Excerpt from the Proceedings of the COMSOL Conference 2010 Boston

Hydro-Mechanical Modelling of a Shaft Seal in a Deep Geological Repository

Deni G. Priyanto*,1
[1]Atomic Energy of Canada Limited
*Corresponding author: Whiteshell Laboratories, Pinawa, Manitoba, Canada, R0E 1L0, priyantd@aecl.ca

Abstract: A shaft seal is one of the engineered barriers considered by Canada's Nuclear Waste Management Organization (NWMO) for use in isolating and containing used nuclear fuel in a Deep Geological Repository (DGR). This paper presents hydraulic-mechanical (HM) numerical simulation of a shaft seal installed in hypothetical geosphere using COMSOL. Two different stages are considered in the simulations undertaken. Stage 1 and 2 simulate the groundwater flow into an open shaft and after installation of shaft sealing-components, respectively. This paper presents the numerical formulation that couples the unsaturated flow with structural analysis. This formulation successfully simulated the HM behavior of an unsaturated triaxial specimen in a laboratory and was used to simulate a shaft seal at both stages.

Keywords: hydraulic, mechanical, unsaturated, shaft seal, repository.

1. Introduction

A shaft seal is one of the engineered barriers considered for use by Canada's Nuclear Waste Management Organization (NWMO) in isolating and containing used nuclear fuel in a Deep Geological Repository (DGR). A shaft seal would be installed at strategic locations, such as significant fracture zones, to limit the potential for fast movement of groundwater from repository level to the surface via the shaft. Two different stages should be considered in the simulation of a shaft seal. Stage 1 simulates the groundwater flow into an open shaft to determine the groundwater and stress conditions at the geosphere prior to the installation of shaft sealing-components. Stage 2 simulates groundwater flow after installation of shaft sealing-components.

The main objective of the study presented in this paper is to evaluate the capability of COMSOL to simulate the hydraulic and mechanical (HM) behavior of a shaft seal installed at a fracture zone in a hypothetical geosphere. In order to simulate HM behavior of a shaft seal using COMSOL, the following challenges must be solved. First, the shaft-sealing components are unsaturated at installation, so coupling the unsaturated flow formulation with structural analysis is required. Secondly, properties and conditions at the seal location change abruptly between Stages 1 and 2, thus a method to apply this change is required. Finally, evaluation of the long-term performance of a shaft seal must be assessed. The durations of Stages 1 and 2 considered in this study are anticipated to be in the order of 100 years and 1,000,000 years, respectively.

Numerical modeling of an actual shaft seal will ultimately involve a more complex geometry and more processes will need to be included in the analysis (e.g., thermal or solute transport) than are considered in the current study. Consequently, given the ultimate complexity that will be needed for a complete numerical simulation, the duration of the solution time required to complete the basic analysis presented in this study should be reasonably short. If this is accomplished then this will leave room for extending the capability/ complexity of the models while still obtaining results in a timely manner.

This paper presents an algorithm to couple unsaturated flow formulation (i.e., Richard's equation) with stress-strain analysis using COMSOL. This algorithm was then used to simulate infiltration process of triaxial specimen of one of the sealing components in a laboratory. The results were compared with the measurement to verify the formulation. Finally, this formulation was used to simulate a shaft seal installed in a hypothetical geosphere.

2. Description of a Shaft Seal Considered in the Numerical Modeling

The selection of the geometry and configuration of sealing materials used in the shaft seal will ultimately be a site specific and depend on the design requirements of the DGR.

For the purpose of this study, the geometry and configuration of a shaft seal located in a hypothetical geosphere was assumed and illustrated in Figure 1.

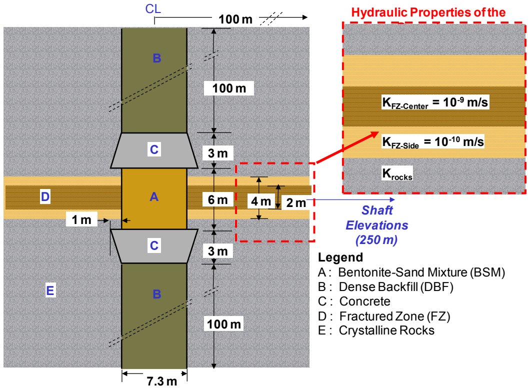


Figure 1. Geometry of the shaft seal in hypothetical geosphere considered in the numerical modeling

The following assumptions were made in defining the shaft seal modeled in this study. The geosphere was crystalline (granitic) rock. The fracture zone that intersected the shaft was perfectly horizontal and located at a depth of 250 m. The shaft diameter was 7.3 m and the center of the shaft seal was located at 250 m depth, the same location as the fracture zone. The repository was located at a depth of 500 m and so the shaft seal was assumed to be in an isothermal condition. Consequently, HM numerical simulation using a 2D-axisymetric model within a smaller domain was used to evaluate the shaft seal performance. The domain used in this numerical modeling had a 200-m diameter and a 200-m height (Figure 1).

