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Research paper

Predicting the swelling pressure of MX-80 bentonite

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ABSTRACT

This paper proposes a calculation procedure to estimate the swelling pressure of bentonites. The experimental information needed to obtain the estimations can be obtained from relatively conventional tests, including the determination of the water retention curve, and swelling pressure tests using oedometric sample holders. This allows to obtain physically based predictions of the changes in swelling pressure with environment salinity. To facilitate the calculations, an open access spreadsheet in which the proposed approach has been implemented is attached as Supplementary material. A set of significant swelling pressure tests are modelled, obtaining very good fits. The fits not only build confidence in the proposed methodology, but also improve the validation of the hydro-chemo-mechanical formulation on which the proposed procedure is based.

1. Introduction

In addition to their low hydraulic conductivity, the high adsorption capacity and high swelling potential of bentonites have made these clays an important part of multi-barrier systems that are expected to be used in the deep geological disposal of spent nuclear fuel (e.g., Bennett and Gens, 2008; Sellin and Leupin, 2013; Sanders and Sanders, 2016). Therefore, an important research effort has been conducted in recent years to understand the properties of bentonites, and the results have demonstrated the remarkable dependence of the hydraulic and deformational behaviour of bentonites on the environment salinity (Alawaji, 1999; Di Maio, 1996; Studds et al., 1998). Based on the current trends of modelling techniques (Keyes et al., 2013), a multiphysics approach is advised for modelling the behaviour of bentonites. This approach allows the integration of flow and transport formulations, such as those described by Loret and Huyghe (2004) and Tournassat et al. (2015), with mechanical constitutive models, such as the Barcelona Basic Model (Alonso et al., 1990) and the Barcelona Expansive Model (Gens and Alonso, 1992; Alonso et al., 1999), which are recognized by many researchers (e.g., Wheeler et al., 2002; Sheng et al., 2004; Sołowski et al., 2012) as references for the analysis of the mechanical behaviour of bentonites.

Navarro et al. (2017) presented a multiphysics approach that integrates a mechanical model based on the Barcelona Expansive Model (Navarro et al., 2014) with a electro-chemical formulation based on the use of a Donnan equilibrium approach (Revil et al., 2011; Tournassat and Appelo, 2011). Satisfactory results were obtained despite using a simplified conceptual model to characterize the geochemistry of the system (only Ca^{2+}, Na^{+} and Cl^{-} were considered in addition to the mineral clay), and even though the simulated tests (free swelling of MX-80 bentonites) were challenging for the model because they incorporated significant deformations and notable variations of salinity. Nevertheless, it would be interesting to further validate the formulation by analysing other processes.

With this goal, this paper presents simulations of the swelling pressure tests performed by Karnland et al. (2005, 2006). The satisfactory fits obtained provides additional confidence in the hydro-chemo-mechanical formulation proposed by Navarro et al. (2017). Moreover, the good results obtained imply something more important than this validation. The calculation procedure defines a strategy to determine the swelling pressure, providing a physically based formulation that complements the use of empirically based extrapolations when, for example, sensitivity analyses such as those described by Juvankoski (2013) are performed.

2. Materials and methods. Description and results of swelling pressure tests

The swelling tests performed by Karnland et al. (2005, 2006) were analysed. Karnland et al. (2005) carried out three sets of tests (S2-41-46, S2-51-56, S2-61-66; Fig. 1) using a sodium-purified MX-80 bentonite with a cation exchange capacity (*CEC*) of 0.85 eq/kg clay. Karnland et al. (2006) tested several clays, although in the present study only results obtained with sodium-purified MX-80 "WyNa" (*CEC* of 0.86 eq/kg clay) were used (Fig. 1). Both materials are similar to the MX-80 sodium bentonite analysed by Navarro et al. (2017), which had a *CEC*

