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Modelling of compacted bentonite swelling accounting for salinity effects

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ABSTRACT

This paper presents a formulation to incorporate the influence of water salinity on the swelling behaviour of a MX-80 bentonite into previously developed hydro-mechanical models that can reproduce swelling under dilute conditions. The effects of salinity on macro- and microstructural water chemical potentials were introduced. In addition, a description of solute transport was included to characterise the evolution of the system's salinity. A simplified geochemical model was adopted to idealise the geochemical complexity of bentonite. In addition, the modelling of the destructuration process that occurs during swelling was modified to account for the effect of salinity. The formulation was implemented in a multiphysics partial differential equation finite element solver, and the numerical model was used to simulate several vertical free swelling tests with feed water of different salt contents (deionised, 10, 35 and 70 g/L). The results demonstrate that even though the model can be developed further, it represents a significant improvement over models that do not account for the effects of salinity.

1. Introduction

The highly expansive behaviour and low hydraulic conductivity of bentonites make them good sealing materials for engineered barrier systems in deep geological repositories for spent nuclear fuel. The operation conditions of these systems will vary widely throughout their useful life. It is therefore essential to have a bentonite stress-strain constitutive model that is capable of estimating its long term behaviour. The characterisation of the hydration and swelling of bentonite is particularly important because these properties define its the ability to seal gaps (natural or associated with the construction process) that may exist in engineered barrier systems.

Given the importance of this matter, a significant amount of research has focused on bentonite hydration (see for example the contributions in Tournassat et al., 2015). Most of these studies assume a hierarchical idealisation of the clay fabric (Yong, 1999). However, even in compacted bentonites, the stacking of clay layers to form particles is irregular, which generates micro-voids inside the particles (Cases et al., 1992). Furthermore, the particles split into smaller ones along wetting paths Saiyouri et al. (2004) suggested that swelling is essentially a process of subdivision of the clay particles and not a homogeneous increase in the distance between the layers. Similar processes occur in the particle aggregates (Salles et al., 2009). As a result, the internal topology of bentonite is irregular, and both the particles and the aggregates they form should be considered dynamic functional structures that evolve throughout the hydration process. This evolution conditions the process itself. Swelling is a non-linear (Wang et al., 2015) complex process in which "competition" for water occurs between the hydration of cations, the hydration of the charged surface of the clay, the separation of particles, the adsorption in the intra-aggregate pores (microporosity), the hydration of the inter-aggregate space (macroporosity) and diffuse double layer development (Salles et al., 2009).

Despite significant advances in upscaling techniques based on the Homogenization Theory (Marry and Rotenberg, 2015), the complexity of these phenomena still makes it difficult to define a macroscopic model that will solve engineering-scale problems (i.e., behaviour of the repository) through the integration of microscopic processes. To obtain a macroscopic model, it is necessary to introduce simplifying hypotheses that avoid characterising some of the processes that occur at a microscopic level. The most frequent simplification strategy for compacted bentonite is to consider it as a double porosity medium (e.g., Alonso et al., 1999; Mašín, 2013). This approach is based on the bimodal distribution of porosity observed when the material is analysed using porosimetry techniques (Romero et al., 1999) to identify the macrostructural porosity with the space between the bentonite particle aggregates, and the microstructural porosity with their internal voids. While this fabric evolves throughout the hydration process as a result of

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the previously described microscopic processes (Burton et al., 2015), the double porosity models satisfactorily reproduce the macroscopic effects of these changes on deformability and flow (Gens and Alonso, 1992).

Hydro-mechanical models have typically been used for dilute conditions. However, these models must be modified to describe the response of bentonites to variations in salinity. This topic is important for deep geological repositories, where significant changes in the chemistry of the surrounding groundwater and thus of the interstitial porewater will take place (Hellä et al., 2014). Many experimental studies have been conducted to characterise the effect of porewater salinity on the hydro-mechanical behaviour of bentonite. These studies have confirmed that the swelling pressure decreases when the porewater's ionic strength increases (Karnland et al., 2005; Zhu et al., 2013). Alawaji (1999) showed in swelling tests that the initial strain velocity increases and the swelling capacity decreases as the concentrations increase. In addition, since the seminal work of Quirk and Schofield (1955), several authors have shown that the hydraulic conductivity of bentonites increases when they are saturated with solutions of increasing salinity (Zhu et al., 2013).

