

HYDRO-MECHANICAL MODELLING OF A SHAFT SEAL IN CRYSTALLINE AND SEDIMENTARY HOST ROCK MEDIA USING COMSOL

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ABSTRACT

Shaft seals are components of the engineered barriers system considered for closure of a Deep Geological Repository (DGR). These seals would be installed in strategic locations of the shafts, where significant fracture zones (FZ) are located and would serve to limit upward flow of groundwater from the repository level towards the surface.

This paper presents the results of hydro-mechanical (HM) numerical modelling exercises to evaluate the performance of a shaft seal using a finite element computer code, COMSOL. This study considered a variety of host geological media as part of generic assessments of system evolution in a variety of environments including five hypothetical sedimentary and crystalline host rock conditions. Four simulations of a shaft seal in different sedimentary rocks were completed, including: (1) shale with isotropic permeability; (2) shale with anisotropic permeability; (3) limestone with isotropic permeability; and (4) limestone with anisotropic permeability. The other simulation was a shaft seal in crystalline rock with isotropic permeability. Two different stages were considered in these HM simulations. Stages 1 and 2 simulated the groundwater flow into an open shaft and after installation of shaft sealing components, respectively.

As expected, the models were able to simulate that installation of the shaft seal limits groundwater flow through the shaft. Based on the conditions and assumptions defined for the host media and fracture features examined in this study, the following conclusions can be drawn from the results of the numerical modelling exercises. A shaft that remained open for a longer time was beneficial with respect to delaying of seal saturation because it could reduce the groundwater flow rate around the fracture zone. Delaying saturation time indicates slower movement of the groundwater or other substances that may be transported with the groundwater. The core of the shaft seal (i.e., the bentonite-sand mixture (BSM)) became fully saturated after 90-100 years if the shaft remained open for 100 years before a seal was installed. Only a slight difference between five cases was observed from the results of the numerical modelling exercises for different cases. This may, in part, be the result of limitations in the knowledge regarding the HM characteristics of the geological media evaluated. Defining of more site specific conditions (e.g., depth and geometry of fracture, hydraulic properties of rock and fracture feature, and mechanical characteristics of rock) was recommended in order to more effectively simulate HM behaviour of a shaft seal at the location of a fracture zone.

Keywords: shaft seal, numerical modelling, hydraulic, mechanical, finite element methods.

1. INTRODUCTION

The isolation and containment of used nuclear fuel in a Deep Geological Repository (DGR) is a common approach for international waste management agencies. When a DGR is permanently closed, there will be a need to install sealing materials in the shafts used to access the underground. Shaft seals would be installed at strategic locations, such as significant fracture zones (FZ), to limit the potential for upward groundwater flow along the shaft. The objectives of this study were to develop numerical models to simulate shaft seal evolution and likely performance for a range of hypothetical geological media.

As there is at-yet no site or medium selected for a DGR in Canada, this study considers five different cases of hypothetical crystalline and sedimentary host rocks. Although a variety of processes (e.g., thermal or mass transfer) were important, this study focused on the hydraulic-mechanical (HM) processes. The simulations were done using a finite element computer code, COMSOL. Interpretation of the numerical modelling results was completed in order to assess the ability of this code to predict the performance of a shaft seal under a variety of hydraulic conditions imposed by these host rocks. Other work related to this study has been reported in several papers, but they assumed different conditions than used in the current study ([1], [2]). The methods and algorithms to develop HM models of a shaft seal were discussed in [1]. The sensitivity of different configurations of clay-based sealing materials components for a shaft seal located in a hypothetical crystalline host rock was reported in [2].

2. DESCRIPTION OF A SHAFT SEAL CONSIDERED IN THE NUMERICAL MODELLING

2.1 Shaft seal geometry and configuration

The selection of the geometry and configuration of sealing materials used in the shaft seal would ultimately be 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 hypothetical media were assumed and illustrated in Figure 1a.

Five different cases of hypothetical host rocks were considered in the numerical modelling exercises. The host rock in Case 1 was the crystalline rock media, while the host rock in Cases 2 to 5 were the sedimentary rock media. Case 1 was moderately to sparsely fractured crystalline (granitic) rock (MFR) with isotropic hydraulic conductivity (K). Case 2 and Case 3 were shale with isotropic and anisotropic K, respectively. Case 4 and Case 5 were limestone with isotropic and anisotropic K. All five cases assumed similar geometry (Figure 1a) and homogeneous host rock material throughout the domain.

The FZ was located at a 250-m depth and perfectly horizontal in all the simulations. The FZ intersects a shaft that has a 7.3-m diameter. The centre of the shaft seal was located at 250-m depth, the same location as the FZ. The shape of the seal selected for the numerical models was based on experiences gained in previous field studies and demonstrations where shaft and tunnel seals were constructed [3]. As the FZ was 4-m thick, the shaft seal used 6-m thick of bentonite-sand mixture (BSM) component that was constrained between two massive 3-m thick concrete components. The dense backfill (DBF) was installed above and below the concrete components (Figure 1a). Assuming that the repository level was at 500 m so that there was a considerable distance between the centre of the shaft seal and the repository level, an isothermal condition was assumed for the numerical modelling.

