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Simulation of the hydro-mechanical behaviour of bentonite seals for the containment of radioactive wastes

For submission to Canadian Geotechnical Journal

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Abstract

Geological disposal of radioactive wastes relies on a multiple barrier system to provide long-term containment and isolation of the wastes. The excavation of the repository creates openings and disturbed zones in the host rock formations that need to be properly sealed. Bentonite-based materials are being considered worldwide as a preferred type of sealing material, since they possess desirable characteristics such as low permeability, high sorption capability and swelling potential allowing them to close internal cracks and gaps at interfaces with other materials. The French Institute for Radiation Protection and Nuclear Safety (IRSN) has led an experimental program consisting of a series of laboratory and large in-situ experiments in order to assess the hydro-mechanical behaviour of bentonite seals. The experiments consisted of the forced re-saturation of pre-fabricated blocks of bentonite-sand mixture, with technological voids between bentonite seals and the walls of the steel cell (in the laboratory tests) and the host rock (in the in-situ experiment). Relative humidity and total stress were monitored during both tests. The Canadian Nuclear Safety Commission (CNSC) collaborated with Geofirma Engineering, IRSN and Commissariat à l’énergie atomique (CEA) to develop a mathematical model to simulate the above experiments. The model was developed within the framework of poromechanics, with the inclusion of partial saturation characteristics and swelling potential in order to simulate the behaviour of the bentonite-based material. The model results were in good agreement with the experimental measurements for relative humidity and swelling stresses. The model also predicted the closure of technological voids and gaps due to swelling. Although swelling into the technological voids leads to an increase in permeability, that permeability remains low and insignificant from a safety perspective.

Keywords: Radioactive Waste Disposal, Bentonite, Swelling, Permeability Change

INTRODUCTION

Many countries are considering deep geological disposal as a preferred option for the long-term management of radioactive waste (e.g., Bell 2011; Garisto et al. 2009). A deep geological repository (DGR) relies on a multiple barrier system that includes the host rock and the engineered barriers in order to provide long-term containment and isolation of the wastes (IAEA, 2011). The construction of the DGR requires the excavation of shafts, access tunnels and waste emplacement rooms in the host rock and overlying formations. The excavation process might create preferential flow paths through the excavated openings and through disturbed zones in the rock formations around the openings. Those potential pathways need to be properly sealed and/or considered in the design process to
ensure the long-term safety of the system. Bentonite-based materials are considered (e.g., Alonso et al. 2010) as the preferred type of sealing materials since they possess desirable characteristics such as low permeability, high sorption capability and swelling potential allowing closure of internal cracks and gaps at interfaces with other materials. Therefore, during the last few decades many experimental studies, including laboratory and field tests, have been performed to better understand the hydromechanical properties of bentonite-based seals (Alonso et al. 2005; García-Siñeriz et al. 2015; Popp 2009; Villar et al. 2014; among others) and how they influence the long-term evolution of the seals. The IRSN (Barnichon and Deleruyelle, 2009; Barnichon et al. 2011) is conducting a series of laboratory and large in-situ experiments called SEALEX in order to identify conditions (technical specifications, defects, etc.) that influence the long-term behaviour of bentonite-based seals. The material used in the IRSN’s experimental program is a bentonite-sand mixture, with a weight ratio of 70-30. In this work, the authors focused on experiments where technological voids exist both within the sealing system and between the sealing system and its surrounding enclosure. The experiment considered here is a large in-situ test, called PT-A1, performed at the IRSN’s Underground Research Laboratory (URL) at Tournemire (Aveyron, France). Prior to the in-situ experiment, a small-scale mock-up experiment was performed at the Ecole des Ponts (Paris, France). In both lab- and field-scale experiments, technological voids were introduced between the bentonite-based seals and at their interface with the surrounding medium. In both experiments, forced resaturation of the seals was induced, and relative humidity and total stress were continuously monitored. Many models have been developed to simulate the coupled hydromechanical (HM) processes that occur during resaturation. These models include the swelling process from different perspectives such as physicochemical, multiscale (micro to macro) and semi-analytical analysis (Alonso et al. 2010, 2005; Gens and Alonso 1992; Hoffmann et al. 2007; Xie et al. 2004; among others). Following the approach of previous researchers, the authors developed a model within the framework of poromechanics, including partial saturation characteristics and swelling potential in the seals, in order to simulate the coupled HM processes that prevail in those experiments. The technological voids present special challenges to the numerical solution of the model. The authors used special interface HM models to simulate the voids. The model’s input parameters were determined from characterization tests performed at the Ecole des Ponts ParisTech (Paris, France).

**SUMMARY OF THE EXPERIMENTAL PROGRAM**

A brief description of the experimental program is given here. Each individual experiment will be described in detail in later sections, along with the comparison of the experimental data and modelling results. The main components of the experimental program are:

i) Characterization tests to determine the basic HM properties of the bentonite-sand. These include: water retention tests under constant volume and free swelling conditions; swelling tests under suction controlled conditions; and oedometric compression tests under suction controlled conditions.

ii) An infiltration test in which water was injected at one end of the sample. The relative humidity was continuously monitored at four locations along the length of the sample.

iii) The mock-up test in which water was infiltrated from two ends into a relatively dry bentonite-sand sample. The sample was emplaced in a rigid cylinder with a pre-existing void between the sample and the rigid cylinder. The axial pressure and displacement were measured during the test. The mock-up test is a small-scale, simplified version of the PT-A1 test described next.
iv) The PT-A1 test performed at the URL in Tournemire, was a large scale field test to investigate the infiltration of water into highly compacted bentonite-sand blocks installed inside a 60 cm diameter horizontal borehole excavated in the host shale formation. Technological voids between the blocks, and between the blocks and the host rock were initially present. As water infiltrated from both ends of the seal, the axial stress, radial stress, and relative humidity were measured at various locations within the bentonite-sand system. More details about the tests are presented in Numerical Solution section.

