeability - Two-Phase Flow

For vertical two-phase flow through an element, the concept of relative permeability is adopted (e.g., Bear, 1988), allowing the description of flow of each component to be a function of the effective saturation.

Specifically, assuming that Darcy's law is applicable, the flow of each phase can be conceptually described separately using a relative permeability approach. The representation of Darcy's law for either phase in the vertical direction for 1-D flow through a homogenous solid/feature is:

$$u_\alpha = \frac{k_{r\alpha} k_t}{\mu_\alpha} (-\nabla p_\alpha + \rho_\alpha g) \tag{B-4}$$

where

α = the phase, either wetting or nonwetting (w or n)

u_α = phase Darcy velocity or specific discharge (discharge per unit area)

$k_{r\alpha}$ = relative permeability for phase α

μ_α = phase viscosity

ρ_α = phase density

k_t = total permeability

∇p_α = pressure gradient for phase

g = standard acceleration due to gravity

The relative permeability of a phase, $k_{r\alpha}$, is defined as the ratio of the phase permeability to the total permeability:

$$k_{r\alpha} = \frac{k_\alpha}{k_t} \tag{B-5}$$

As defined, the relative permeability is always less than or equal to 1.0.

For a defined area or cell, the vertical flow in NSealR, the discharge (volume/time), Q_i, is equal to the specific discharge over the total area for the specific cell, A_i, for the phase under consideration (α), with upward flow as positive:

$$Q_i = u_{\alpha i} A_i \tag{B-6}$$

For a period of time when the discharge is constant (Δt), the rate of mass transport (mass flux) for the cell, Γ_i, becomes:

$$\Gamma_i = Q_i \rho_\alpha [\Delta t] \tag{B-7}$$

The resulting mass transport for each phase is expressed in terms of metric tonnes per year by NSealR.

B.3 Brooks-Corey 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 ($\boldsymbol{\lambda}$) and bubbling pressure (P_b). The equations were originally developed for a liquid-gas system, but are considered applicable for a fluid-fluid 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 as 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 (Equation 3, Brooks and Corey, 1966):

$$P_c \equiv P_n - P_w \tag{B-8}$$

The effective saturation is related to the capillary pressure though a simple power-relationship (Equation 12 of Brooks and Corey, 1966):

$$S_e = \left[\frac{P_b}{P_c}\right]^{\lambda} \qquad \text{if } P_c \geq P_b \tag{B-9a}$$

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:

$$S_e = 1.0 \qquad \text{if } P_c < P_b \tag{B-9b}$$

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:

$$S_e = \left[\frac{P_b}{P_c}\right]^{\lambda} \qquad \text{if } P_c \geq P_e \tag{B-10a}$$

$$S_e = 1.0, \qquad \text{if } P_c < P_e \tag{B-10b}$$

This revised form is shown, e.g., in Corey and Brooks (1999, Equation 1), 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, Equation 26):

$$k_{rw} = S_e^{\left[\frac{2+3\lambda}{\lambda}\right]} \tag{B-11}$$

Similarly, the relative permeability is defined for the nonwetting phase as (Brooks and Corey, 1966, Equation 32):

$$k_{rn} = (1 - S_e)^2 \left\{1 - S_e^{\left[\frac{2+\lambda}{\lambda}\right]}\right\} \tag{B-12}$$

An example of the relationship of capillary pressure and effective saturation for the Brooks-Corey model is shown in Figure B-3 for λ=2.0. The rapid decrease in the effective saturation becomes a single line in a log-log plot of this relationship with a slope of λ and an x-axis intercept of 1. The relationship of relative permeabilities to effective saturation is shown in Figure B-4 for λ=2.0 and residual saturations of 10%. Note that x-axis is reversed in the figure to more clearly represent the drainage progress for the viewer as the eye moves from left to right.

B.4 Implementation of the Brooks-Corey Model

The implementation of the Brooks-Corey model in NSealR can be described as a series of tasks performed for each time interval over which the inputs (carbon dioxide pressure and saturation) are assumed constant. Looping over each active cell of the grid, the following tasks are performed:

1. From the source text file, the relevant input from the reservoir model provides the nonwetting pressure and saturation for supercritical carbon dioxide. A check is made to ensure that this pressure is defined within target region.
2. Using Equation B-1, the wetting saturation is computed.
3. The effective saturation is evaluated using the residual wetting phase saturation and the residual nonwetting phase saturation taken from Dashboard input. If the wetting saturation is less than the residual wetting saturation, the effective saturation is set equal to zero; if the wetting saturation is more than the upper bound (i.e., 1 - residual nonwetting saturation), the effective saturation is set equal to 1.0. Otherwise, the effective saturation is computed using Equation B-2.
4. Using the effective saturation, S_e, and the bubbling pressure, P_b, the capillary pressure is computed by re-writing Equation B-9 to solve for the capillary pressure, P_c. The equation is limited to values of $S_e \geq 0.01$ in NSealR for numerical stability:

$$P_c = \left\{\frac{P_b}{(S_e)^{\frac{1}{\lambda}}}\right\} \qquad \text{if } S_e \geq 0.01 \tag{B-13a}$$

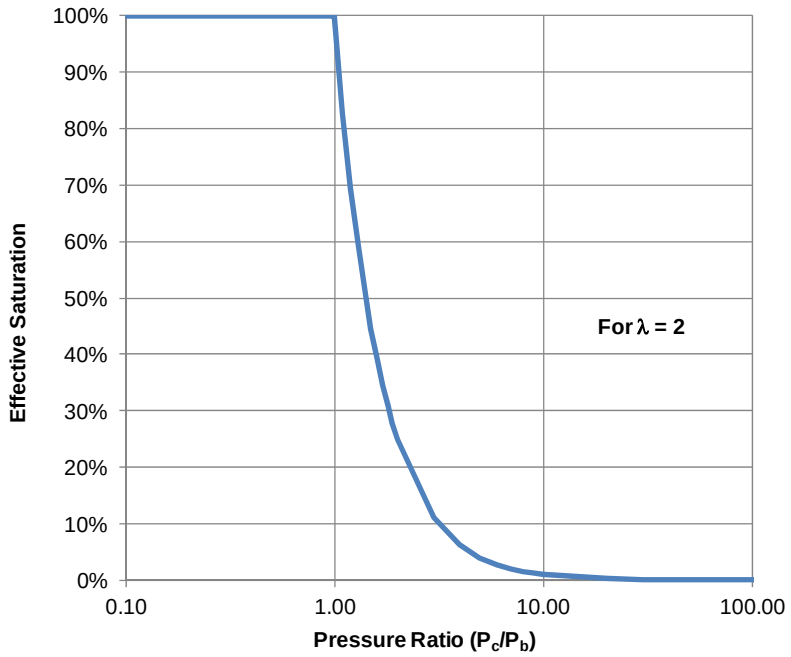


Figure B-3: The Brooks-Corey relationship of effective saturation to capillary pressure.

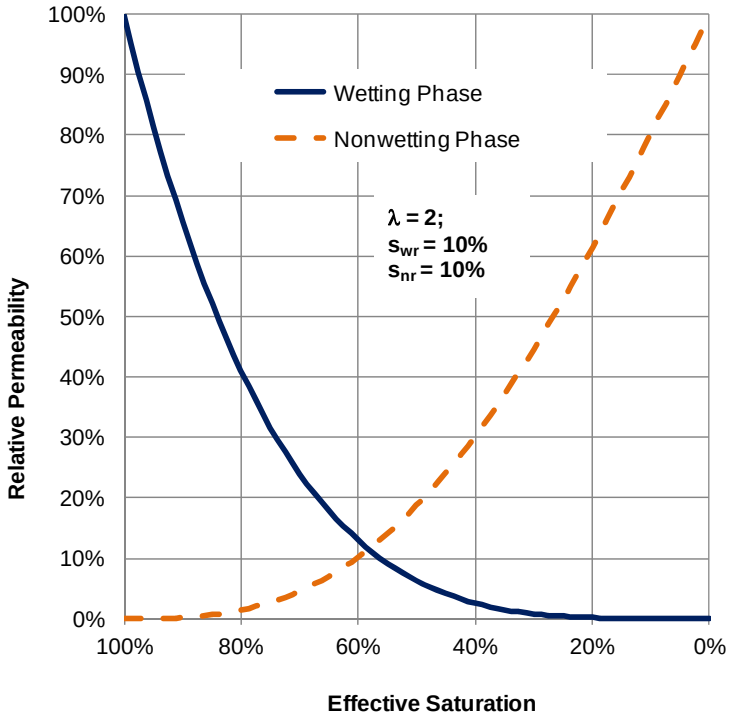


Figure B-4: Brooks-Corey relationship of relative permeabilities to effective (wetting) saturation.

and arbitrarily set to a upper limit capillary pressure at lower saturations, defined as:

$$P_c = \left\{ \frac{P_b}{(0.01)^{\frac{1}{\lambda}}} \right\} \qquad \text{if } S_e < 0.01 \qquad \text{(B-13b)}$$

The wetting phase pressure is computed from Equation B-8, re-written to solve for the wetting phase pressure, i.e.:

$$P_w = P_n - P_c \qquad \text{(B-14)}$$

A check is performed to ensure that this pressure is above minimum pressure for the target region.