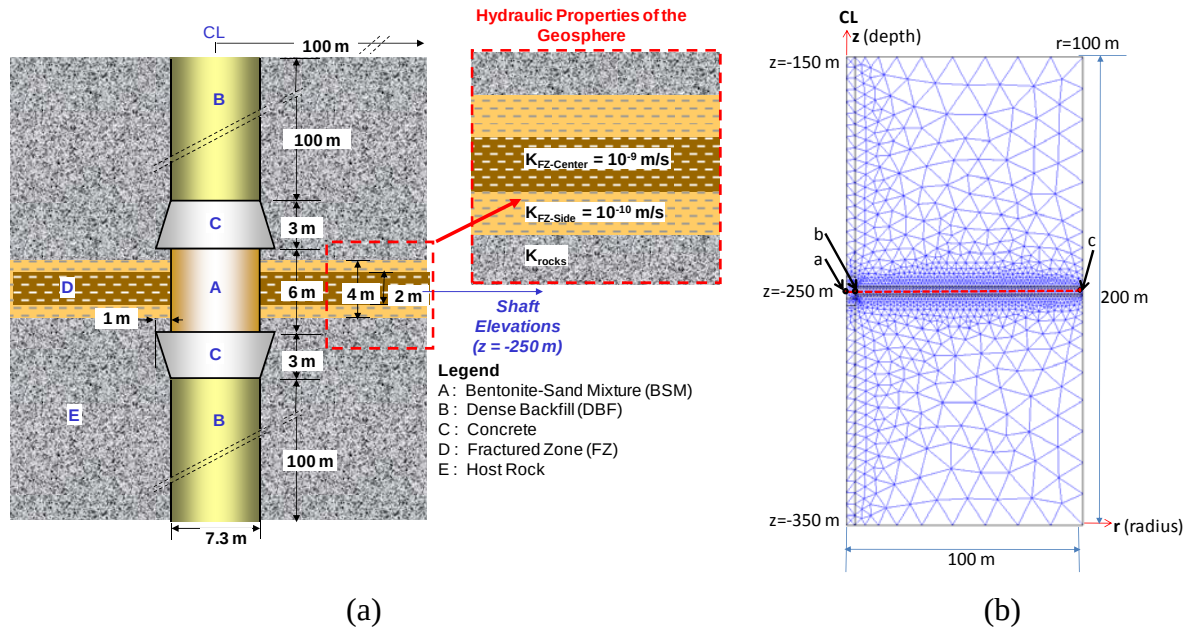


Figure 1. Geometry of the shaft seal considered in numerical modelling exercise.

2.2 Selection of material properties

2.2.1 Intact host rock and fracture zone

Selection of the hydraulic conductivity for the host rock is described below. The horizontal hydraulic conductivity (K_h) of the shale and limestone were deemed to be typical values. The horizontal flow was assumed to be dominant following the direction of FZ. The ratio of hydraulic conductivity in vertical to horizontal (K_v/K_h) of the limestone and shale was estimated based on the laboratory measurements [4]. Table 1 summarizes the remaining HM parameters, which are based on available references (e.g., [4], [5], and [6]).

In all five cases, the fracture zone had an isotropic hydraulic conductivity (K), which was based on the range of hydraulic conductivity measured around the excavation damage zone (EDZ) at the Atomic Energy of Canada Limited (AECL)'s Underground Research Laboratory (URL) [7]. For intact granitic rock having K in the range of 10^{-12} to 10^{-13} m/s, K around the EDZ could increase up to 10^{-9} m/s [7]. For the purpose of this study, the 4-m thick FZ was divided into two different zones: FZ-centre having K of 10^{-9} m/s (2-m thick), and FZ-side having K of 10^{-10} m/s (1-m thick) (see Figure 1). For simplicity, the K was similar for all five cases and the remaining HM properties of the FZ were similar as the intact rock for each case.

Table 1. HM parameters of the geological media.

Case	1	2	3	4	5
Host Rock	MFR	Shale, Isotropic	Shale, Anisotropic	Limestone, Isotropic	Limestone, Anisotropic
Saturated Hydraulic Conductivity, Horizontal, K_h (m/s)	10^{-12} [6]	10^{-11}	10^{-11}	5×10^{-11}	5×10^{-11}
Hydraulic Conductivity, Vertical, K_v (m/s)	$K_v = K_h$	$K_v = K_h$	$K_v = 5.2 \cdot K_h$ [4]	$K_v = K_h$	$K_v = 0.2 \cdot K_h$ [4]
Bulk Density, ρ_{bulk} (Mg/m ³)	2.7 [6]	2.6 [5]	2.6 [5]	2.6 [5]	2.6 [5]
Porosity, n (%)	0.3 [6]	7 [4]	7 [4]	2 [4]	2 [4]
Young's Modulus, E (GPa)	45 [6]	12 [5]	12 [5]	30 [5]	30 [5]
Poisson's Ratio, ν	0.25 [6]	0.3 [5]	0.3 [5]	0.3 [5]	0.3 [5]