The bentonite used in this work is MX80 Na–bentonite from Wyoming, USA, and the sand is pure quartz from the regions of Eure and Loire, France. Table 1 summarizes the main characteristics of the bentonite and the sand (Wang et al. 2013a and 2013b). The mixture was prepared in a dry weight proportion of 70/30 (bentonite/sand) at a water content of 11%. More information about the characteristics of the bentonite-sand mixture can be found in Wang et al. (2013a and 2013b).

MODELLING APPROACH AND GOVERNING EQUATIONS

The SEALEX in-situ experiments aim to simulate the behaviour of bentonite seals during their resaturation in repository conditions. Depending on the initial properties of the seal material, and the emplacement conditions, the resaturation process will have a different influence on the seals long-term properties. The supply source in repository conditions comes from the host rock formation. Consequently the rate and mechanisms of saturation also depends on the properties of the rock mass and its pore water. The resaturation process might take hundreds to thousands of years due to the low permeability of the host rock. Therefore, in the SEALEX tests, water is artificially injected into the seal material. Since the bentonite seal material is initially unsaturated, an air phase is present in its pores. The water must displace the air in order to resaturate the bentonite seal. A schematic pore-scale representation of the bentonite seal adopted from Ichikawa et al. (2004) is reproduced and shown in Figure 1. The macro-grains would represent the sand particles. The clay aggregates constitute the main components of the bentonite, and consist of stacks of clay layers. Water is sorbed into those aggregates by the strong physico-electro-chemical forces that exist in them.

The water that infiltrates through the pores moves simultaneously with the air, and some would be trapped into the aggregates. The latter mechanism is responsible for the swelling observed in bentonite-based materials. During resaturation, the pressure of both water and air will change and, in addition to the swelling process, this will lead to a change in the forces of interaction between the clay and sand particles. Therefore, the hydraulic and mechanical processes are fully coupled, and this coupling was integrated into the mathematical model developed by the authors as follows.

In order to simulate the coupled HM processes in the SEALEX experiment, we consider the general theoretical framework of two-phase flow in deformable porous media (e.g., Nguyen and Le, 2015). The system of governing partial differential equations was derived based on the considerations of quasi-static equilibrium of the solid skeleton, and mass conservation for the pore water and air. In this work, it is assumed that only the water pressure changes, and the air pressure remains constant and equal to atmospheric pressure. The governing equations from Nguyen and Le (2015) then reduce to:
\[
\rho \left( \frac{C_m}{\rho g} + S e S \right) \frac{\partial \tilde{p}}{\partial t} + \nabla \cdot \rho \left( -\frac{k_s}{\mu} k_r (\nabla p + \rho g \nabla D) \right) = Q_m
\]

(1)

\[
\nabla \cdot (\sigma^' + B \tilde{p} I) = 0
\]

(2)

With:

\[
Q_m = B \times \rho \times S \times \frac{\partial \epsilon_v}{\partial t}
\]

\[
\tilde{p} = \text{Max}(0, p_r), \ p_r \text{ is the pore water pressure (negative in unsaturated conditions)};
\]

\[
I \quad \text{identity matrix};
\]

\[
\sigma^' \quad \text{effective stress tensor};
\]

\[
C_m \quad \text{specific storage capacity (m}^{-1}\text{)};
\]

\[
S_e \quad \text{effective saturation (-)};
\]

\[
S \quad \text{storage coefficient (m}^{-1}\text{)};
\]

\[
\rho \quad \text{fluid density (water) (kg/m}^3\text{)};
\]

\[
k_r \quad \text{water relative permeability coefficient (-)};
\]

\[
\kappa_s \quad \text{intrinsic permeability (m}^2\text{)};
\]

\[
g \quad \text{gravitational acceleration (m/s}^2\text{)};
\]

\[
D \quad \text{elevation direction (m)};
\]

\[
\mu \quad \text{fluid dynamic viscosity (Pa.s)};
\]

\[
\epsilon_v \quad \text{volumetric deformation (-)};
\]

\[
Q \quad \text{fluid mass source (kg.m}^{-3}\cdot\text{s}^{-1}\text{)};
\]

\[
B \quad \text{biot poroelastic constant (-)}; \text{ and}
\]

\[
t \quad \text{time (s)}.
\]

The stress strain relationship can be written in matrix notation as:
\[ \{d\sigma'\} = [D_e]\{d\varepsilon - d\varepsilon_{vs} - d\varepsilon_p\} \quad (3) \]

With:

- \(d\sigma'\) is the effective stress increment;
- \(d\varepsilon\) is the strain increment (\(vs\) and \(p\) denote swelling and plastic strain, respectively); and
- \(D_e\) is the elastic stiffness matrix.

The swelling process is represented by the following equation which relates the change in suction \((ds)\) to swelling induced volume change \(d\varepsilon_{ps}\) as follows:

\[ d\varepsilon_{vs} = -B_s ds \quad (4) \]

Where the parameter is:

\[ B_s \quad \text{swelling coefficient (Pa}^{-1}). \]

\(B_s\) is in general a function of suction and void ratio, and can be derived by a state surface equation (Lloret and Alonso, 1995). In this work we assumed a constant value for simplicity. The sign convention for Equations 2-4 considered force and displacement components to be positive if directed in the positive direction of the coordinate axes (tensile stresses are positive and compressive stresses are negative) with hydrostatic pressure and suction pressure with positive sign.