5. At this point, the wetting phase density and viscosity are computed, considering a computed average (wetting) pressure for the cell, together with the average seal temperature and salinity.
6. The relative permeability for the wetting phase is computed from Equation B-11.
7. The wetting phase (brine) flux is then computed using the established relationships. The Darcy velocity is computed from Equation B-4, the discharge from the cell using Equation B-6, and the mass transport for the cell using Equation B-7.
8. The nonwetting phase is then examined.
    a. If the nonwetting phase pressure is less than the entry pressure, the mass transport for the nonwetting phase is set to zero (the drainage case is assumed). For this case, additional steps are skipped and the cycle is completed.
    b. If the nonwetting phase pressure is greater than or equal to the entry pressure, then the nonwetting phase density and viscosity are computed from nonwetting pressure and the average seal temperature.
9. The relative permeability for the nonwetting phase is computed from Equation B-12.
10. Then the nonwetting phase (brine) flux is computed using the established relationships. The Darcy velocity is computed from Equation B-4, the discharge from the cell using Equation B-6, and the mass transport for the cell using Equation B-7. If the flow of brine is upward (positive), the amount of dissolved CO_2 is computed using the solubility factor for the existing conditions and assuming a fully saturated condition, and this amount is added to the CO_2 mass transport for the cell.
11. The wetting phase and nonwetting phase flux from this interval are stored and the process steps are repeated until the last time step is completed.

B.5 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, Equation 3):

$$S_e = \left\{\frac{1}{1+(\alpha h)^n}\right\}^m \tag{B-15a}$$

or alternately,

$$S_e = \{1+(\alpha h)^n\}^{-m} \tag{B-15b}$$

where α, 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:

$$m \equiv \left(1-\frac{1}{n}\right) \qquad \text{for } 0 < m < 1 \tag{B-16}$$

Introducing a capillary pressure term to replace pressure head in the equation, the form becomes (e.g., White and Oostrom, 2000, Equation 4.10.3):

$$S_e = \left\{1+\left(\alpha\left[\frac{P_c}{\rho_w g}\right]\right)^n\right\}^{-m} \qquad \text{if } P_c \geq 0 \tag{B-17}$$

where

P_c = capillary pressure
ρ_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, Equation 11):

$$S_e = \left\{1+\left(\alpha\left[\frac{P_c}{\rho_w g}\right]\right)^n\right\}^{-m} \qquad \text{if } P_c \geq P_e \tag{B-18a}$$

$$S_e = 1 \qquad \text{if } 0 < P_c < P_e \tag{B-18b}$$

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

$$S_e = \left\{1 + \left(\alpha \left[\frac{P_c}{\rho_w g}\right]\right)^{\left[\frac{1}{1-m}\right]}\right\}^{-m} \qquad \text{if } P_c \geq P_e \tag{B-19}$$

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

$$P_c = \frac{1}{\alpha'}\left\{S_e^{\left(-\frac{1}{m}\right)} - 1\right\}^{1-m} \qquad \text{for } 0 < m < 1 \tag{B-20}$$

and the constants are merged into a single term, α':

$$\alpha' = \frac{\alpha}{g\rho_w} \tag{B-21}$$

Extending the theoretical development represented by Equation B-15, van Genuchten developed a relationship for wetting phase permeability, k_{rw}, in terms of effective saturation (van Genuchten, 1980, Equation 9):

$$k_{rw} = (S_e)^{\frac{1}{2}}\left[1 - \left(1 - (S_e)^{\frac{1}{m}}\right)^m\right]^2 \tag{B-22}$$

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; Equation 17). Luckner et al. (1989) also provided an expression for the nonwetting phase relative permeability using a second characteristic parameter, γ ((Luckner et al., 1989; Equation 18).

These two equations (as presented by Finsterle and Pruess, 1995; Equation 9) are:

$$k_{rw} = (S_e)^{\beta}\left[1 - \left(1 - S_e^{\left(\frac{1}{m}\right)}\right)^m\right]^2 \tag{B-23}$$

$$k_{rn} = (1 - S_e)^{\gamma}\left[1 - S_e^{\left(\frac{1}{m}\right)}\right]^{2m} \tag{B-24}$$

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 using Equations B-4, B-6 and B-7.

To implement the modified van Genuchten-Mualem model as described, four characteristic parameters are required: α', β, γ and m. The remaining term, *n*, mentioned earlier is defined in terms of m (per Equation B-17). Referring to Equation B-20, some authors redefine the inverse

of α' as the entry pressure (i.e., specifically as the air entry pressure or capillary air pressure) (e.g., Finsterle, 2007, p. 47; Cinar, 2006, Equation 4), but this approach is considered inappropriate for describing an accurate relationship (see Ippisch et al., 2006) and is not adopted here.

The van Genuchten-Mualem model is illustrated in Figures B-5 and B-6 for specific parameter values. Figure B-5 provides an example of the relationship of capillary pressure and effective saturation for the van Genuchten-Mualem model. In comparison to the Brooks-Corey model (see Figure B-3), the curve is more gradual transition in slope at higher wetting saturations, but otherwise similar at low values of effective saturation.

The relationship of relative permeabilities to effective saturation for the van Genuchten-Mualem model is shown in Figure B-6. The terms β and γ were set both equal to 2.0, which reduces the wetting phase equation to the original form by van Genuchten (1980). Note that x-axis is reversed in the figure to more clearly represent the drainage progress for the viewer as the eye moves from left to right. The representation in this case is similar to the Brooks-Corey model (see Figure B-4).

B.6 Implementation of the Modified van Genuchten-Mualem Model

The implementation of the modified van Genuchten-Mualem model in NSealR is similar to the implementation of the Brooks-Corey model. The process can be described as a series of tasks performed for each time interval over which the inputs (carbon dioxide pressure and saturation) are assumed constant. Looping over each active cell of the grid, the following tasks are performed:

1. From the source text file, the relevant input from the reservoir model provides the nonwetting pressure and saturation for supercritical carbon dioxide. A check is made to ensure that this pressure is defined within target region.
2. Using Equation B-1, the wetting saturation is computed.
3. The effective saturation is evaluated using the residual wetting phase saturation and the residual nonwetting phase saturation taken from Dashboard input. If the wetting saturation is less than the residual wetting saturation, the effective saturation is set equal to zero; if the wetting saturation is more than the upper bound (i.e., 1 - residual nonwetting saturation), the effective saturation is set equal to 1.0. Otherwise, the effective saturation is computed using Equation B-2.
4. Using the effective saturation, S_e, and the terms m and α'as defined by the user, the capillary pressure is computed from Equation B-20 for values of $S_e \geq 0.001$ in NSealR for numerical stability. For smaller effective saturation values, S_e is arbitrarily set to 0.001 and computed.
5. The wetting phase pressure is computed from Equation B-8. A check is performed to ensure that this pressure is above minimum pressure for the target region.