2.2.2 Sealing materials

Table 2 shows the HM parameters of the sealing materials used in numerical modelling exercises. The sealing material components include the BSM, DBF, and concrete seal. The BSM was a mixture of bentonite and sand with 40/60 ratio by dry mass proportions, compacted to a dry density (ρ_{dry}) of 1.80 Mg/m³ and gravimetric water content (w) of 12%, corresponding to the degree of saturation (S_w) of 65%. The ability to install the BSM with similar specification had been demonstrated at the AECL's URL shaft seal [3].

The DBF was composed of 70% crushed granite, 25% glacial clay, and 5% bentonite clay (montmorillonite content of ~80%) by dry mass proportion [8]. The DBF was compacted to a ρ_{dry} of 2.1 Mg/m³ and w of 7% corresponding to S_w of 86%.

The concrete components in the shaft seals to be modelled were composed of low-heat high-performance concrete (LHPC), the type used in the Tunnel Sealing Experiments (TSX) [9] and Enhanced Sealing Project (ESP) [3].

3. DEVELOPMENT OF A SHAFT SEAL MODEL USING COMSOL

The HM analyses presented in this study were performed using a finite element computer code, COMSOL version 3.5a with Earth Science and Structural Mechanics Modules. As the shaft sealing components were initially unsaturated, modelling of a shaft seal required coupling of HM formulation under unsaturated conditions. Detail formulations are provided in [1] so they would not be repeated; some of the equations are presented here for completeness of the presentation.

Table 2. Properties and HM parameters of the shaft sealing components.

	Bentonite-Sand Mixture (BSM)	Dense Backfill (DBF)	Concrete
Properties at Installation			
Specific Gravity, G _s	2.7	2.65	
Dry Density, ρ _{dry} (Mg/m ³)	1.80	2.10	
Gravimetric Water Content, w (%)	12	8.5	
Bulk Density, ρ _{bulk} (Mg/m ³)	2.02	2.28	2.35
Degree of Saturation (%)	65	86	5
Total Porosity, n (%)	33	21	0.9
HM Parameters			
Parameter α (1/m)	0.002	0.02	50
Parameter n	1.4	1.4	1.5
Parameter L	0.5	0.5	0.5
Saturated Hydraulic Conductivity, K (m/s)	10 ⁻¹²	10 ⁻¹¹	10 ⁻¹²
Young's Modulus, E (MPa)	100	200	38,000
Poisson's Ratio, ν	0.1	0.1	0.24

3.1 HM formulations for unsaturated media

The unsaturated flow is described using Richard's equation:

$$[C + S_e S] \frac{\partial H_p}{\partial t} + \nabla \cdot [-k \cdot \nabla (H_p + D)] = Q_s \quad (1)$$

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 unsaturated hydraulic conductivity (m/s), Q_s is a fluid source, D is the vertical elevation, and H_p [m] is pressure head. The unsaturated hydraulic conductivity (k) is

$$k = K \cdot k_r \quad (2)$$

K is the hydraulic conductivity at saturated conditions (m/s). For the BSM and DBF, K is dependent on the total porosity (θ). The relationship of K and θ is defined using Kozeny's model:

$$K = k_0 \frac{\theta^3}{(1-\theta)^2} \frac{(1-\theta_0)^2}{\theta_0^3} \quad (3)$$

k_r in Equation 2 is the relative permeability described using the equations below [10]:

$$k_r = \begin{cases} S_e^L \left[1 - (1 - S_e^{1/m})^m \right]^2 & \text{for } H_p < 0 \\ 1 & \text{for } H_p \geq 0 \end{cases} \quad (4)$$

S_e and C are calculated using these equations below:

$$S_e = \begin{cases} \frac{1}{\left[1 + |\alpha H_p|^n\right]^m} & \text{for } H_p < 0 \\ 1 & \text{for } H_p \geq 0 \end{cases} \quad (5)$$

$$C = \begin{cases} \frac{\alpha m}{1-m} (\theta_s - \theta_r) S_e^{\frac{1}{m}} \left(1 - S_e^{\frac{1}{m}}\right)^m & \text{for } H_p < 0 \\ 0 & \text{for } H_p \geq 0 \end{cases} \quad (6)$$

θ_s and θ_r are the saturated and residual volumetric water content. α , n , and L are fitting parameters and $m=1-1/n$. Parameters K , α , n , and L for BSM, DBF and concrete are listed in Table 2.