In addition to the swelling strain, the elastic and plastic strain components must be defined. In this work, we used both a simplified approach with a linear elastic model, and an elastoplastic model approach based on the Barcelona Basic Model (BBM). The BBM model is a modified Cam-Clay model which includes volume change and variation in module parameters as a function of changes in suction and volumetric deformation (usually using the void ratio as a measuring parameter). The BBM was developed by Alonso et al. (1990) and later modified by Alonso et al. (2011). The BBM has been successfully used by many researchers in the simulation of coupled thermal, hydraulic and mechanical processes in unsaturated bentonite-based materials. This work is mainly based on the Alonso et al. (2011) model.

The equation of the yield surface in the BBM is:

\[ q^2 - M^2 (p + p_s) (pc - p) = 0 \quad (5) \]

\[ \kappa(s) = \kappa_{po} (1 + \alpha_s \cdot s) \quad (6) \]

\[ p_{co} = pc \left( \frac{p*}{pc} \right)^{\frac{\lambda(0) - \kappa(s)}{\lambda(s) - \kappa(s)}} \quad (7) \]
\[ P_{Co} = P_o^* (1 + \alpha_p \cdot s) \]  
(8)

\[ P_c = P_c^0 \times \text{Exp} \left( \frac{- (1 + e_o) \cdot \eta_{vp}}{(\lambda - \kappa(s))} \right) \]  
(9)

\[ -p_s = -k \cdot s \]  
(10)

Where parameters are:

- \( q \): deviatoric stress \((=\sigma_2-\sigma_3)\) where \( \sigma_1, \sigma_3 \) are respectively major and minor principle stresses;
- \( p \): net mean stress \(=(\sigma_1+\sigma_2+\sigma_3)/3\); where \( \sigma_2 \) is the intermediate stress.
- \( P_{Co} \): initial preconsolidation stress;
- \( P_c \): preconsolidation stress;
- \( P_o^* \): initial preconsolidation stress for saturated conditions;
- \( e_0 \): initial void ratio;
- \( \eta_{vp} \): plastic volumetric strain;
- \( M \): slope of critical state line;
- \( P_s \): increase in cohesion with suction;
- \( p_c \): reference pressure (Pa);
- \( k \): parameter describing the increase in cohesion with suction;
- \( \kappa(s) \): slope of the unloading curve (Pa\(^{-1}\)) as a function of suction;
- \( \lambda(s) \): slope of the compression curve (Pa\(^{-1}\)) as a function of suction;
- \( \lambda(0) \): slope of the compression curve (Pa\(^{-1}\)) for saturated conditions;
- \( \kappa_{po} \): slope of the unloading curve (Pa\(^{-1}\)) for saturated conditions;
- \( \alpha \): parameter describing the change in \( \kappa(s) \) with suction \( s \); and
- \( \alpha_{po} \): parameter describing the change in \( P_o \) with suction \( s \).

In this work, the parameters of the model, in particular, \( \lambda(s) \), \( \kappa(s) \), and \( P_c \) were calibrated from three oedometric tests performed under three different values of suction.
The retention characteristics of the buffer-based material were considered using the van Genuchten model (van Genuchten, 1980). The set of equations of the van Genuchten model used in this work is as follows:

\[
\theta = \begin{cases} 
\theta_s + S_e(\theta_s - \theta_r) & Hp < 0 \\
\theta_s & Hp \geq 0 
\end{cases}
\]  

(11)

\[
S_e = \begin{cases} 
1 & Hp < 0 \\
\left[\frac{1}{1 + \alpha EMDD H_p}\right]^m & Hp \geq 0 
\end{cases}
\]  

(12)

\[
C_m = \begin{cases} 
\frac{\alpha m}{1 - m}(\theta_s - \theta_r)S_e \left(\frac{1}{1 - S_e^m}\right)^m & Hp < 0 \\
0 & Hp \geq 0 
\end{cases}
\]  

(13)

\[
k_r = \begin{cases} 
S_e^l & Hp < 0 \\
1 & Hp \geq 0 
\end{cases}
\]  

(14)

Where the parameters are:

- \( \theta \) liquid volume fraction (-);
- \( \theta_s \) saturated liquid volume fraction (-);
- \( \theta_r \) residual liquid volume fraction (-);
- \( H_p \) pressure head (m); and
- \( \alpha \) \((m^{-1})\), \( l \) (-), \( N \) (-) and \( m \) (-) are parameters of the van Genuchten model. \(1/\alpha\) is the apparent air entry pressure (m).

Equations 11-13 are from the original van Genuchten model. However, equation 14 for the relative permeability \( k_r \) is based upon the relative permeability expression from Brooks and Corey (1964). This expression for relative permeability was found to better fit the experimental data.

The original van Genuchten model is applicable for saturation-desaturation processes under constant volume conditions (Baumgartner, 2006). In the mock-up and PT-A1 tests, large technological voids exist in the initial state, therefore resaturation induced important volume change (and change in dry density) during those tests. Baumgartner suggested that the original van Genuchten model could be adapted to variable volume conditions by setting the parameters of the model, in particular the apparent air entry pressure parameter \( \alpha \), as a function of the effective montmorillonite dry density (EMDD), as follows:
\[ EMDD = \frac{f_m f_c \rho_d}{1 - \left( \frac{f_c}{G_a \rho_w} \right) - \left( \frac{1 - f_m}{G_n \rho_w} \right)} \]  

(15)

\[ \alpha = \left( 0.0705 \times EMDD^2 - 0.3065 \times EMDD + 0.313 \right) \times F_{Corr} \]  

(16)

Where:

- **EMDD** effective montmorillonite dry density (Mg/m³);
- **f_m** mass fraction of montmorillonite in clay fraction f_c (-);
- **f_c** mass fraction of clay in dry solid (-);
- **\rho_d** dry bulk density (Mg/m³);
- **\rho_w** water density (Mg/m³);
- **G_a** relative density of aggregate component (specific gravity) (-);
- **G_n** relative density of non-montmorillonite clay component (2.65, range from 2.64-2.7) (-);
- and
- **F_{Corr}** calibration parameter (50) (-).