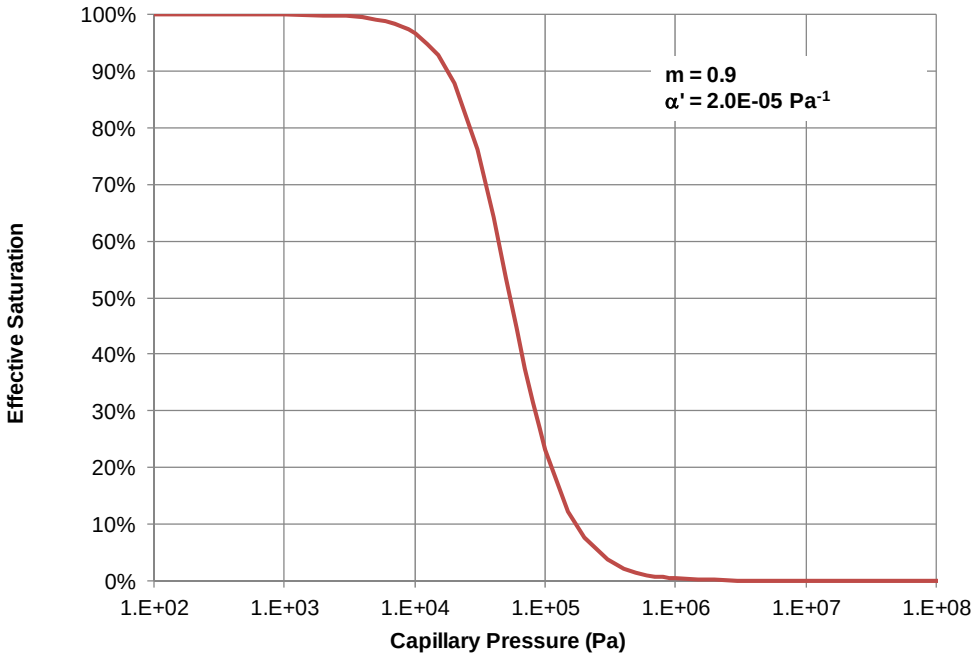


Figure B-5: van Genuchten-Mualem relationship of effective saturation to capillary pressure.

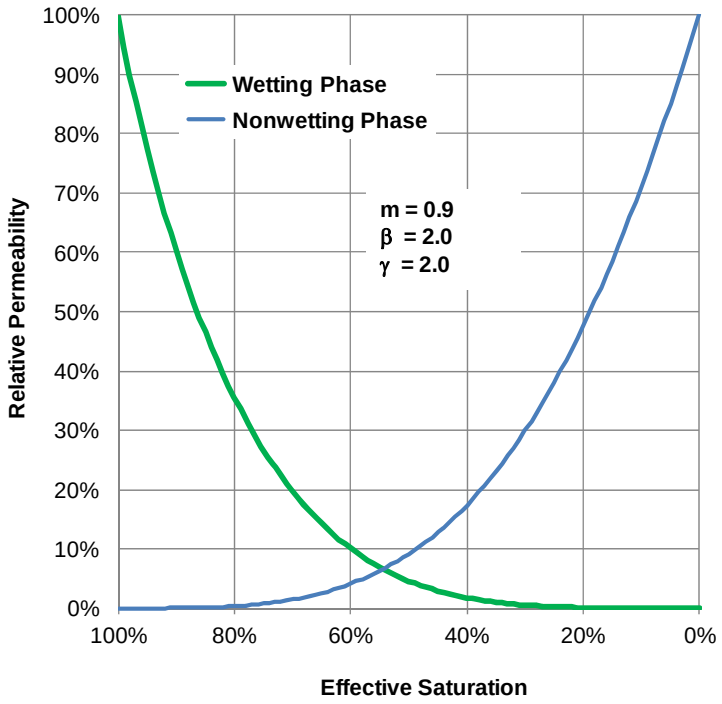


Figure B-6: van Genuchten-Mualem relationship of relative permeabilities to effective (wetting) saturation.

6. At this point, the wetting phase density and viscosity are computed, considering a computed average (wetting) pressure for the cell, together with the average seal temperature and salinity.
7. Using m and β defined by the user, the relative permeability for the wetting phase is computed from Equation B-23.
8. The wetting phase (brine) flux is then computed using the established relationships. The Darcy velocity is computed from Equation B-4, the discharge from the cell using Equation B-6, and the mass transport for the cell using Equation B-7.
9. The nonwetting phase is then examined.
    a. If the nonwetting phase pressure is less than the entry pressure, P_e, the mass transport for the nonwetting phase is set to zero (the drainage case is assumed). For this case, additional steps are skipped and the cycle is completed.
    b. If the nonwetting phase pressure is greater than or equal to the entry pressure, then the nonwetting phase density and viscosity are computed from nonwetting pressure and the average seal temperature.
10. Using m and γ defined by the user, the relative permeability for the nonwetting phase is computed from Equation B-24.
11. Then the nonwetting phase (brine) flux is computed using the established relationships. The Darcy velocity is computed from Equation B-4, the discharge from the cell using Equation B-6, and the mass transport for the cell using Equation B-7. If the flow of brine is upward (positive), the amount of dissolved CO_2 is computed using the solubility factor for the conditions and assuming a fully saturated condition, and this amount is added to the CO_2 mass transport for the cell.
12. The wetting phase and nonwetting phase flux from this interval is stored and the process steps are repeated until the last time step is completed.

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APPENDIX C: DLL FILES

NSealR code incorporates 17 dynamic link libraries (DLLs) to increase efficiency and to perform specific operations not available in GoldSim. These libraries are code written in C++ and compiled independently of GoldSim using Microsoft Visual Studio. The libraries are linked to NSealR operation using GoldSim External elements, where input and output variables are defined.

For efficiency of computations, NSealR employs five DLLs files for the definition of fluid properties, as listed in Table C-1. These files are located in the "\fluid_properties" directory. These DLLs describe property variability as a function of temperature and stress. Three of these DLLs, those for brine density, brine viscosity, and CO_2 solubility[33], provide values as a function of brine salinity as well. These DLLs use a lookup table (LUT) approach to define values for reduced computation times (versus computing values using an equation of state correlation from source references). In comparison to the use of these DLLs, employing Lookup Table elements in GoldSim (linked to separate Microsoft Excel worksheets) would incur additional run times.

NSealR employs six additional DLLs for specific computations. These DLLs are listed in Table C-2 and the files are located in directory, "\dll_folder." The source code for each library DLL is provided under named locations in the subdirectory, "\source code." While this approach is not as transparent to the user as would be the use of GoldSim Script elements, these DLLs substantially shorten computation times.

Further, six DLLs are used to provide formatted output files for post processing by other graphic computer codes. These DLLs are described in Table C-3 and these files are also located in directory, "\dll_folder." The source code for each library code is provided in subdirectory, "\source code"

Listings of all DLLs are also provided in an addendum to this guide.

[33] Note that the aspect of CO_2 solubility in brine is not used in the current version of NSealR, as the two phases are assumed immiscible. It is expected, however, that this assumption will be changed in future versions of NSealR and therefore CO_2 solubility is included in discussions of fluid properties.

Table C-1: Dynamic Link Library Files for Fluid Properties in Directory "\fluid_properties"

DLL File Name	Purpose
LUT_brine_density_DLL.dll	Provides density of a saline solution as a function of temperature, pressure, and salinity
LUT_brine_viscosity_DLL.dll	Provides viscosity of a saline solution as a function of temperature, pressure, and salinity
LUT_CO2_density_DLL.dll	Provides density of carbon dioxide as a function of temperature and pressure
LUT_CO2_solubility_DLL.dll	Provides solubility of carbon dioxide in water as a function of temperature, pressure, and salinity
LUT_CO2_viscosity_DLL.dll	Provides viscosity of carbon dioxide as a function of temperature and pressure

Table C-2: Dynamic Link Library Files for Computations in Directory "\dll_folder"

DLL File Name	Purpose
compute_defined_flux.dll	Computes the brine and CO_2 flows for a constant flux across the seal horizon for cells that have experienced a pressure change in the reservoir.
Compute_eq_driven_conditions.dll	Computes the brine pressure and CO_2 saturation along the upper boundary of the seal horizon.
compute_flows.dll	Computes the brine and CO_2 flows based on Darcy's equations and user defined permeability and thickness of each cell.
compute_fractured_perm.dll	Computes the equivalent permeabilities for each cell using fractured rock option and related variables. Includes stress-dependency option in generating fracture apertures and computes stress normal to each fracture using horizontal principal stresses as basis.
compute_smooth_array.dll	Computes and adjusted cell thickness across the entire horizon using a two-pass averaging system and adjusting the values to restore the user-specified standard deviation of the population. In effect, the process smoothes the thickness variability across the horizon, providing a semblance of autocorrelation.
compute_static_conditions.dll	Computes the (brine) hydrostatic stress at the top of each cell given a reference fluid pressure at a given depth (input from Dashboard).[34] Assigns a zero value for CO_2 saturation along the upper boundary as well.