The shape of the shaft seal in this paper was based on actual construction experiences where shaft and tunnel seals were constructed (Dixon et al. 2009), but dimensions and material configuration considered in the model differed. Materials used in the shaft seal include: bentonite-sand mixture (BSM), dense backfill (DBF), and concrete. The BSM was constrained between two massive concrete segments (Figure 1). The DBF was installed above and below the concrete components of the shaft seal (Figure 1).

Keying of the rock to install the concrete components provides mechanical stability to the construction and facilitates distribution of any stresses developed within the shaft/ tunnel uniformly into the rock. The concrete components were designed to provide a mechanical constraint to the swelling clay materials, thereby preventing discernible loss of clay density and in so doing, maintain the low-permeability characteristics of the shaft sealing volume.

3. Development of HM Coupling and Verification

Prior to HM simulation of a shaft seal using COMSOL, the development of HM coupling for unsaturated clay and verification of the formulation using the laboratory test results were completed.

3.1 Coupling HM Formulations for Unsaturated Soil

Due to the high swelling capacity of clay-based sealing material components, in particular the BSM, it is significant to couple mechanical and hydraulic process to simulate a shaft seal.

The coupling of HM formulation to simulate saturated soil was provided in COMSOL 3.5a, Earth-Science Module. This formulation was modified in order to simulate unsaturated soil. This study developed custom-additions in COMSOL to couple Richard's equation and linear elastic model and to implement user-defined SWCC (soil water characteristics curve) and permeability models that were based on results of laboratory testing of the BSM (Siemens 2006, Priyanto and Dixon 2009).

The governing equations used in the analysis are as follows. Unsaturated flow is described using Richard's equation:

$$\left[C + S_e S\right]\frac{\partial H_p}{\partial t} + \nabla \cdot \left[-K\nabla\left(H_p + D\right)\right] = Q_s \qquad (1)$$

C denotes specific moisture capacity [m^{-1}], S_e is the effective saturation, S is the storage coefficient (m^{-1}), t is the time, K is the hydraulic conductivity (m/s), and D is the vertical elevation, H_p [m] is pressure head, which can be related to the pore water pressure (p) using:

$$p = H_p/(g \cdot \rho_f) \qquad (2)$$

ρ_f is the fluid density. Assuming pore air is constant and equal to 0, suction is equal to negative porewater pressure (s = -p) and hence $H_p = -s \cdot g \cdot \rho_f$.

In Equation 1, the first term represents the change in storage in the unsaturated material, while the second term represents Darcy's law with a hydraulic conductivity that is dependent upon saturation. S is the specific storage, which is set as follows.

$$S = \rho_f g\,(\chi_p + \theta \chi_f) \tag{3}$$

ρ_f is the fluid density, g is the gravitational acceleration, χ_p and χ_f are the compressibility of the solid particles and fluid, respectively. The hydraulic conductivity, K is:

$$K = k_w^{sat} \cdot k_r \tag{4}$$

k_w^{sat} is the hydraulic conductivity at saturated conditions [m/s] and dependent on the total porosity (θ). The relationship of k_w^{sat} and θ is defined using Kozeny's model:

$$k_w^{sat} = k_0 \frac{\theta^3}{(1-\theta)^2} \frac{(1-\theta_0)^2}{\theta_0{}^3} \tag{5}$$

k_r in Equation 4 is the relative permeability described using van Genuchten (1980) equations.

$$k_r = \begin{cases} S_e{}^L \left[1 - \left(1 - S_e{}^{1/m}\right)^m\right]^2 & \text{for } H_p < 0 \\ 1 & \text{for } H_p \geq 0 \end{cases} \tag{6}$$

S_e and C are also calculated using van Genuchten (1980) equations.