In order to consider the effect of swelling on the intrinsic permeability (\( \kappa \)), the Kozeny-Carman equation was used (Carman 1941; Kozeny 1927). This equation links these two processes through the change in porosity caused by swelling:

\[ \kappa = \kappa_0 \left( \frac{n^3}{1 - n} \right) \times \frac{1 - n_0}{n_0^3} \]  

(17)

Where the parameters are:

- **\kappa_0** intrinsic permeability (m²) at the reference porosity \( n_0 \); and
- \( n_0, n \) initial and current porosity (-). The current porosity evolves as a function of volumetric strain.

**NUMERICAL SOLUTION**

The mathematical model described in the previous section was implemented in a general-purpose equation solver, COMSOL Multiphysics (COMSOL, 2012). The COMSOL software solves coupled partial differential equations, with their boundary and initial conditions, using the finite element method. It allows the user to define all auxiliary equations related to the adopted constitutive relationships and their parameters.

**Calibration of Material Properties and Model Parameters from characterization tests**

Many of the HM parameters of the model were calibrated from characterization tests (Wang et al. 2013a, 2013b), which were water retention tests under constant volume and free swelling conditions,
swelling tests under suction controlled conditions, and oedometric compression tests under suction controlled conditions.

**Water retention characteristics**

Two types of tests were performed (Wang et al. 2013a) to characterize the water retention of the investigated bentonite-sand mixture. Tests of the first type were performed under constant volume conditions, and therefore the initial dry density also remained constant. In the second type, the sample was allowed to swell freely, and therefore the dry density changed during the test. Figure 2 shows the calibration and prediction of the EMDD dependent water retention curve (WRC) using equation 16 for three different constant dry densities (1.2, 1.67, and 1.97 Mg/m$^3$ corresponding to EMDD of 0.8, 1.26, and 1.6 Mg/m$^3$) and for the free swelling test. The model predictions for the constant dry density and free swelling are in good agreement with measurements as shown in Figure 2. It is worth mentioning that the infiltration test was performed at a constant volume with 1.67 Mg/m$^3$ dry density. On the other hand, in the mock-up and PT-A1 tests, the initial dry density was 1.97 Mg/m$^3$ (corresponding to an EMDD of 1.6 Mg/m$^3$). Due to swelling to fill the technological voids, that density decreased to a final average density of 1.65 Mg/m$^3$ (corresponding to an EMDD of 1.26 Mg/m$^3$). The water retention model we used takes into account this variation of EMDD during the course of the mock-up and PT-A1 experiments. Each line in Figure 2 represents the water retention curve at a specific EMDD (0.8 to 1.6) Mg/m$^3$.

**Swelling characteristics**

Swelling tests under suction control conditions were used to characterize the swelling characteristics of the bentonite-sand mixture. In these tests, suction was imposed on a sample, and the volumetric deformation for each suction level was determined. The first series of tests were performed in an oedometer, with a constant axial load of 0.1 MPa (triangle symbols in Figure 3), while the second series of tests was performed on free swelling samples (square symbols in Figure 3). These results are used to calibrate the swelling coefficient $B_s$ in Equation 4 with an estimated $B_s$ value of 2E-9 Pa$^{-1}$.

**Oedometric compression**

Figure 4 shows the calibration of Equations 5 to 10 to the experimental data of compression tests at different suctions (from Wang et al. 2013a).

Table 2 shows the calibrated BBM parameters for the investigated bentonite-sand mixture for a range of suction values (0 to 38 MPa).

Numerical simulation for the infiltration, mock-up and PT-A1 tests, as presented next, was performed using the input parameters in Table 2 to estimate the parameters shown in Table 3 by fitting the results to the experimental data. As previously described, these parameters were estimated from the calibration of the characterization tests. However, some of the parameters needed to be adjusted to take into account differences between the infiltration, mock-up and PT-A1 tests due to the following factors: i) simplified assumptions in boundary conditions (for example gap simulation), ii) uncertainties in the actual initial conditions, and iii) differences in sample sizes and sample preparation methods.
**Infiltration Test**

The infiltration test is a simple hydration test to study resaturation processes of the seals. A pre-compactsed bentonite-sand specimen (70/30 bentonite/sand), 50 mm in diameter and 250 mm in height, was used in the test (Wang et al. 2013b). The initial dry density was 1.67 Mg/m$^3$ and initial gravimetric water content was 11%, corresponding to a water saturation of 47%, and a suction of 65 MPa according to the water retention model previously described. During the test, water was allowed to infiltrate from the bottom of the sample, while the top of the sample was kept open to the atmosphere. Throughout the test, the sample was confined in a rigid cell. The reduction in suction as water infiltrated upwards was measured indirectly using a set of relative humidity sensors (RH1 to RH4 inserted into the sample as shown in Figure 5).