[34] Fluid pressure in the seal layer at the start of the realization is defined by specifying a fluid stress at a specific depth, on the other flow properties Dashboard.

Table C-3: Dynamic Link Library Files for Output in Directory "\dll_folder"

DLL File Name	Purpose
brine_out.dll	Writes brine mass flux data at specified intervals to a text file, *brine leakage-step_zzz.txt*, where zzz is the simulation step for the selected realization. Results are placed in directory, *"\results\brine"*
CO2_out.dll	Writes CO_2 mass flux data at specified intervals to a text file, *CO2 leakage-step_zzz.txt*, where zzz is the simulation step for the selected realization. Results are placed in directory, *"\results\CO2"*
conditions_out.dll	Writes seal barrier dimensions, salinity, temperature and depth, together with two-phase parameters and in situ stress to a text file, *NSealR conditions.txt* at a selected realization. Results are placed in directory, *"\results\input"*
fluid_out.dll	Writes average seal fluid property values to a text file, *NSealR fluid properties.txt* at a selected realization. Results are placed in directory, *"\results\input"*
perm_out.dll	Writes the intrinsic permeability and porosity arrays to a text file, *NSealR permeability-porosity grid.txt* at a selected realization. Results are placed in directory, *"\results\input"*
thick_out.dll	Writes the seal barrier thickness array to a text file, *NSealR thickness grid.txt* at a selected realization. Results are placed in directory, *"\results\input"*

APPENDIX D: FLUID PROPERTY VARIABILITY

To provide the user with guidance on the variability of fluid properties, various parameter relationships are shown in Figures D-1 to D-10. The figures represent plots from fluid properties' tabular data incorporated into DLLs.

Figure D-1 indicates a strong variation of CO_2 density with temperature, and the relationship of which is also significantly changed by pressure. The CO_2 Critical Temperature (31°C) is shown by a vertical blue dashed line in this figure. Figure D-2 also indicates a strong dependence of CO_2 density on pressure and the nature of which also changes with increased temperature. The CO_2 Critical Pressure (7.4 MPa) is shown by a vertical blue dashed line in this figure.

The variability of CO_2 viscosity with temperature and pressure is shown in Figures D-3 and D-4. The variability of CO_2 viscosity is relatively smaller than that of CO_2 density with respect to small changes in conditions. Critical parameters are again shown by a vertical blue dashed line.

Figures D-5 and D-6 illustrate the variability of brine density with temperature, pressure and salinity concentration. Pressure-dependency appears relatively small and variability with temperature is roughly linear at temperatures above 60°C.

Figures D-7 and D-8 illustrate the variability of brine viscosity with temperature, pressure, and salinity concentration. Brine viscosity decreases significantly with temperature, but stress-dependency is essentially negligible and concentration dependence is only minor.

Figures D-9 and D-10 illustrate the variability of CO_2 solubility in brine with varying temperature, pressure, and salinity concentration. The trends are not straightforward for this parameter; for example, CO_2 solubility can first decrease and then increase with increasing temperature as shown in Figure D-9 for pure water (salinity = 0) at 35 MPa. However, CO_2 solubility in brine can steadily decrease with increasing temperature at higher salinity concentrations or at decreased pressures (also shown in Figure D-9).

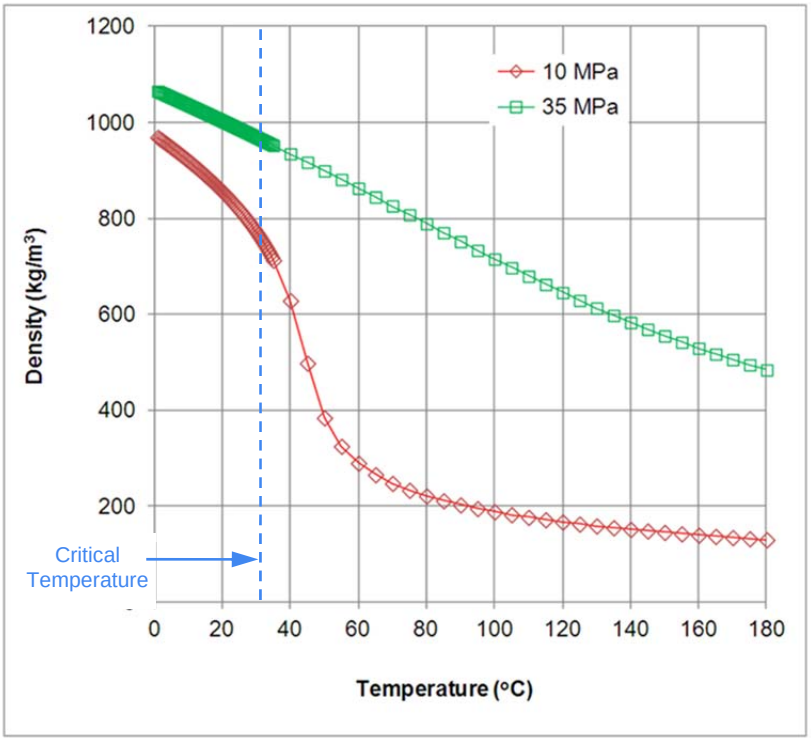

Figure D-1: CO_2 density versus temperature at two pressures (CO_2 critical temperature = 31°C).

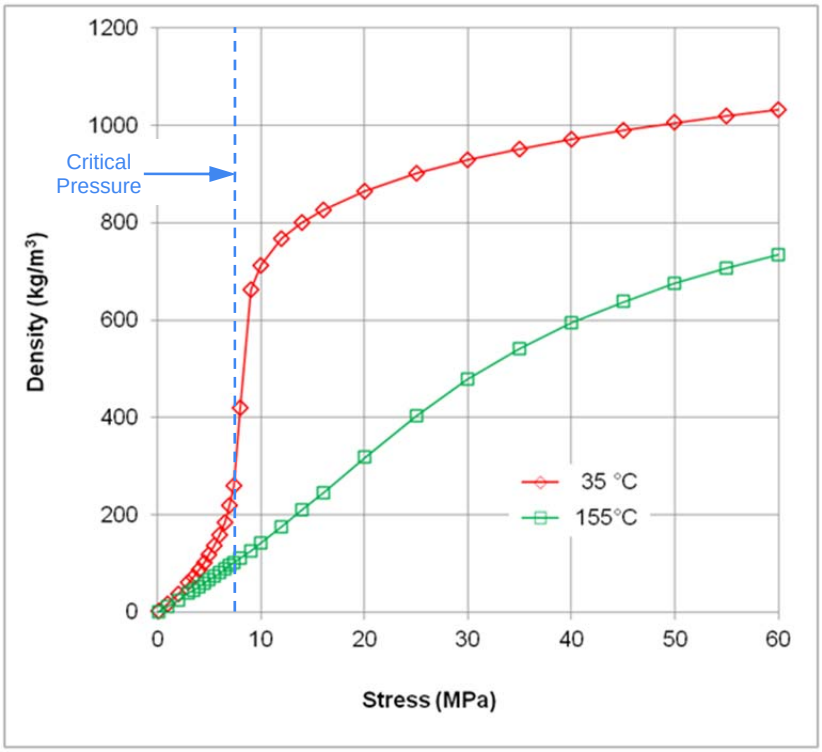

Figure D-2: CO_2 density versus pressure at two temperatures (CO_2 critical pressure = 7.4 MPa).