$$S_e = \begin{cases} \dfrac{1}{\left[1 + \left|\alpha H_p\right|^n\right]^m} & \text{for } H_p < 0 \\ 1 & \text{for } H_p \geq 0 \end{cases} \tag{7}$$

$$C = \begin{cases} \dfrac{\alpha m}{1-m} \left(\theta_s - \theta_r\right) S_e^{\frac{1}{m}} \left(1 - S_e^{\frac{1}{m}}\right)^m & \text{for } H_p < 0 \\ 0 & \text{for } H_p \geq 0 \end{cases} \tag{8}$$

α, m, n, and L are fitting parameters. θ_s and θ_r are the saturated and residual volumetric water contents. In this analysis saturated volumetric water content (θ_s) is equal to the current total porosity (θ) that is calculated using:

$$\theta = (v-1)/v \tag{9}$$

v is the total specific volume and calculated from the mechanical analysis using:

$$v = v_{initial} \cdot (1+\varepsilon_v) \tag{10}$$

$v_{initial}$ ($=1/(1-\theta_{initial})$) is the initial specific volume. ε_v is the volume strain.

The mechanical to hydraulic (MH) coupling is done by substitution of the flow (Q_s) in Equation 1 with the following equations:

$$Q_s = -\alpha_b \cdot \frac{\partial}{\partial t}(\nabla \cdot u) \tag{11}$$

$\frac{\partial}{\partial t}(\nabla \cdot u)$ is the time rate change of strain, u is the displacement vector and α_b is a constant usually termed as Biot-Willis coefficient.

The hydraulic to mechanical (HM) coupling is done by application of the body force induced by the hydraulic process.

$$\mathbf{F} = -\alpha_b\, \rho_f\, g\, \nabla H \tag{12}$$

In this analysis a linear elastic model is used. The results of the laboratory test of BSM specimen indicate that the maximum degree of saturation (S_{max}) depends on the total porosity, where S_{max} increases with an increase of θ (Siemens 2006, Priyanto and Dixon 2009). With known value of S_{max}, the residual volumetric water content and the current degree of saturation (S_w) are equal to:

$$\theta_r = (1-S_{max}) \cdot \theta \tag{13}$$

$$S_w = S_e\,(\theta - \theta_r)/\,\theta \tag{14}$$

3.2 Modelling Laboratory-Scale Test

In order to verify the formulation presented previously, it was used to simulate HM behavior of a BSM specimen in a triaxial test (Siemens

2006). Figures 2a, 2b, and 2c show the dimensions of triaxial specimen, the hydraulic and mechanical boundary and initial conditions used in the numerical modeling. The specimen had a cylindrical shape, 50-mm diameter and 100-mm height (Figure 2a). Due to its symmetrical shape, only half of the specimen was simulated in the numerical models using axisymmetric geometry. Thus the numerical model simulated a radius of 25 mm and a height of 50 mm. The top of the specimen and the symmetry line were assumed to be impermeable. A pore water pressure of 0.2 MPa was applied around the specimen perimeter during the test. The initial gravimetric water content was 18.75% (corresponding to an initial degree of saturation of 70%). The initial mean stress was 0.5 MPa. Roller mechanical boundary conditions were assumed at the top, symmetry line, and perimeter of the model (Figure 2c). Application of these mechanical boundary conditions resulted in constant total volume, but allows the displacement of the internal grids to investigate the variation of dry density along radial and axial direction. Parameters used in this numerical modelling are summarized in Table 1.

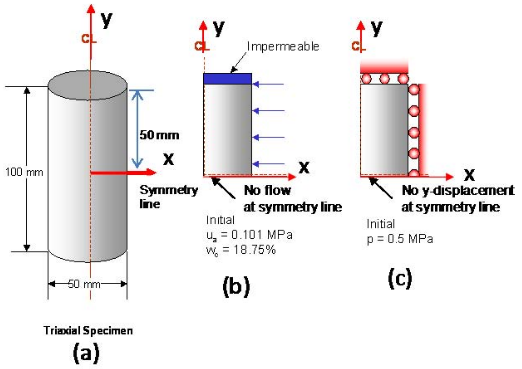


Figure 2. Infiltration test of the BSM specimen: (a) triaxial specimen; (b) hydraulic and (c) mechanical boundary and initial conditions.

Figure 3 shows the result of the numerical simulation using COMSOL compared with laboratory test results. The use of Richard's equation in this study induced some limitation of this formulation due to its assumption of constant poreair pressure, which can be different from the laboratory test. The volume of water input to the specimen for approximately the first 5 days was underestimated by COMSOL analysis (Figure 3). Unlike the laboratory test results where smooth transition of the volume of water added to specimen was observed, COMSOL analysis showed a clear change in water uptake behavior at approximately 5 days (Figure 3). Using another computer code, smooth transition can be obtained when using two-phase flow formulation (Priyanto and Dixon 2009). Future studies to couple the two-phase flow formulation with mechanical constitutive model in COMSOL are recommended to generate this smooth transition, as it was observed in the laboratory test results.