3.2 Initial and boundary conditions

The finite element computer code (COMSOL) was used to simulate the transient HM responses of the shaft seal up to 1000 years following installation. The model used a two-dimensional axisymmetric geometry with a 100-m radius and 200-m thick (depth (z) of -150 m to -350 m) (Figure 1b).

Two different stages were considered in the shaft seal. Stage 1 simulated the groundwater flow into an open shaft. The simulation time of Stage 1 was equal to the duration of the shaft being in operation. In this study, it was assumed that the shaft remained open for 100 years before a seal was installed.

Stage 2 simulated groundwater flow after the shaft sealing components (BSM, DBF, and concrete) were installed. The results of the Stage 1 in the host rock components were the initial condition for Stage 2. In the sealing components, the initial condition was assigned equal to the properties (i.e., density, water content, suction, stress) at installation. In this study, the simulation time of Stage 2 was 1000 years. For simplicity, the perfect seal between the interfaces of different sealing components was assumed. The saturation period of this numerical model can be expected to be longer than what would be observed in an actual shaft seal since at least some degree of contact variability could be expected to exist.

Mechanical boundary conditions for Stage 1 and Stage 2 were assumed as follows. An axial symmetry boundary condition was assigned at the centre line. Rollers boundary conditions were assigned at the top, bottom, and perimeters. Hydraulic boundary conditions were assumed as follows:

- An axial symmetry boundary condition was assigned at the centre line.
- Constant porewater pressure was assigned at the perimeter.
- No flux boundary conditions were assigned at the top and bottom.

The initial stress conditions in the host rock for Stage 1 was based on the equation provided in [11], which described measured in situ stress measurements in Canada. The horizontal (σ_h) and vertical stresses (σ_v) varied with depth (z) and were defined by equations below.

$$\sigma_h = 0.071 * z - 5.768 \quad (7a)$$

$$\sigma_v = 0.034 * z \quad (7b)$$

In Equations 7 and 8, depth (z) had a unit [m], (-) sign represented downward direction with zero z located at the ground surface; σ_h and σ_v had a unit of [MPa] and (-) sign represented compression. The initial porewater pressure (p_w) varied with z and was calculated using

$$p_w = -\rho_w * g * (z + 80 \text{ m}) \quad (8)$$

where ρ_w was water density ($\sim 1 \text{ Mg/m}^3$) and g was gravimetric acceleration ($\sim 9.81 \text{ m/s}^2$). The initial conditions of Stage 2 were the results of the analyses of Stage 1 at a simulation time of 100 years.

4. RESULTS AND DISCUSSION

The results of the Stage 1 and Stage 2 simulations are discussed below. It should be remembered that the discussion in this paper is limited to the conditions and assumptions defined for this study. In reality the HM responses will deviate from those predicted in this study due to site-specific conditions.

4.1 Stage 1, groundwater flow into open shaft

Figure 2 shows the porewater pressure contour due to groundwater flow into open shaft after 0, 1, 10 and 100 years for the MFR host rock (Case 1). The groundwater flow into an open shaft caused the porewater pressure at the open shaft contact and the region extending into the rock to decrease with time (draw-down). Since the fracture zones had a greater K (10^{-9} to 10^{-10} m/s) compared to the intact rock ($K \sim 10^{-12} \text{ m/s}$), the decrease of the groundwater flow around the FZ was greater than the intact rock.

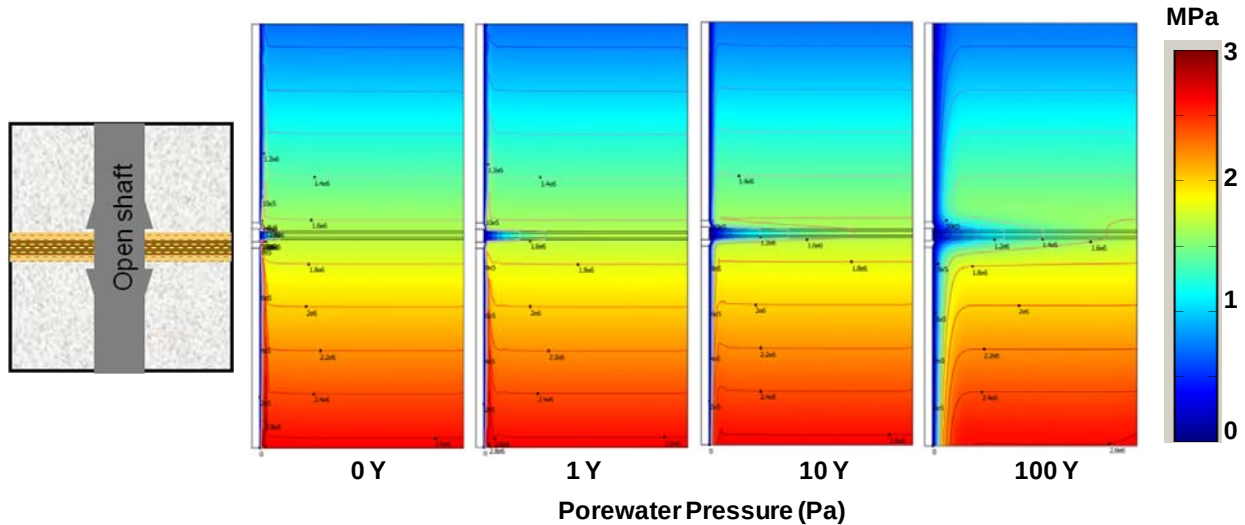


Figure 2. Porewater pressure contour due to groundwater flow into an open shaft (Stage 1, Case 1).