Since the sample was radially and axially confined, its total volume remained constant during the test. However, local density variations are possible, resulting in a heterogeneous distribution of volume and permeability during water infiltration. Therefore, the infiltration test was simulated using the fully coupled HM model previously described. The finite element model is shown in Figure 6. The simulated geometry is only one-eighth of a cylinder, assuming radial symmetry around the axis of the cylinder. This domain was discretized into 250 prismatic elements. Initial suction was set at 65 MPa. The boundary conditions for the governing equations were based on the corresponding laboratory conditions. Those boundary conditions are shown in Figure 6.

Figure 7 shows the modelled versus measured (Wang et al. 2013b) values of suction at the four observation points (corresponding to the locations of relative humidity sensors RH01 to RH04). The results show that the modelled suction at the middle sensors (RH02 and RH03) was overestimated at early times and underestimated at later times. At the two outer observation points, RH01 and RH04, the model performed much better, predicting the observed evolution of suction with much greater accuracy. This behaviour may be attributable to the assumption of Kozeny-Carman estimation of intrinsic permeability using Equation 17. Estimation of the intrinsic permeability could be better represented by a non-linear function considering other factors such as changes in pore size distribution resulted from swelling, which would also improve the ability of the model to reproduce experimental observations.

**Mock-up Test**

The mock-up test (see Wang et al. 2013c) is a small-scale (1/10) laboratory version of the in-situ SEALEX PT-A1 experiment. The mock-up test was performed on a pre-compactsed bentonite-sand specimen with an initial dry density of 1.97 Mg/m$^3$. The specimen, with dimensions of 55.5 mm in diameter and 120 mm in height, was placed in a rigid hydration cell with a 60 mm inner diameter. The larger diameter of the hydration cell simulated the initial technological void present in the full-scale SEALEX in-situ test. The testing apparatus is shown in Figure 8.

The 1/10 scale generic mock-up test included three phases as described below and illustrated in Figure 9:
Phase 1, Initial saturation: Water was injected into the hydration cell from the bottom and the vertical deformation was restrained to maintain constant volume.

Phase 2, Recovery of the vertical void: The confinement (vertical load) was removed, allowing the sample to swell freely until the axial deformation reached 20% of the sample height (approximately 25 mm). Phase 2 simulates a possible failure in the repository confinement system which could lead to limited free swelling conditions (20%). Phase 2 was subdivided to two parts, Phase 2a, with a free swelling up to 2.8% and Phase 2b with a free swelling up to 20% and water being injected from both the bottom and from the top of the sample.

Phase 3, Confinement: Vertical deformation of the sample was once again restrained, as in Phase 1. The vertical piston load required to restrain further sample deformation represents residual swelling pressure after 20% swelling. Phase 3 assessed the possible residual swelling pressure that could develop when confinement is re-established after a period of free swelling.

The sample was induced to swell by injecting water from the bottom during initial saturation and initial free swelling (Phase 1 and Phase 2a) and from the top and bottom during additional free swelling and reconfinement (Phase 2b and Phase 3). A 60 mm mechanical piston equipped with a load cell was used to restrain the vertical displacement and measure the swelling pressure. A linear variable differential transformer (LVDT) was installed to measure the swelling strain when needed, as shown in Figure 8.

The geometry of the experiment was represented in a 3D quarter cylinder model discretized into 1260 elements, as shown in Figure 10. Although the mock-up test could be modelled as an axisymmetric problem, a 3-D finite element discretization was chosen in order to better prepare for the subsequent PT-A1 field test which is a true 3-D problem. Initial conditions and properties of the bentonite-sand mixture were as follows:

- Initial dry density is 1.97 Mg/m$^3$
- Initial gravimetric water content is 11%
- Grain specific gravity of bentonite/sand (70/30) is 2.734
- Initial water saturation is calculated to be 73%
- Initial water suction pressure is calculated using van Genuchten equation as 56 MPa
- Initial intrinsic permeability is 1E-21 m$^2$ (calibrated value)

The boundary conditions for the water flow equation (as shown in Figure 10), were set based on the corresponding experimental conditions. The initial volume of injected water was sufficient to fill the technological void surrounding the sample (Wang et al. 2013c). This means that initially, a constant pressure, fully water saturated boundary condition was appropriate for the sides of the sample. The side boundary conditions were changed to no-flow boundaries as the sample swelled and made contact with the wall of the hydration cell. The base of the sample, which was in contact with a saturated porous stone, was assumed to be a zero pressure, fully water saturated boundary. The top of the sample, in contact with the piston, was set as a no flow boundary for Phase 1 and Phase 2a, and switched to a zero pressure, fully water saturated boundary in Phase 2b and Phase 3 as the
water was allowed to flow into the sample from the top during these phases. For the mechanical process, the sides and top mechanical boundaries were represented as elastic interfaces (supported by springs), while at the bottom, zero normal displacement was assumed (roller interface). The springs’ stiffness (k2 shown in Figure 10) at the top (in contact with the piston) was set as a variable as a function of time k2(time) using user defined function in COMSOL to simulate the movement of the piston during the test (high stiffness when no movement is allowed, low stiffness when movement is allowed). The top boundary is assumed to be completely free without the weight of the piston. For the side boundaries, springs with variable stiffness were also used in order to represent the technological void. The stiffness was initially very low (0 MPa) and increased to 4 GPa when the maximum displacement of 0.25 mm (thickness of the technological void) was reached. This change in properties of the spring was meant to simulate the initial free swelling of the sample as it expanded into the technological void, followed by the restraint of the sample as swelling brought it into contact with the wall of the hydration cell.