To introduce these processes into constitutive models, simplified models of the geochemical configuration of the clay have been adopted (see Guimarães et al., 2013, for instance), which often assume a system that is composed of two basic cations (usually Na^+ and Ca^{2+}) and a single anion (typically, Cl^-). This has allowed researchers to characterise the response of the material to simple "chemical loads" and to better understand the importance of hydro-mechanical-chemical coupling on the deformational behaviour of bentonites. Currently, thermo-hydro-mechanical and chemical models are being developed with a broader geochemical basis (Zheng et al., 2015).

However, those formulations are primarily aimed at confined conditions and not at free swelling conditions that may occur in the presence of voids or erosion processes (Navarro et al., 2016). This paper proposes a hydro-chemo-mechanical formulation that is capable of reproducing the free swelling behaviour of an MX-80 bentonite under different water salinity conditions. To illustrate its applicability, a set of vertical free swelling tests were simulated to demonstrate the scope and limitations of the proposed formulation.

2. Vertical free swelling tests on MX-80

2.1. Materials and methods

Wyoming MX-80 bentonite was used in the vertical free swelling tests. Its properties are similar to the material called Be-Wy–BT007-1-Sa-R that was used by Kiviranta and Kumpulainen (2011). Table 1 shows the main mineralogical, chemical, and physical properties of this natural sodium bentonite.

This material was used to produce cylindrical samples 40 mm in height and 50 mm in diameter. The initial bulk density and water content of the samples were 2.05 g/cm^3 and 17%, respectively. Deionised (DI) water was used to increase the original bentonite water content up to this value. The compacted blocks were placed at the bottom of a transparent test cell that was 50 mm in diameter (Fig. 1). Water with the desired salinity was poured on top of the samples, which allowed them to swell freely in the vertical direction. The water solutions used in the tests included DI water (one test), a 10 g/L solution (two tests), a 35 g/L solution (two tests) and a 70 g/L (one test). These solutions contained only two cations (sodium and calcium) and a common anion (chloride); their characteristics are shown in Table 2. The 10 g/L solution was a brackish-saline groundwater simulant for Olkiluoto, which is the site of the Onkalo deep geological repository for spent nuclear fuel in Finland, at the repository depth during the operational phase (based on Hellä et al., 2014). The 35 g/L solution represents the maximum expected salinity of the groundwater at the repository depth (Hellä et al., 2014) and corresponds to saline

Table 1
Properties of the tested material (Kiviranta and Kumpulainen, 2011).

Chemical composition (weight %)	
SiO_2	59.82
Al_2O_3	21.27
Fe_2O_3	3.62
Na_2O	2.86
MgO	2.77
CaO	1.49
K_2O	0.55
FeO	0.49
TiO_2	0.15
Mineralogical composition (weight %). Phases present only as traces are not shown	
Smectite	87.6
Plagioclase	4.2
Quartz	4.1
K-feldspar	1.8
Rutile	0.9
Calcite	0.6
Pyrite	0.6
Illite	0.1
Other properties	
CEC (eq/kg)	0.84
$Na^+/K^+/Ca^{2+}/Mg^{2+}$ (eq/kg)	0.58/0.02/0.25/0.08
Bentonite density $\rho_{mineral}$ (g/cm^3)	2.78
Liquid limit	510
Plastic limit	50
Plasticity index	470

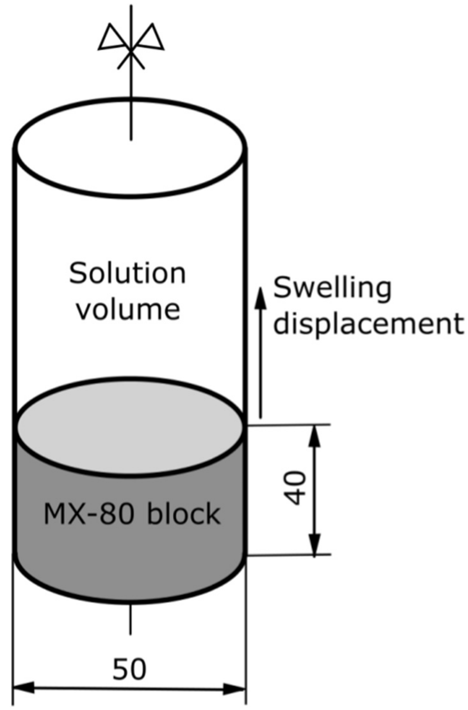

Fig. 1. Setup of the vertical free swelling test (initial dimensions in mm).

Table 2
Compositions of the permeant solutions used in the tests.

Solution	TDS (g/L)	NaCl (g/L)	$CaCl_2$ (g/L)	Number of tests
Brackish-saline water	10	6.47	3.53	2
Saline water	35	16.75	18.25	2
Highly saline water	70	26.58	43.42	1

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