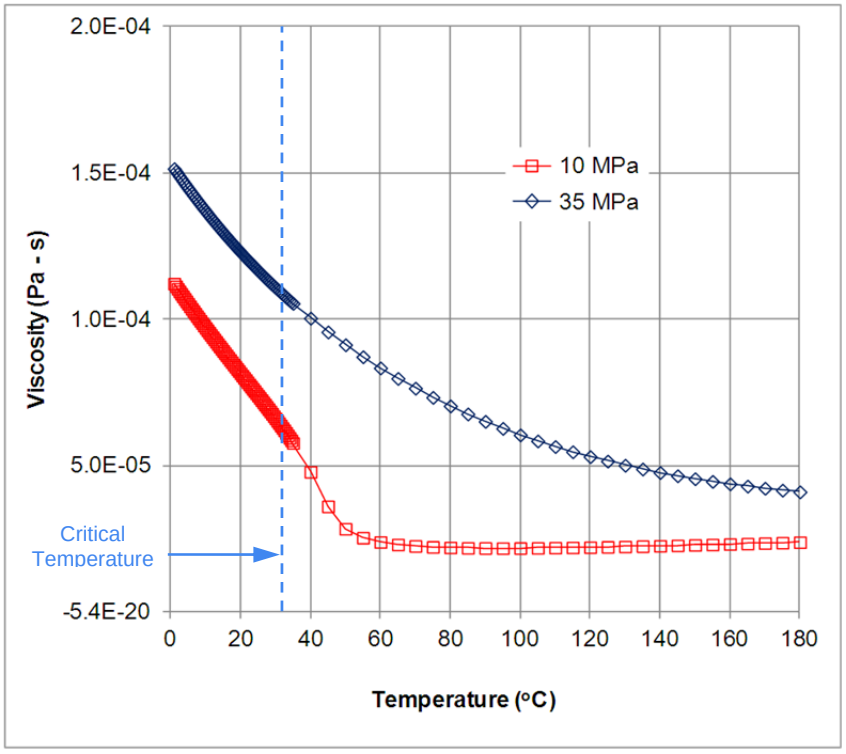

Figure D-3: CO_2 viscosity versus temperature at two pressures (CO_2 critical temperature = 31°C).

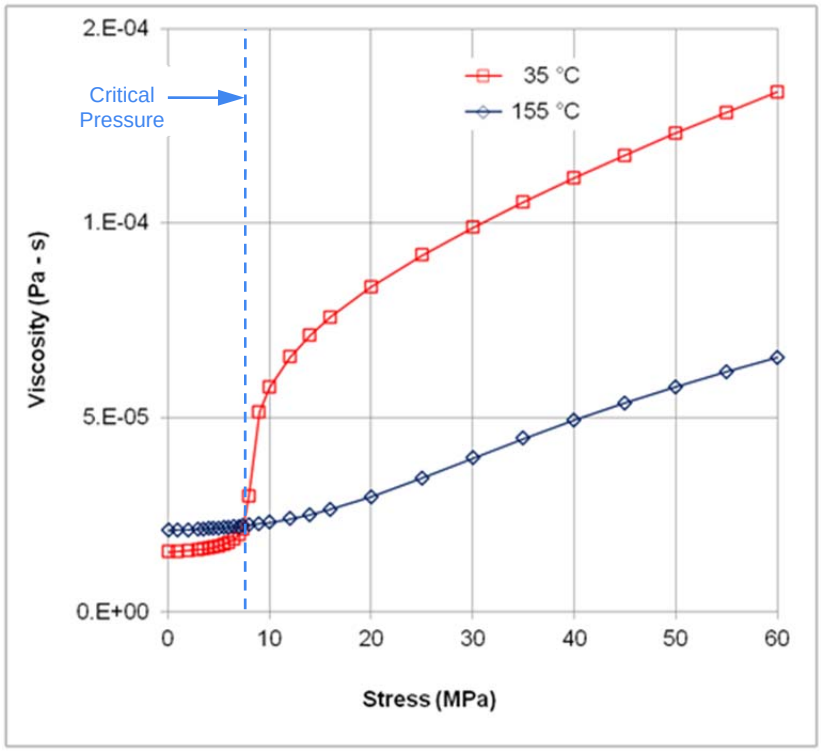

Figure D-4: CO_2 viscosity versus pressure at two temperatures (CO_2 critical pressure = 7.4 MPa).

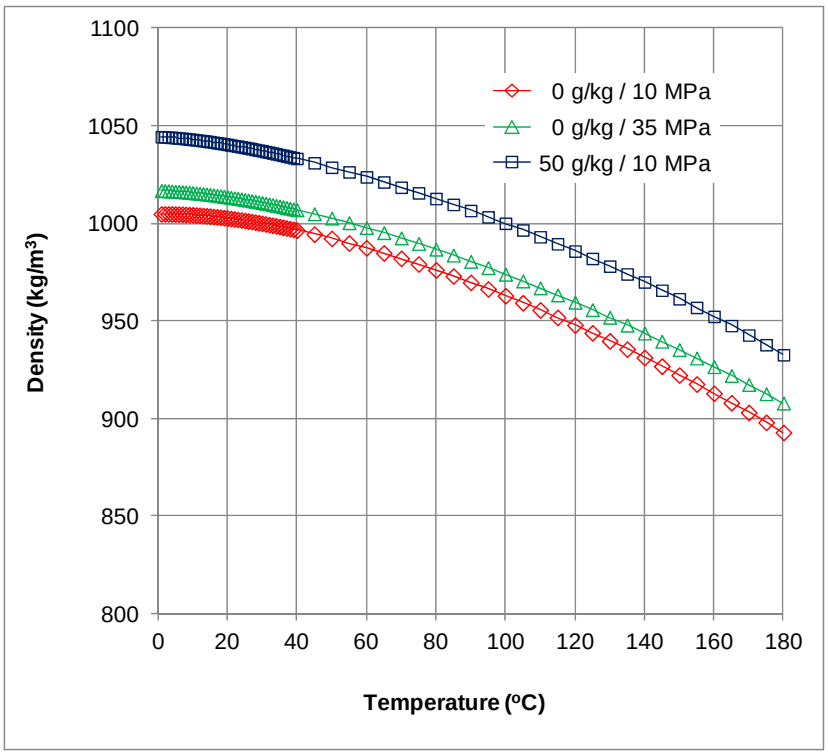

Figure D-5: Brine density versus temperature at different pressures and salinity concentrations.

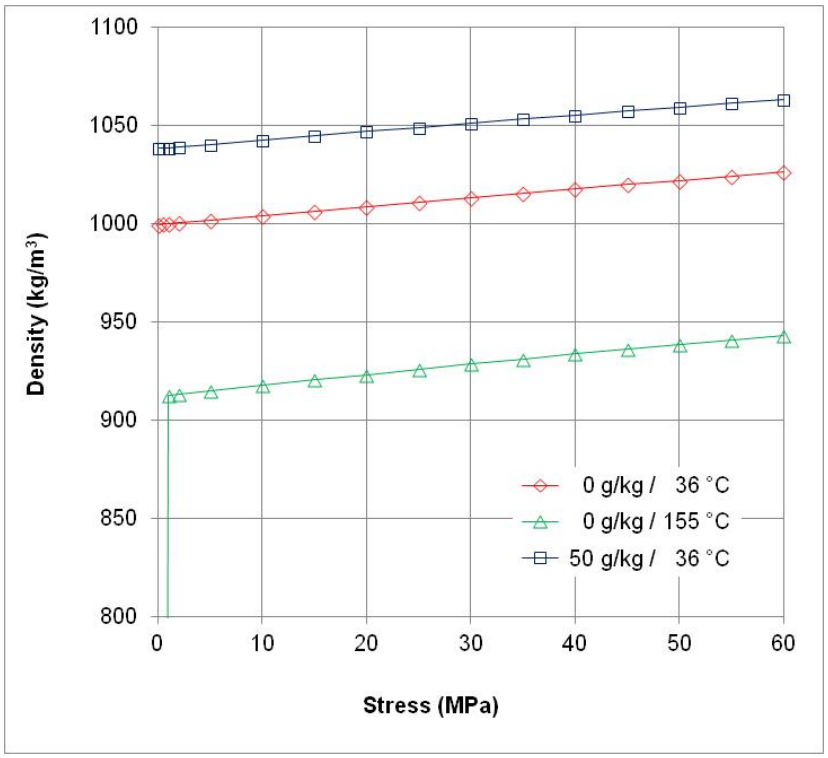

Figure D-6: Brine density versus pressure at different temperatures and salinity concentrations.