Phase 1 included the initial saturation of the sample and the measurement of swelling pressure. The piston force was simulated by assuming a vertical spring with a high spring constant = $1 \times 10^20$ N/mm$^2$. During Phase 2a, and Phase 2b of the experiment from 350 to 400 days, free swelling was allowed until the sample reached a vertical displacement of about 20% of the height of the sample (0.2x120=24 mm). This phase was simulated by reducing the spring constant smoothly to zero over a short time period. In Phase 3 (from 400 to 520 days) the conditions were once again set to constrained swelling conditions by increasing the spring constant to a higher value gradually in a short time period.

For this case, two mechanical models were used and the results for swelling pressure (piston pressure) during Phase 1, Phase 2a, Phase 2b and Phase 3 are presented in Figure 11. Using the linear elastic model, the results of Phase 1 showed good agreement in terms of swelling pressure development. The maximum swelling pressure of 1.75 MPa after 350 days was also in good agreement with the maximum swelling pressure from the experimental data. The stepped reduction in swelling pressure after 350 days is a numerical artifact. The unloading at 350 days was applied in two steps to avoid numerical problems. At early times, laboratory results showed an increase in the swelling pressure followed by a drop. The linear elastic model did not reproduce this observed drop in swelling pressure. This decrease in measured swelling pressure may be attributable to the collapse of the sample prior to swelling. This hypothesis was tested and validated using the BBM (red line results) which showed a very good agreement in both pressure response and maximum swelling pressure. The results of Phase 2 (350 to 400 days) showed zero swelling pressure as expected under free swelling for elastic model and BBM model. In Phase 3 (from 400 to 520 days) the BBM model also provided a better prediction of the swelling pressure. However, both models showed steeper increases in swelling pressure as compared to the measured data. This may be attributed to the approach we used to simulate the injection of water at Phase 2b (the variation in top hydraulic boundary condition).

The BBM yield surface, given by Equations 5 to 10, can be plotted in q-p-s space (Figure 12) or in the p-q space (Figure 13) for different values of suction.
The model results using the BBM showed an increase in swelling pressure to approximately 1.5 MPa, followed by a drop to approximately 0.6 MPa around 35 days, and then a gradual increase to a maximum of 1.8-1.9 MPa as shown in Figure 11.

The drop in swelling pressure can be attributed to the collapse phenomenon resulting from the saturation process that led to shrinking of the yield surface (Figure 14). This is illustrated by following the stress paths for a number of points along the radius of the sample at its top boundary, as shown in Figure 14. The sample started swelling first at its side boundary, with an increase in p and q under the initial high suction, however the stress state was still within the yield surface. Subsequently, the increase in saturation resulted in a reduction in suction (increase in saturation), which induced a shrinkage of the yield surface leading to the collapse.

**PT-A1 test**

The PT-A1 test was performed at the Tournemire URL, France, within a borehole also named PT-A1. Borehole PT-A1 was filled with eight pre-compacted bentonite-sand discs, each of which was 56 cm in diameter and 15 cm thick (total seal length was 120 cm as shown in Figure 15). The initial dry density of the bentonite block without considering the gap was 1.94 Mg/m$^3$ and the reported initial saturation was 73%. The overall average density after the gaps are filled would be 1.65 Mg/m$^3$. At the time of installation (June and July 2013), there was a significant and non-uniform gap with a maximum distance of 4 cm separating the bentonite-sand discs and the borehole wall (see Figure 15 D). During the test, water was allowed to infiltrate from both sides of the borehole to fill the initial gap between the discs and the surrounding rock. In addition to this gap, there were additional voids within the testing borehole, including a gap between the downstream lid and the end of the borehole, gaps between bentonite discs, and gaps inside discs where sensors were installed. Initially, all of these gaps will have filled with the injected water. The injected water volume, total stress and relative humidity were measured at specific locations shown in Figure 15 (B, C and D). These measurements were compared with the modelling results in order to verify the mathematical model.

For the purpose of numerical solution, the model domain was simulated using a 3D geometry. Assuming symmetry, only half of the domain was simulated. The meshing algorithm was designed to generate radial mesh with finer mesh elements close to the boundary conditions as well as close to the disc-to-disc interface as shown in Figure 16.

The bentonite-sand mixture was pre-fabricated to the following specifications:

- Dry density = 1.94 Mg/m$^3$
- Gravimetric water content of 11% corresponding to an estimated initial saturation of 73%

An initial saturation of 73% was used to estimate the initial suction of 56 MPa using the water retention equations for the bentonite-sand mixture presented in Summary of Experimental Program section. The calculated initial suction corresponds to initial relative humidity (RH) of approximately 66%. However, the measured RH values range of 60-62% suggests that the actual water content of the bentonite-sand blocks could be slightly lower than the reported 73%.
Figure 17 shows the hydraulic and mechanical boundary conditions. A description of each of the boundary conditions (B.C.) follows:

**Mechanical boundary conditions:**

- B.C.1: The bentonite-sand is supported from both sides and movement is only allowed in the direction parallel to the support; a roller boundary condition is assigned.

- B.C.3: This surface represents the internal surface of the excavated borehole, it is assumed that the stiffness of the rock is high enough to prevent any deformation caused by swelling pressure; a zero displacement boundary conditions is assigned.

**Hydraulic boundary conditions:**

- B.C.1: This boundary represents the water saturated filter plate at which the water is applied to the bentonite-sand mixture; a zero pressure boundary condition is assigned.

- Pervious layer: This surface is located at the interface between the bentonite-sand domain and the water filled gap domain. This surface allows water to infiltrate into the bentonite-sand discs with a water pressure of zero as long as the gap is open. A zero pressure boundary condition is assigned at time zero; the boundary condition is converted to no-flow when the gap is closed. The pervious layer is assigned with a changing hydraulic conductance starting with a high value at a larger gap opening and a low value when the gap is closed by assuming that the conductance is a linear function of the closure ratio (closure/initial gap).