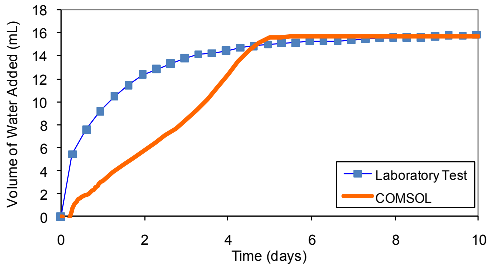


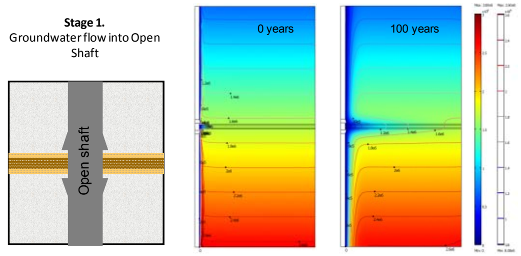
Figure 3. Volume of water added to the specimen from COMSOL simulation compared with the laboratory test

Despite of this limitation, the general behaviour of the BSM specimen can be captured using the formulation presented in this study. The total amount of water added to the specimen based on COMSOL simulation was similar to that measured in laboratory testing. Since the COMSOL and laboratory tests showed such close matches for periods beyond a few days the water uptake formulation was then used to simulate a shaft seal in a hypothetical geosphere.

4. Development of a Shaft Seal in a Hypothetical Geosphere Model

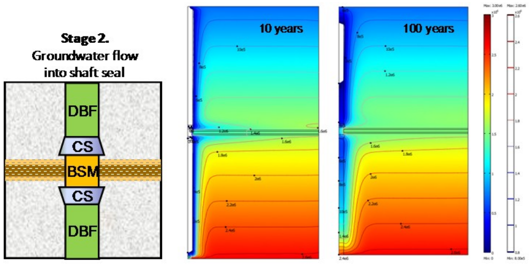
The HM formulation presented previously was used to simulate a shaft seal installed in a hypothetical geosphere. Two different stages were considered in this HM numerical modelling of a shaft seal. Stage 1 simulated the groundwater flow into an empty shaft, prior to shaft seal installation (Figure 4a). Stage 2 simulated the groundwater flow into the shaft seals (Figure 5a). Table 2 summarizes the parameters used in the simulation.

The shaft seal was assumed to be constructed after 100 years of shaft operation (i.e., open hole). Stage 1 was a time-dependent HM analysis simulating 0 to 100 years after the completion of shaft construction, but prior to the shaft sealing construction (Figure 4a). A very large hydraulic conductivity (i.e., K = 1 m/s) and very low Young's modulus (i.e., E = 1 Pa) were assigned to represent an empty shaft (Figure 4a). Porewater pressure on the interface between the geosphere and the empty borehole was assumed as a constant atmospheric pressure (= 0.1 MPa).



(a) **(b)**

Figure 4. Porewater pressure contour at stage 1



(a) **(b)**

Figure 5. Porewater pressure contour at stage 2

The initial horizontal stress (σ_h), vertical stress (σ_v) and porewater pressure (p) in the intact rock prior excavation were assumed to be varied with depth according to Equations 15, 16 and 17, respectively.

$$\sigma_h\,(z) = 0.071 \text{ MPa/m} * z + 5.768 \text{ MPa} \qquad (16)$$

$$\sigma_v\,(z) = 0.034 \text{ MPa/m} * z \qquad (17)$$

$$p(z) = \rho_w \cdot g \cdot (z + 80) \qquad (18)$$

Stage 2 simulated groundwater flow into the shaft seal. The results of the analysis in Stage 1 at time 100 years were used as the initial conditions for Stage 2. Time-dependent HM analyses in Stage 2 simulated 0 to 1,000,000 years after installation of the shaft seal (Figure 5a).

In Stage 2, the empty shaft was filled with the BSM, DBF, and concrete. The parameters for these materials in Table 2 were used as an input in Stage 2. The initial porewater pressures for BSM, DBF, and concrete components were set to negative value representing unsaturated conditions of these materials at the installation of the shaft sealing components. These negative porewater pressures correspond to the initial degree of saturation of each material calculated using SWCC of the van Genuchten (1980) model.