Figure 3 shows the porewater pressure at the centre of the fracture zone ($z = -250 \text{ m}$, line b-c in Figure 1b) at different times in the ranges of 0 to 100 years due to groundwater flow into the open shaft for Case 1. The slope of the porewater pressure, equal to the porewater pressure

gradient, decreased with time (Figure 3). As the flow rate around the fracture zone decreased with time, a longer duration of the shaft remaining open was beneficial for the shaft seal construction and installation.

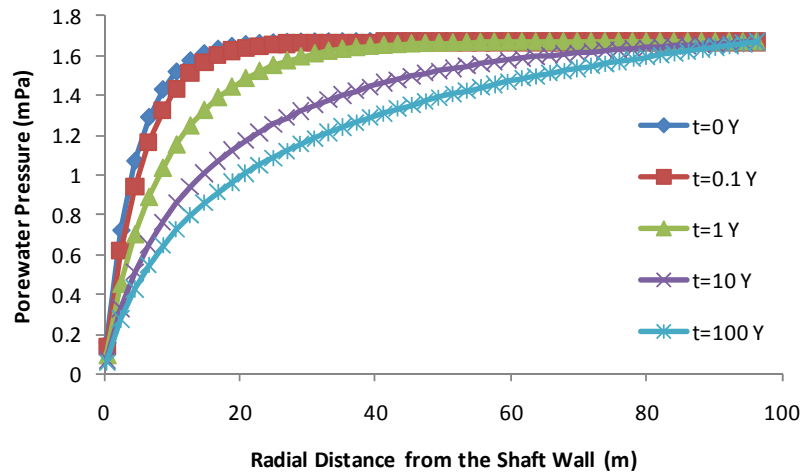


Figure 3. Porewater pressure at the centre of fracture zone (Line b-c in Figure 1b) due to groundwater flow into open shaft at different times (Stage 1, Case 1).

For the cases considered in this study, there was only slight variation on the porewater pressure at the centre of the fracture zone intersecting an open shaft after 100 years (see Figure 4). Compared to the other cases, Case 3 and Case 1 showed the greatest and lowest porewater pressure along the radial distance, respectively. Case 1 was the MFR with isotropic permeability and had the lowest hydraulic conductivity ($K_h=K_v=10^{-12}$ m/s). Case 3 was shale with anisotropic hydraulic conductivity ($K_v=5.2K_h$ and $K_h = 10^{-11}$ m/s).

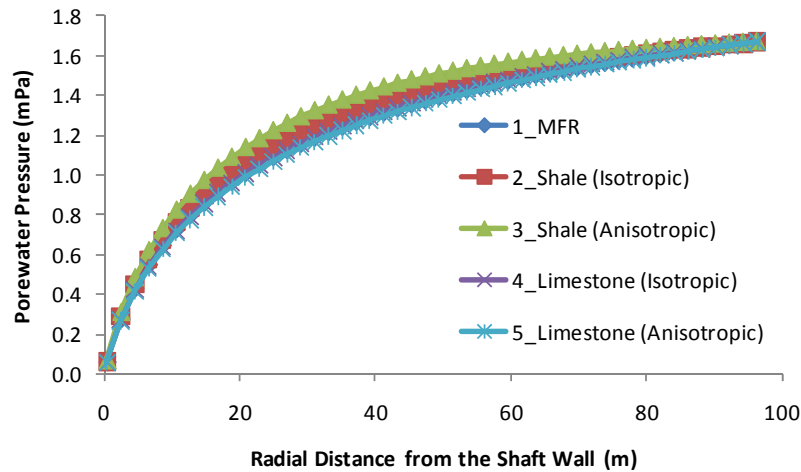


Figure 4. Porewater pressure at the centre of fracture zone (Line b-c in Figure 1b) after 100 years of groundwater flow into open shaft for different cases.

The groundwater flow rates at the FZ wall for different cases were calculated. Figure 5 shows normalized flow rate at stage 1, which is the ratio of the groundwater flow rate into an open shaft at different times compared to the initial flow rate at the centre of fracture zone immediately after completion of shaft construction. There was only slight variation between the different cases. Figure 5 illustrates how a longer duration of open shaft conditions can reduce the groundwater flow rate in the fracture zone where it intersects the shaft. The groundwater flow rate at the fracture zone could be reduced up to approximately 35% to 40% of the initial flow rate if the shaft remained open for 100 years before a seal was installed.