- B.C.3: This surface represents the internal surface of the excavated borehole. It is assumed that the rock hydraulic conductivity is very low and the flow into the rock is negligible; a no-flow boundary conditions is assigned.

For the mechanical process, the gap between the bentonite discs and the rock was simulated as an elastic material with a high porosity (n=1). It was originally assigned a very low Young’s modulus which increased progressively with a decrease in volume, in order to mimic the closing of the gap. The disc-to-disc interfaces (shown in Figure 17) were simulated as joints with a porosity of 1. From the mechanical perspective, both sides of the joint were always in contact. From the hydraulic perspective, the joint was assumed to be permeable with an initial permeability of $10^{-14}$ m$^2$ (approximately equivalent to a fracture aperture of 3 µm using aperture dependent permeability $k = a^2/12$, where a is the aperture). The permeability was set to be variable as a function of swelling pressure development, reaching a permeability of $10^{-21}$ m$^2$ at full swelling pressure.

Figure 18 shows the change in saturation for six different times (0, 50, 100, 200, 250 days and 10 years). There is an increase in saturation on the outer wetting boundaries, as well as along the disc-disc interfaces. However, it is noted that during the initial period (0 to 50 days) the saturation within the internal part of the discs decreased from an initial value of 73% to about 65%. This reduction could be attributed to the increase in porosity resulting from swelling as shown in Figure 19.
Figure 19 shows the change in porosity for six different times: (a) at 0 days; (b) at 50 days; (c) at 100 days; (d) at 200 days; (e) at 250 days; and (f) at 10 years. The porosity changed from an initial value of 0.28 to a maximum of 0.38. The porosity distribution was not uniform: the highest porosity (0.38 at 10 years) was found in the material that swelled into the gap, while in the core the porosity increase was smaller (from 0.27 to 0.33). At 10 years the porosity distribution seemed not stabilized yet.

Figure 20 shows the change in permeability for six different times (0, 50, 100, 200, 250 days and 10 years). The permeability changed from an initial value of 1.6E-21 m² to a maximum of 6.0E-21 m². Figure 20 shows that the final permeability at 250 days was heterogeneous, with a higher permeability close to the original void. This is caused by the increase in porosity due to free swelling into the technological void. However, the model predicts that this heterogeneity would gradually be reduced and a homogenous permeability would be reached at approximately 10 years.

The experimental setup was equipped with eight relative humidity (RH) sensors at the locations shown in Figure 15. The RH measurements showed only two sensors providing a reasonable reading (22_2 and 52_1). The other sensors show unrealistic values (such as a flat response as a function of time) due to technical failure. Therefore, only sensors 22_2 and 52_1 were used for direct comparison between modelled and measured values.

Figure 21 shows the modelled RH (%) at the 52-1 sensors location between 0 and 250 days. These results were obtained using the given initial water saturation of 73%. It can be seen that the actual measured initial RH of 62% is lower than the estimated 66% based on the given saturation. This could explain the overestimate of the initial RH modelled results.

The experimental setup was equipped with five pressure cells located as shown in Figure 15. The experimental stress measurements showed that only one sensor provided a reasonable reading (S-120). Two concepts used to identify the reasonableness of the measurements, first, the maximum measured compared with the expected maximum swelling based on literature, second is trend of increase in swelling pressure. Therefore, only S-120 pressure cell data were used for direct comparison of modelled and measured values.

Figure 22 shows the modelled stress (in MPa) at the selected cell location between 0 and 250 days. The S-120 cell was selected for comparison of the measured axial swelling pressure with the expected swelling pressure based on the EMDD after Baumgartner (2006). The EMDD for the bentonite-sand mixture was approximately 1.25 Mg/m³ and the water used for the experiment was synthetic water with a TDS of 5.7 g/l. According to Baumgartner (2006), the expected swelling pressure is 2-3 MPa which is consistent with the recorded pressure at cell S-120.

The radial stresses σ_R (at positions shown in Figure 23) are shown in Figure 24 for the pressure cell S_60_0_3, S_60_0_1 and S_60_0_2. The radial stress results show good agreement with the measured values.

CONCLUSION

A HM model for coupled two-phase flow in porous, deformable and expansive media was developed and used to simulate experiments for simulating the behavior of bentonite-based seals material. A set of equations were proposed, in which the van Genuchten air entry pressure parameter was made dependent on the EMDD. In addition, a simple relationship for swelling-dependent intrinsic
permeability of the bentonite block interfaces was implemented. The results showed good agreement between modelled and measured values for all tests for the evolution of relative humidity and swelling stress. A further confirmation that the model produces physically realistic results was obtained by comparison with the estimated swelling pressure after Baumgartner (2006). Both linear elastic and elasto-plastic models using the BBM were able to predict the main features of the hydromechanical response of the bentonite-sand mixture. However, the collapse phenomenon in the mock-up test could only be reproduced by the BBM model. Both modelling and experimental swelling pressure results show that given sufficient water the bentonite seal is able to swell and fill the technological gaps in a relatively short time. However, under anticipated repository conditions, the swelling process will depend on the availability of water, and the full swelling process might take hundreds to thousands of years if the host rock has very low permeability. On the other hand, gap closure is a function of both swelling potential and initial gap size. The overall bentonite-sand permeability is predicted to increase as a result of swelling if technological voids exist. In the mock-up and in-situ PT-A1 experiments considered in this paper, there is a rather large gap of 7% and 8% of the sample diameter, respectively. In most repository designs, those gaps would be smaller and/or filled (for example with bentonite pellets). The results of our modelling indicate that the overall increase in permeability would be insignificant from a safety perspective.