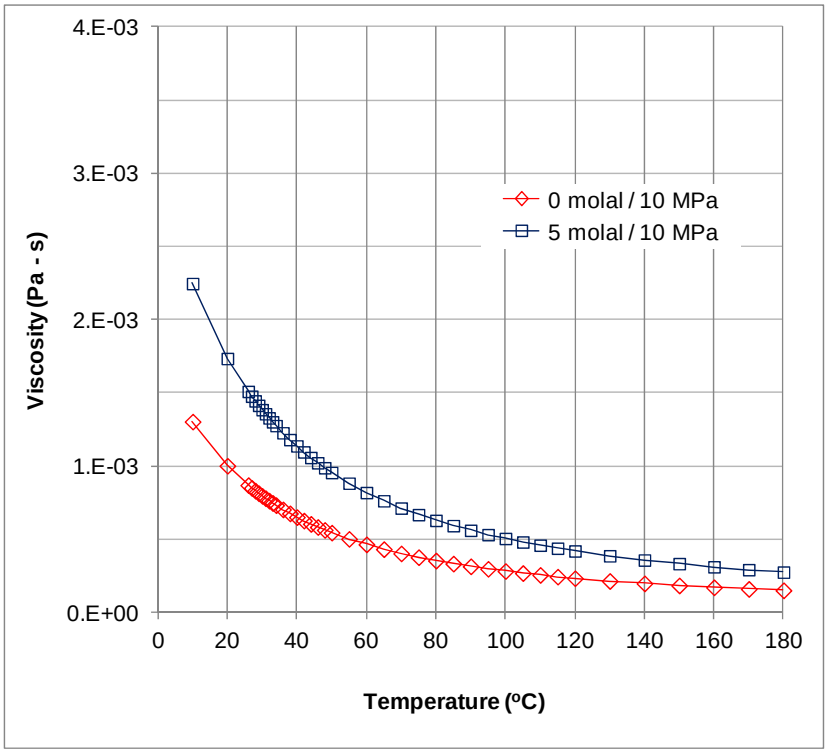

Figure D-7: Brine viscosity versus temperature at different salinity concentrations.

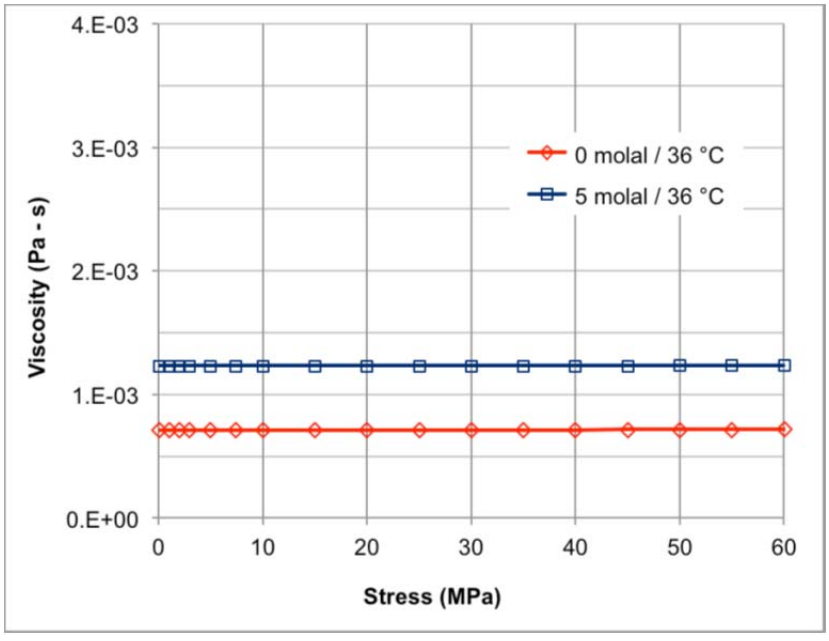

Figure D-8: Brine viscosity versus pressure at different salinity concentrations.

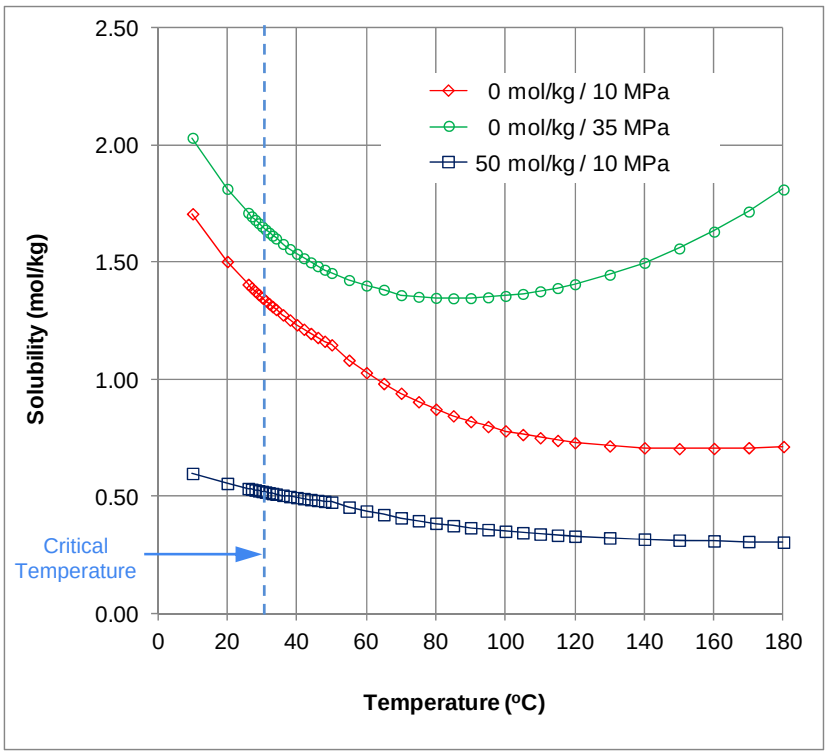

Figure D-9: CO_2 solubility in brine versus temperature at differing pressures and salinity concentrations.

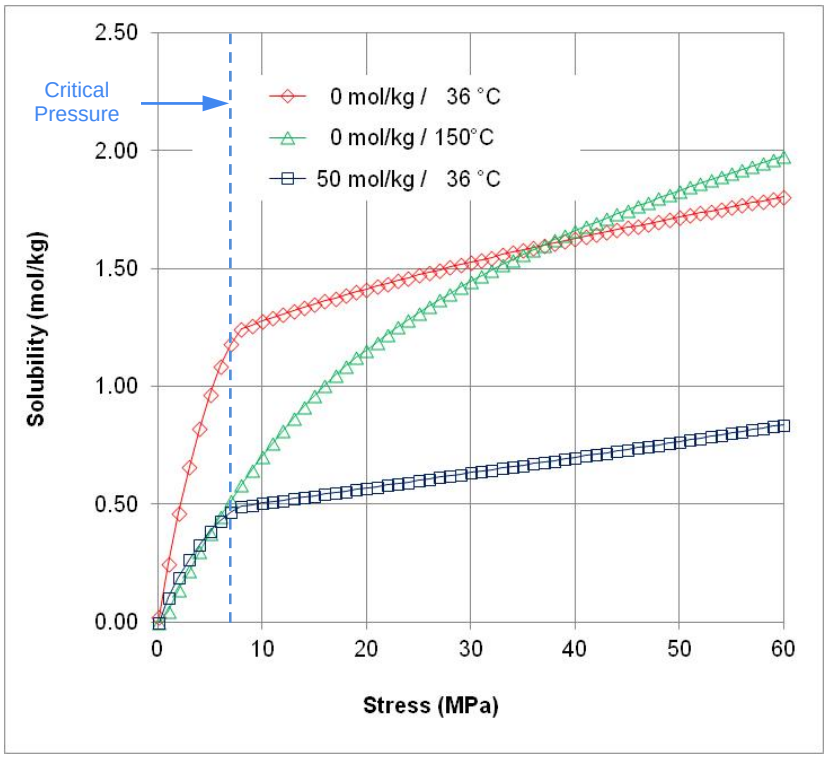

Figure D-10: CO_2 solubility in brine versus pressure at differing pressures and salinity concentrations.