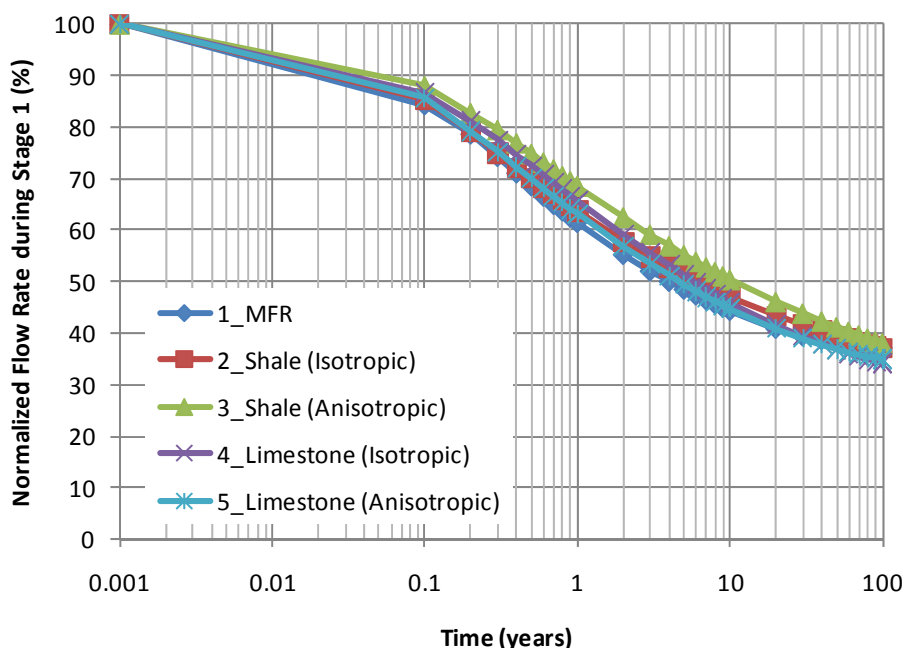


Figure 5. Normalized flow rates during stage 1 (prior to shaft backfilling).

4.2 Stage 2, groundwater flow into shaft sealing component

Stage 2 simulates groundwater flow after the installation of the shaft-sealing components at several times between 0 to 1000 years. The initial condition in the rock was the results of Stage 1 simulation. Figure 6 shows porewater pressure contour due to groundwater flow into shaft sealing components at time 1, 10, 100 and 1000 years for Case 1 (moderately to unfractured granitic rock with isotropic hydraulic conductivity). After 1000 years simulation time (Stage 2), the porewater pressure around the fracture zone that was decreased during Stage 1 tended to recover to the condition prior to the construction of the shaft.

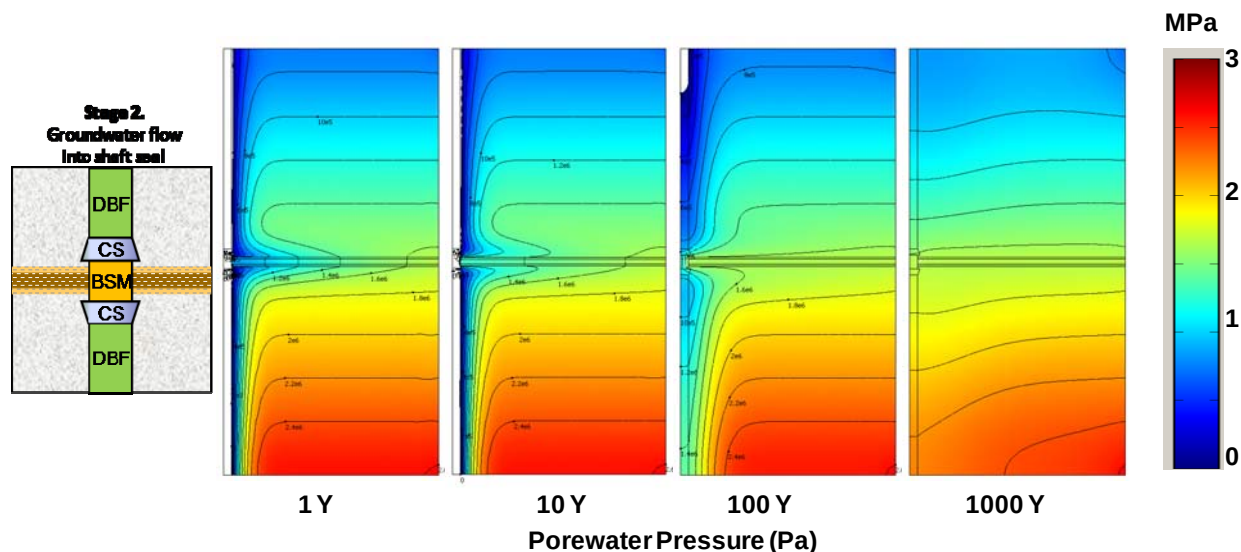


Figure 6. Porewater pressure contour due to groundwater flow into shaft sealing components (Stage 2, Case 1).