5. Results and Discussion

Some of the HM simulation results of a shaft seal in a hypothetical geosphere are illustrated in Figure 4b, 5b, 6, and 7. Figure 4b shows the porewater pressure during Stage 1 at time 0 (immediately after shaft excavation) and 100 years (after shaft excavation). Stage 1 represents the period when the groundwater is removed from the shaft during shaft operation. The groundwater flow from the host rocks to empty borehole causes a decrease of porewater pressure in the host rock surrounding this excavation and the area affected increases with time (Figure 4b).

Stage 2 simulates groundwater flow at time 0 to 1,000,000 years after shaft seal installation. One of the challenges mentioned previously for simulating a shaft seal was an abrupt change of material properties and conditions from Stage 1 to Stage 2. The porewater pressure result at the geosphere domains (i.e., crystalline rock and fracture zones) from the end of Stage 1 analyses (100 years) are applied as the initial conditions in Stage 2 in these domains. However, this condition is not applied at the shaft seal domain.

In order to apply this initial condition of Stage 2, a function was created from the results of the Stage 1 analysis at time of 100 years and applied at the geosphere domain. This function is applied as the initial value in the sub domain. At the shaft sealing components domains (BSM, DBF, and concrete), negative porewater pressure are applied as the initial conditions of stage 2 to represent unsaturated conditions. Different material properties listed in Table 2 are assigned at each domain.

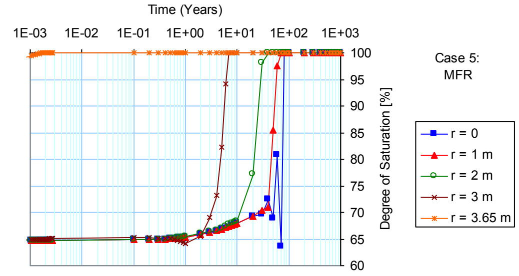


Figure 6. Degree of saturation evolution in the BSM at 250-m depth (stage 2)

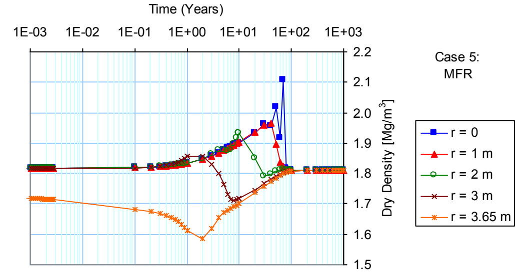


Figure 7. Dry density evolution in the BSM at 250-m depth (stage 2)

Figure 5b shows the porewater pressure at times 0 and 100 of Stage 2. Due to the unsaturated condition of the BSM at the beginning of stage 2, porewater pressure was initially (-12.5 MPa). The porewater pressure in the BSM increases due to the saturation process. Similarly, the porewater pressure at the geosphere components near the shaft seal also increases.

Figure 6 shows the evolution of the porewater pressure at the centre of the fracture zone (z = -250 m) in the BSM in four different locations (r = 0, 1, 2, 3, 3.65 m) from time 0 to 1000 years of Stage 2. Figure 7 shows evolution of the dry density at the same locations and stage. The evolution of the degree of saturation indicated that the BSM is fully saturated approximately 80 years after shaft seal installation (Figure 7). The time when the center of BSM was fully saturated can be used as an indicator to show an effectiveness of the shaft sealing system (Priyanto 2009).

As expected due to abrupt property changes between Stage 1 and Stage 2, the dry density at the BSM adjacent to the rock decreased immediately, due to the saturation and swelling of the material in this region (see r=3.65 m in Figure 7). This swelling of the BSM in this region caused compression of the BSM material next to it and increased its dry density (see r = 0, 1, 2, 3 m in Figure 7). Since the BSM material was simulated using a linear elastic model, after 100 years, all the material equilibrate at similar dry density of ~1.8 Mg/m^3, equal to the dry density at installation. This may not be the case if a mechanical constitutive model incorporating plasticity was used and the results will be more representative to material behavior. Coupling of the unsaturated flow formulation with a model with plasticity feature are recommended in the future study.

6. Conclusions and Recommendations

This study has developed custom-additions in COMSOL to couple Richard's equation and the linear elastic model and to implement a custom SWCC (soil water characteristics curve) and permeability model observed from the results of laboratory testing of the BSM.