APPENDIX E: INPUT FILE STRUCTURE - LOOKUP FILES

Special files (primarily text files) are used for importing data where user-defined data is specified by Dashboard selections. These files are located in the Lookup_Tables directory. The current set of lookup files is listed in Table E-1.

The numeric values provided in the text lookup files are comma-delimited and have a line structure as specified by GoldSim. Examples are provided in Table E-2 with explanatory text in ***blue***; the blue text is not shown or maintained in the file when prepared for use.

For reservoir-based text files, the row and column headers are coordinates for the location of the array values. For seal-based text files, the header files are simple index values. The logic of NSealR allows for the seal grid to be independent of the reservoir input grid, where seal values are interpreted from the reservoir location coordinates using GoldSim's Lookup Table elements.

Seal elevations are computed internally to NSealR and therefore, no text file for seal elevations is required for NSealR operation; seal elevations are computed as the sum of the elevations of the top of reservoir and the thickness of the seal barrier. Note that this convention differs from CO_2-PENS.

Example text files are provided together with the code files. Note that the current version of NSealR does not use the time series text file as an option; rather time series input is defined using an Excel file, formatted in the same fashion as shown for the text file option.

All arrays in NSealR are dimensioned for a 100 x 100 grid of elements which reflects the basic CO_2-PENS assumption for grid size.[35] For time step input files, values for time are in seconds, assuming a Julian calendar per GoldSim.[36]

[35] The data structure within these input text files are extremely wide and long, and in general, not well viewed with standard Window text software such as Notepad or Microsoft Word. Other text processing software, such as Notepad++© or Microsoft's WordPad© are better suited as they maintain the column structure in viewing.

[36] Time values in seconds are based on 365.25 days per (Julian) year, for 3.15576 x 10^7 seconds per year or 31.56 Ms/yr.

Table E-1: Input Files Used by NSealR in Directory "\Lookup_Tables"

Input Parameter	File Name
Directory: Lookup_Tables\reservoir	
Land Surface Elevations (with Coordinates)	*Lookup_land_surface.txt*
Reservoir Elevations of Top Surface (with Coordinates)	*Lookup_reservoir_elev.txt*
Directory: Lookup_Tables\seals	
User-Designated Active/Inactive Cells	*Lookup_seal_active.txt*
Areas of Seal Grid Elements	*Lookup_seal_grid_area.txt*
Center Coordinates of Seal Grid Elements	*Lookup_seal_grid_coord.txt*
Intrinsic Permeability of Seal Grid Elements	*Lookup_seal_perm*
Porosities of Seal Grid Elements	*Lookup_seal_porosity.txt*
Height/Thickness of Seal Grid Elements	*Lookup_seal_thick.txt*
Brine Pressure Values at the Top of the Seal Horizon for Each Time Step	*Lookup_seal_top_press.txt*
CO_2 Saturation Values at the Top of the Seal Horizon for Each Time Step	*Lookup_seal_top_sat.txt*
Directory: Lookup_Tables\transfer_data	
CO_2 Pressure Values at Top of Reservoir (with Coordinates) for Each Time Step	*Lookup_reservoir_CO2press.txt*
CO_2 Saturation Values at Top of Reservoir (with Coordinates) for Each Time Step	*Lookup_reservoir_CO2sat.txt*
Time In Years For Each Time Step	*Lookup_times_series.txt*

Table E-2: File Formats

Lookup_land_surface.txt

```
! Land Surface Elevation File …     Comment Line
2                                   Array Dimension
100, 100                            Number of Rows (Y) and Columns (X)
   0.0,  100.0,  200.0,  300.0, ... 9900.0          X Coordinates (100 values - labels for columns)
   0.0,  100.0,  200.0,  300.0, ... 99000,          Y Coordinates (100 values - labels for rows)
((Land Surface Elevation Values (m - NAVD88) in 100 Column x 100 Row Array))
  3200.00,  3163.32,  3161.32,  3159.32,  3157.32,  3155.32,  3153.32,  3151.32,
3149.32,  3147.32,  3145.32,  3150.18, ...      Column Values for First Row
...     ((98 Rows))
  3167.08,  3165.08,  3163.08,  3161.08,  3177.21,  3175.21,  3173.21,  3182.19,
3156.56,  3154.56,  3152.56,  3150.56, ...      Column Values for 100th Row
```

Lookup_reservoir_elev.txt

```
! Reservoir Elevation File          Comment Line
2                                   Array Dimension
100, 100                            Number of Rows (Y) and Columns (X)
   0.0,  100.0,  200.0,  300.0, ... 9900.0          X Coordinates (100 values - labels for columns)
   0.0,  100.0,  200.0,  300.0, ... 9900.0          Y Coordinates (100 values - labels for rows)
((Reservoir Elevation Values (m - NAVD88) in 100 Column x 100 Row Array))
  -1001.00,  -1001.00,  -1003.00,  -1003.00,  -1000.00,  -1000.00,  -1000.00,  -
1000.00,  -1000.00,  -1000.00,  -1000.00, ...   Column Values for First Row
...     ((98 Rows))
  -1000.00,  -1000.00,  -1010.00,  -1010.00,  -1010.00,  -1020.00,  1020.00,  -
1030.00,  -1030.00,  -1030.00,  -1040.00, ...   Column Values for 100th Row
```

time_series.xlsx / time_series.txt

```
! Time series for case 1     Comment Line
1                            Array Dimension
33                           Number of Values
((Index and Time Values (yr) in Vector Form))
  1,  2,  3,  4,  5,  6,  7,  8, ... 32,  33   Step Index Number
  0,  1,  2,  5,  10,  15,  20,  25, ... 175, 200     Time (yr)
```

Table E-2: File Formats (Continued)

Lookup_seal_grid_area.txt

```
! User-Defined Seal Grid Area File          Comment Line
2                                           Array Dimension
100, 100                                    Number of Rows (Y) and Columns (X)
  1,  2,  3,  4,  5,  6, ... 99, 100        Column Index Values (100)
  1,  2,  3,  4,  5,  6, ... 99, 100        Row Index Values (100)
((Area (m2) in 100 Column x 100 Row Array))
  900.00,  900.00,  900.00,  900.00,  900.00,  900.00,  900.00,  900.00,  900.00,
900.00,  900.00,  900.00,  900.00, ...      Column Values for First Row
...     ((98 Rows))
  900.00,  900.00,  900.00,  900.00,  900.00,  900.00,  900.00,  900.00,  900.00,
900.00,  900.00,  900.00,  900.00, ...      Column Values for 100th Row
```

Lookup_seal_grid_coord.txt

```
! User-Defined Grid Element Center Coordinates File     Comment Line
3                                           Array Dimension
100, 100, 2                                 Number of Rows (Y), Columns (X), and Depth (Z) of Array
  1,  2,  3,  4,  5,  6, ... 99, 100        Index Values - Columns
  1,  2,  3,  4,  5,  6, ... 99, 100        Index Values - Rows
  1,  2                                     Index Values - Depth
((X Coordinates (m) in 100 Column x 100 Row Array))
  15.00,  45.00,  75.00,  105.00,  135.00,  165.00,  195.00,  225.00,  255.00,
285.00,  315.00,  345.00,  Column Values for First Row
....15.0,      ((Total of 100 Rows))
((Y Coordinates (m) in 100 Column x 100 Row Array))
  15.00,  15.00,  15.00,  15.00,  15.00,  15.00,  15.00,  15.00,  15.00,  15.00,
15.00,  15.00, ...  Column Values for First Row
....15.0,      ((Total of 100 Rows))
```

Table E-2: File Formats (Continued)

Lookup_seal_perm.txt

```
! User-Defined Seal Permeability File      Comment Line
2                                          Array Dimension
100, 100                                   Number of Rows (Y) and Columns (X)
 1, 2, 3, 4, 5, 6, 7, ... 99, 100          X Index Values
 1, 2, 3, 4, 5, 6, 7, ... 99, 100          Y Index Values
((Permeability (mD) in 100 Column x 100 Row Array))
 5.021, 4.981, 4.958, 4.725, 5.056,  5.071, ...        Column Values for First Row
...     ((98 Rows))
 5.040, 5.090, 5.032, 4.947, 5.003, 4.894, ... Column Values for 100th Row
```