Figure 7 shows the degree of saturation at the BSM components for Case 1 at simulation times between 0 to 100 years. In this figure, the white contour indicates that the degree of saturation has reached 100%. As the main source of the groundwater flow was located on the fracture zone, the wetting of the BSM component started from the perimeter and migrated to the centre. In Case 1, the BSM became fully saturated after 100 years.

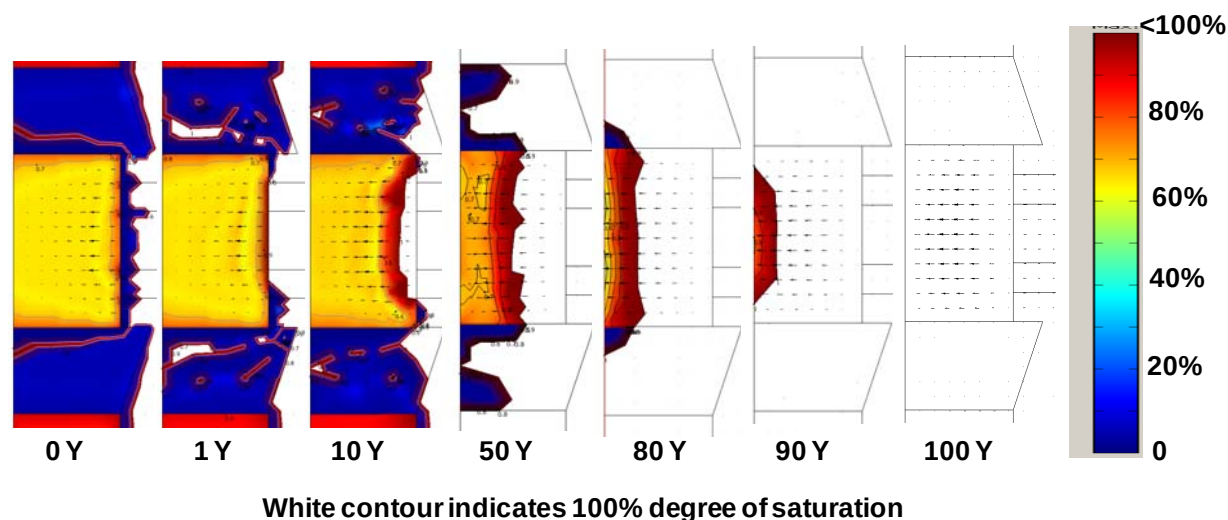


Figure 7. Degree of saturation at the shaft sealing components at different times.

Figure 8 shows the degree of saturation close to the centre of the BSM for 5 different cases. The key output of the simulations was that only slight variation of the degree of saturation was observed for different cases (Figure 8) and the core of the BSM component became fully saturated after approximately 90-100 years. Further study using site-specific data to characterize the fracture zone may result in different HM responses than were observed in this study.

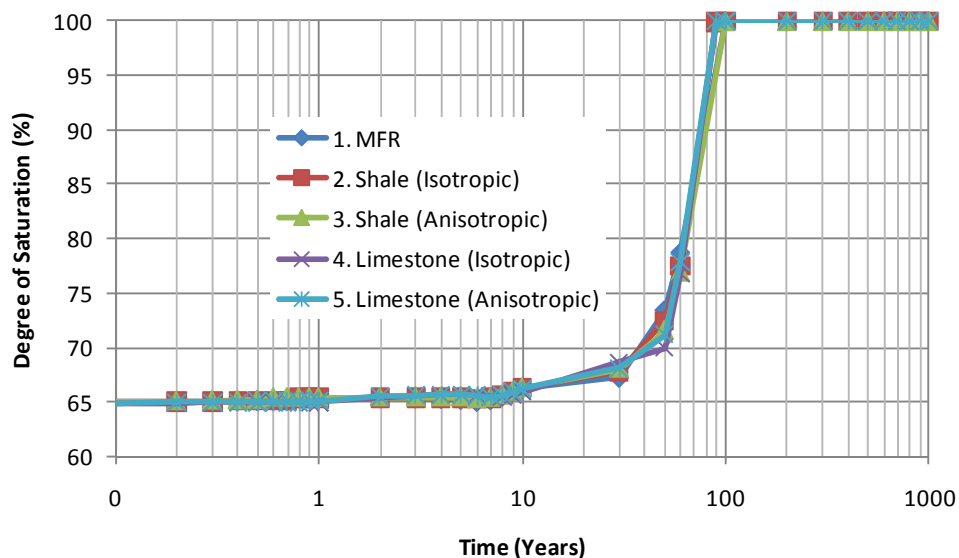


Figure 8. Degree of saturation near the centre of shaft seal.