ACKNOWLEDGMENT

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REFERENCES


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Figure Captions

Figure 1: Pore scale representation of bentonite seal material (modified after Ichikawa et al. 2004).

Figure 2: Modelled water retention of the bentonite compared with measurements from Wang et al. (2013a).

Figure 3: Experimental results for swelling tests under controlled suction.

Figure 4: Calibration of the BBM with Void ratio – Pressure relationship at different suctions: (a) Suction = 0 MPa; (b) Suction = 4.2 MPa; (c) Suction = 12.6 MPa; (d) Suction = 38 MPa.

Figure 5: Illustration of the infiltration test.

Figure 6: Finite element model and boundary conditions for infiltration test.

Figure 7: Observed and modelled evolution of suction at the four monitoring points.

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Figure 10: Finite element model and boundary conditions for the mock-up test.

Figure 11: Modelled and measured swelling pressure.

Figure 12: BBM Yield Surface in p-q-s space.

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Figure 14: Stress path analysis.

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Figure 16: Model Discretization.

Figure 17: Boundary Conditions.

Figure 18: Calculated water saturation at different times: (a) at 0 days; (b) at 50 days; (c) at 100 days; (d) at 200 days; (e) at 250 days; and (f) at 10 years.

Figure 19: Calculated Change in Porosity at different times: (a) at 0 days; (b) at 50 days; (c) at 100 days; (d) at 200 days; (e) at 250 days; and (f) at 10 years.
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Figure 21: Modelled RH between 0 and 250 days (RH in %).

Figure 22: Simulated evolution of axial swelling pressure during the PT-A1 Test.

Figure 23: Radial stress sensors.

Figure 24: Simulated evolution of radial swelling pressure during the PT-A1 Test at S_60_2 and S_60_3 pressure cell location.
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Figure 9: Illustration of the mock-up test phases.

Hydraulic boundary conditions: No flow for phase 1 and 2a
Mechanical boundary conditions: Non linear elastic spring k2

Figure 10: Finite element model and boundary conditions for the mock-up test

Hydraulic boundary conditions: Zero pressure
Mechanical boundary conditions: Roller
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Figure 21: Modelled RH between 0 and 250 days (RH in %).

Figure 22: Simulated evolution of axial swelling pressure during the PT-A1 Test.
Figure 23: Radial stress sensors.

1 is the location of PT-A1-S-60-0-1 Pressure cell (θ=210°)
2 is the location of PT-A1-S-60-0-2 Pressure cell (θ=90°)
3 is the location of PT-A1-S-60-0-3 Pressure cell (θ=330°)

Figure 24: Simulated evolution of radial swelling pressure during the PT-A1 Test at S_60_2 and S_60_3 pressure cell location.
Table 1: Characteristics of the bentonite and sand used to prepare samples

<table>
<thead>
<tr>
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<th>Specific gravity of solid particles (-)</th>
<th>Liquid limit/plastic limit (%)</th>
<th>Montmorillonite content %</th>
<th>Grain size</th>
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</thead>
<tbody>
<tr>
<td>Bentonite</td>
<td>2.77</td>
<td>575/53</td>
<td>80</td>
<td>84% less than (2 µm)</td>
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<tr>
<td>Sand</td>
<td>2.65</td>
<td>-</td>
<td>-</td>
<td>100% less than 2 mm</td>
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Table 2: Calibrated parameters of BBM model

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<thead>
<tr>
<th>Parameter</th>
<th>$\kappa_{\rho_o}$ (-)</th>
<th>$\alpha_k$ (-)</th>
<th>$P'_{o}$ (MPa)</th>
<th>$\alpha_{p_o}$ (-)</th>
<th>k</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value</td>
<td>0.08</td>
<td>0.013</td>
<td>1.25</td>
<td>0.1</td>
<td>0.2</td>
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Table 3: Values of calibrated parameters used in the simulation of the infiltration, mock-up and PT-A1 tests

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial water content by mass</td>
<td>$11^{A,B,C}$</td>
<td>%</td>
</tr>
<tr>
<td>$B_s$</td>
<td>$1E-9^{A,C}, 7E-10^B$</td>
<td>Pa$^{-1}$</td>
</tr>
<tr>
<td>$\kappa_{ao}$</td>
<td>$8.5E-20^A, 1.0E-21^B, 8E-21^C$</td>
<td>m$^2$</td>
</tr>
<tr>
<td>$n_{o},$ initial porosity</td>
<td>$0.38^A, 0.41^B,C$</td>
<td>-</td>
</tr>
<tr>
<td>parameters of the van Genuchten equation</td>
<td></td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>$1.16^{A,B,C}$</td>
<td>-</td>
</tr>
<tr>
<td>m</td>
<td>$(1-(1/N))^{A,B,C}$</td>
<td>-</td>
</tr>
<tr>
<td>l</td>
<td>$9^A, 20^B, 8^B,C$</td>
<td>-</td>
</tr>
<tr>
<td>$E_s$, elastic modulus</td>
<td>$3.5E7^{A,C}, 2.5E7^B$</td>
<td>Pa</td>
</tr>
<tr>
<td>$\nu$, Poisson’s ratio</td>
<td>$0.2^{A,B,C}$</td>
<td>-</td>
</tr>
</tbody>
</table>

A: infiltration test, B: Mock-up test (non-linear elastic), C: PT-A1 test