Lookup_seal_porosity.txt

```
! User-Defined Seal Porosity File         Comment Line
2                                          Array Dimension
100, 100                                   Number of Rows (Y) and Columns (X)
 1, 2, 3, 4, 5, 6, 7, ... 99, 100          X Index Values
 1, 2, 3, 4, 5, 6, 7, ... 99, 100          Y Index Values
((Porosity (decimal) in 100 Column x 100 Row Array))
 0.021, 0.354, 0.358, 0.225, 0.295, 0.302, ... Column Values for First Row
...     ((98 Rows))
 0.265, 0.211, 0.320, 0.288, 0.301, 0.255. ... Column Values for 100th Row
```

Lookup_seal_thick.txt

```
! User-Defined Seal Thickness File        Comment Line
2                                          Array Dimension
100,100                                    Number of Rows (Y) and Columns (X)
 1, 2, 3, 4, 5, 6, 7, ... 99, 100          X Index Values
 1, 2, 3, 4, 5, 6, 7, ... 99, 100          Y Index Values
((Seal Element Thickness / Height (m) in 100 Column x 100 Row Array))
  30.00,  30.00,  30.00,  30.00,  30.00, 30.00, ...
  43.00,  43.00,  43.00,  43.00,  43.00,  43.00, ...  Columns Values for 100th Row
```

Table E-2: File Formats (Continued)

Lookup_reservoir_CO2pres.txt

```
! Reservoir CO2 Pressure Data File        Comment Line
3                                         Array Dimensions
100,100,33                                Number of Rows (Y), Columns (X), and Time Steps
   0.0,  150.0,  250.0,  350.0, ...  9950.0          X Coordinates (100 values - labels for columns)
   0.0,  200.0,  400.0,  600.0, ... 198000.0         Y Coordinates (100 values - labels for rows)
   0.0,  3.155760E+07,  6.311520E+7,                 Time Step Values (in seconds)
For each time step: CO2 Pressure Values (MPa) at Top of Reservoir in 100 Column x 100 Row Array))
   10.5,   10.5,   10.5,   10.5,   10.5,   10.5,     ((100 columns x 100 rows) for each  time step))
```

Lookup_reservoir_CO2sat.txt

```
! Reservoir CO2 Saturation Data File     Comment Line
3                                        Array Dimensions
100,100,33                               Number of Rows (Y) Columns (X), and Time Steps
   0.0,  150.0,  250.0,  350.0, ...  9950.0          X Coordinates (100 values - labels for columns)
   0.0,  200.0,  400.0,  600.0, ... 198000.0         Y Coordinates (100 values - labels for rows)
   0.0,  3.155760E+07,  6.311520E+7,                 Time Step Values in seconds
For each time step:  CO2 Saturation Values (decimal) at Top of Reservoir in 100 Column x 100 Row Array
   0.10,   0.10,   0.10,   0.10,   0.10,   0.10,     ((100 columns x 100 rows) for each time step))
```

Lookup_seal_active.txt

```
! User-defined Active/Inactive Cells -- << 0 = Inactive >> … Comment Line
2                    Array Dimension
100, 100             Number of Rows (Y) and Columns (X)
1, 2, 3, 4, 5, 6, 7, ... 99, 100          X Index Values
1, 2, 3, 4, 5, 6, 7, ... 99, 100          Y Index Values
((Active/Inactive Designation in 100 Column x 100 Row Array for Each Cell))
  0.0,  1.0,  1.0,  1.0,  1.0,  1.0,  1.0,  1.0,  1.0,..      Column Values for First Row
  0.0,  0.0,  0.0, ... ((Total: 100 Rows))
```

Table E-2: File Formats (Continued)

Lookup_seal_top_press.txt

```
! Brine Pressure at Top of Seal Horizon File     Comment Line
3                                                Array Dimensions
100,100,33                                       Number of Rows (Y), Columns (X), and Time Steps
   1, 2, 3, 4, 5, 6, 7, ... 99, 100              X Index Values
   1, 2, 3, 4, 5, 6, 7, ... 99, 100              Y Index Values
   0.0,  3.155760E+07,  6.311520E+7,             Time Step Values (in seconds)
For each time step: Brine Pressure Values (MPa) at Top of Seal in 100 Column x 100 Row Array
   12.7,   12.7,   12.7,   12.7,   12.7,   12.7,    ((100 columns x 100 rows) for each time step))
```

Lookup_seal_top_sat.txt

```
! CO2 Saturation at Top of Seal Horizon File     Comment Line
3                                                Array Dimensions
100,100,33                                       Number of Rows (Y) Columns (X), and Time Steps
   1, 2, 3, 4, 5, 6, 7, ... 99, 100              X Index Values
   1, 2, 3, 4, 5, 6, 7, ... 99, 100              Y Index Values
   0.0,  3.155760E+07,  6.311520E+7,             Time Step Values (in seconds)
For each time step: CO2 Saturation Values (decimal) at Top of Seal in 100 Column x 100 Row Array
   0.10,   0.10,   0.10,   0.10,   0.10,   0.10,    ((100 columns x 100 rows) for each time step))
```

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APPENDIX F: PROGRAMMING AND DEVELOPMENT ENVIRONMENT

F.1 Installation Requirements

In establishing a new installation of NSealR on another computer system, please note the following:

1. The directory structure of the NSealR source code must be preserved on the new installation as is, or new links must be established for all input and output files using GoldSim.
2. Excel must reside on the same PC as NSealR for GoldSim operations with Excel.
3. The DLLs for NSealR output were written in C++. These files can be revised using the source code supplied and compiled using Visual C++ from Microsoft© Visual Studio Professional 2013 for Windows Desktop. Note that the files must be compiled as a "Release" version. Visual Studio files can be downloaded from Microsoft at URL: http://www.visualstudio.com/downloads/download-visual-studio-vs (accessed 05 March 2014).
4. If the user does not have access to GoldSim, the player version of the code can be run by installing the GoldSim Player program from GoldSim Technology Group LLC website at URL: http://www.goldsim.com/forms/playerdownload.aspx (accessed 05 March 2014). This allows the Player version of NSealR (*.gsp) to be run, but without the ability to change the source code. If permitted by security settings, the code structure of NSealR can be viewed with GoldSim Player by clicking on the "Go" label on the GoldSim Run Controller (separate window) and selecting, "Go to Model Root..."

F.2 Development Environment

This version of NSealR was developed on a desktop personal computer running Microsoft© Windows 7, Service Pack 3 with an Intel® Xeon® CPU E5-2670, running at 2.6 gigahertz and with 16.0 gigabytes of random access memory.

The development code was GoldSim, Version 11.0.3. Also installed on the same computer was Microsoft© Excel© 2010, stand-alone Version 14.0.6123.5001 (32-bit).

DLLs were written in Visual C++ using the Microsoft© Visual Studio Professional 2013 environment, Version 12.0.21005.1 Release.

F.3 Run Notes

In performing a new analysis with NSealR, please note the following:

1. For each new reservoir data set, new input files must be provided for reservoir input and the relevant input elements must be re-linked.
2. The input data files for the reservoir input are located in directory, "... \Lookup_Tables\transfer_data." The CO_2 pressure values at top of reservoir (with coordinates) for each time step are to be included in file, *Lookup_reservoir_CO2pres.txt.* The CO_2 saturation values at top of reservoir (with

coordinates) for each time step are to be included in file *Lookup_reservoir_CO2sat.txt*.

3. The lookup table elements that are to be adjusted for a new reservoir data set are located in NSealR container, "import_reservoir_results"; the files: *Lookup_reservoir_CO2_sat* and *Lookup_reservoir_CO2_pres*[37] will require re-linking.
4. All changed lookup table elements must re-linked in NSealR, per the GoldSim Manual.
5. Time steps (for control of reservoir saturation and pressure) are defined in an Excel file, titled "time_series.xlsx", which is located in the directory "\Lookup_Tables\transfer_data." The specific times for each time step are entered in row format, starting in column 2, with input descriptions in column 1. Input will stop at the first blank cell.
6. The default data set (null case) provides a set of "zero" results.

[37] Note that these re-linked files can be renamed differently for each test case, but it is recommended that prefix names be retained, i.e. such as for example, renaming a file as: *reservoir_CO2_sat - constant pressure case.txt*.

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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