The inflow rate into the location of the shaft seal before and after installation of the shaft seal components were calculated. Figure 9 shows normalized flow rate at stage 2, which is the ratio of flow rates into shaft seal at different times after seal installation to the flow rate prior to the seal installation at the centre of the fracture zone (i.e., $z = -250$ m, $r = 3.65$ m). As expected, the models were able to simulate that the installation of the shaft seal limits groundwater flow through the shaft. One year after shaft seal installation, groundwater flow decreased up to approximately 20% – 35% of the initial inflow rate prior to shaft seal installation. Comparison between different cases showed that the decrease of flow rate was the greatest in Case 1 (MFR, 80% decrease after 1 year) and the least in Case 3 (shale with anisotropic permeability, 65% decrease after 1 year) (Figure 9).

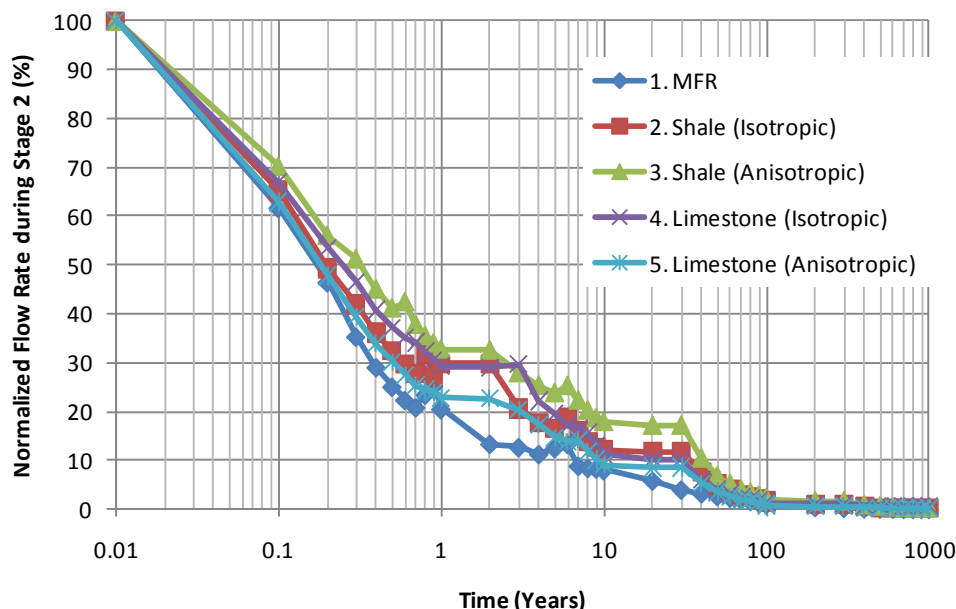


Figure 9. Normalized flow rate in closed shaft (stage 2).

5. SUMMARY AND CONCLUSIONS

This paper presented the results of numerical simulations of hydraulic and mechanical (HM) processes associated with a shaft seal installed in crystalline and sedimentary host rock using a finite element code, COMSOL. Five different cases had been considered in the analyses, including moderately to unfractured granitic crystalline host rock (MFR), shale with isotropic and anisotropic hydraulic conductivity, and limestone with isotropic and anisotropic hydraulic conductivity. The models provided predictions for HM mechanisms at two different stages of the shaft seal evolution. Stage 1 simulated groundwater flow into an open shaft (0 to 100 years). Stage 2 simulated groundwater flow after shaft-seal construction with a duration up to 1000 years simulation time.

As expected, the models were able to simulate that the installation of the shaft seal limits groundwater flow through the shaft. One year after shaft seal installation, groundwater flow decreased up to approximately 20% – 35% of the initial inflow rate prior to shaft seal installation. Based on the conditions and assumptions defined for the host media and fracture features examined in this study, the following conclusions can be drawn from the results of the numerical modelling exercises:

- The longer a shaft remains open, the better are the hydraulic conditions with respect to limiting short-term water movement towards the location of a shaft seal via the fracture feature. The groundwater inflow rate at the fracture zone intersection can be reduced by approximately 35% to 40% of initial flow rate if the shaft remains open for 100 years before a seal is installed.
- The core of the shaft seal (i.e., the bentonite-sand mixture (BSM)) becomes fully saturated after 90-100 years. Delaying saturation time indicates slower movement of the groundwater or other substances that may be transported with the groundwater.

- Only slight differences between five cases were observed from the results of the numerical modelling exercises for the 5 different cases examined in this study. Defining more site specific conditions (e.g., depth and geometry of fracture, hydraulic properties of rock and fracture feature, and mechanical characteristics of rock) is recommended in order to more effectively simulate HM behaviour of a shaft seal at the location of a fracture zone. This may result in a greater degree of divergence in the HM evolution predicted for a shaft seal.

ACKNOWLEDGEMENTS

Technical reviews provided by D.A. Dixon and R. Guo are greatly appreciated.

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