This formulation has been verified to simulate hydraulic and mechanical processes in the laboratory test of an unsaturated bentonite-sand mixture (BSM) specimen and used to simulate a shaft seal in a hypothetical geosphere.

The results of the numerical modeling of a shaft seal using COMSOL show a logical pattern of development of hydraulic and mechanical conditions. This indicates that COMSOL can be used as a tool for further study of the evolution and performance of a shaft seal in a deep geological repository. Moreover, using current computer capability, the solution time required to complete the analysis to simulate 1,000,000 years of HM behavior of a shaft seal described in this study was relatively short (i.e., less than 60 minutes), which is beneficial in building more complex models and formulations to simulate an actual shaft seal in actual geosphere conditions.

Limitations associated with the formulations used to simulate a shaft seal have been observed in this study. Development of coupling formulation for multi-phase flow with a mechanical constitutive model having a plasticity feature is recommended in order to improve HM simulation and more closely simulate conditions anticipated to be present in an actual shaft seal.

7. References

1. Dixon, D.A., J.B. Martino and D.P. Onagi, Enhanced Sealing Project (ESP): Preliminary design and construction plan. *Nuclear Waste Management Organization Technical Report* **(NWMO APM-REP-01601-0001)** (2009)

2. Priyanto, D.G. and Dixon,D.A, Hydraulic-mechanical (HM) numerical modelling of triaxial tests of unsaturated clay-based sealing material using three computer codes. *Nuclear Waste Management Organization Technical Report* **(In review)** (2009)

3. Priyanto, D.G, Numerical modelling of shaft seal in sedimentary and crystalline rocks. . *Nuclear Waste Management Organization Technical Report* **(In review)** (2009)

4. Siemens, G.A., Influence of boundary conditions on the hydraulic-mechanical behaviour of an unsaturated swelling soil. *Ph.D Thesis, Dept. Civil Engineering, University of Manitoba, Winnipeg, Manitoba.*

5. van Genuchten, M.Th, A closed form equation for predicting the hydraulic conductivity of unsaturated soils, *Soil Sc. Soc. Am. J.* **44**, 892-898 (1980)

8. Acknowledgements

The numerical modeling presented in this paper is part of the work funded by Nuclear Waste Management Organization (NWMO).

9. Appendix

Table 1: Parameters used to simulate laboratory-scale test of the BSM specimen

Variables	Units	Descriptions	Value
g	m/s^2	Gravity	9.82
ρ_f	kg/m^3	Fluid density	1000
χ_p	$m\cdot s^2/kg$	Compressibility of solid particles	10^{-8}
χ_f	$m\cdot s^2/kg$	Compressibility of fluid particles	$4.4\cdot 10^{-10}$
α	m^{-1}	Alpha parameter	0.00327
n		N parameter	1.39
m		1-1/n	0.28
L		L parameter	0.5
$\theta_{initial}$		Initial porosity	0.42
k_{sat}	m/s	Kozeny's Equation (Substitution of k_0 = 5e-10 m/s, θ_0 = 0.42 in Equation 5)	Function of θ

Table 2: Parameters used to simulate a shaft seal in a hypothetical geosphere

	Host Rock	Concrete	Bentonite-Sand Mixture (BSM)	Dense Backfill (DBF)
Properties at Installation				
Gravimetric Water Content [%]			12	8.5
Dry Density [Mg/m^3]			1.80	2.10
Bulk Density [Mg/m^3]	2.7	2.35	2.02	2.28
Specific Gravity		2.35	2.7	2.65
Void Ratio, e			0.500	0.262
Specific Volume, V			1.500	1.262
Porosity, θ	0.003	0.009	0.33	0.21
Degree of Saturation, S_w [%]	100	5	65	86
SWCC and Relative Permeability Curve				
Effective Saturation, S_e	0.05	0.05	0.65	0.86
Initial Suction [MPa]	0.1063	0.1063	12.85	0.39
Parameter α [1/m]	50	50	0.001962	0.01962
Parameter m	0.33	0.33	0.28	0.28
Parameter n	1.49	1.49	1.39	1.39
Parameter L	0.5	0.5	0.5	0.5
Saturated Hydraulic Conductivity, K [m/s]	1e-12 (intact) 1e-10 (FZ-side) 1e-9 (FZ-center)	1e-12	1e-12	1e-11
Mechanical Parameters				
Young Modulus [MPa]	45,000	38,000	100	200
Poisson's Ratio	0.25	0.24	0.1	0.1