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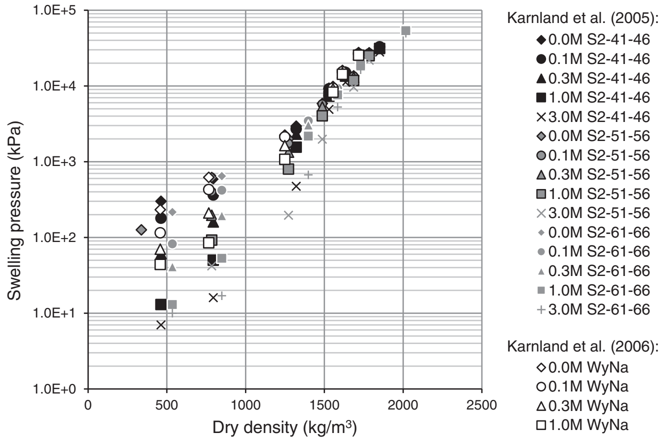

Fig. 1. Experimental results obtained by Karnland et al. (2005, 2006).

of 0.84 eq/kg clay. The similarity is demonstrated by the chemical and mineralogical composition data included in Karnland et al. (2005, 2006) and Navarro et al. (2017). An average mineral density, ρ_{mineral}, of 2780 kg/m^3 was assumed (Navarro et al., 2017).

In all of the tests, after compacting the bentonite, it was initially saturated with deionized water in an oedometric sample holder that prevented volumetric deformation. This equipment and isochoric conditions were maintained throughout the tests. Small samples (1.6 cm^3, Karnland et al., 2005; 4.8 cm^3, Karnland et al., 2006) were used to reduce the time required to reach equilibrium in the different testing steps. After saturation, the salinity of the interstitial water was progressively increased by contacting the sample top and bottom boundaries with an aqueous solution of controlled salinity. The salinity of the boundary solution was increased after the swelling pressure (measured with a load cell) reached a constant value, obtaining the results synthesized in Fig. 1.

3. Conceptual model and numerical solution

As is customary when analysing the behaviour of compacted bentonite, a double porosity medium was considered (e.g., Alonso et al., 1999; Lemaire et al., 2004; Sedighi and Thomas, 2014), which idealizes the macro- and microstructure as the inter-aggregate and intra-aggregate void space, respectively (see Fig. 2). Although it is reasonable to assume at least two different hierarchical levels of voids in the microstructure, interlamellar voids and interstack voids (following the notation in Neretnieks et al., 2009), only one macroscopic variable, the microstructural void ratio e_m (volume of voids in the microstructure per volume of mineral) was considered for characterising the intra-aggregate porosity (microporosity). The internal complexity of the microstructure is abstracted, adopting the aggregate as the support scale (according to Pachepsky et al., 2006). Therefore, different types of microstructural water are not distinguished. Only one microstructural water is considered, which saturates the microstructural space (Gens and Alonso, 1992; Mašín and Khalili, 2016), and does not flow due to hydrodynamic gradients (immobile water of van Genuchten and Wierenga, 1976). On the other hand, the water in the macrostructural pores (inter-aggregate water) does flow under such gradients (free water).

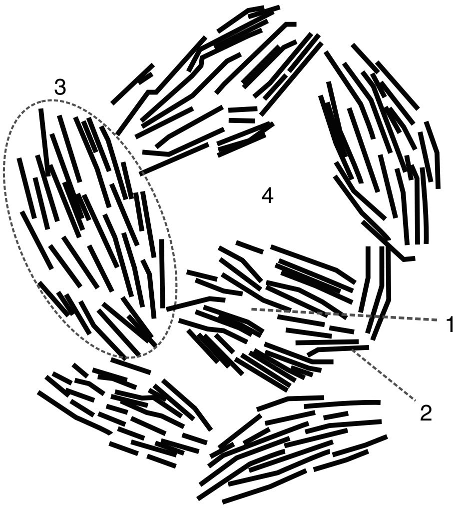

Fig. 2. Schematic particle arrangement in a highly compacted Na-bentonite: 1, intra-aggregate space; 2, bentonite stack; 3, aggregate; 4, inter-aggregate space.
Adapted from Pusch (1987).

In the analysed steps, saturated conditions were maintained with a null macrostructural matric suction (identified by the capillary suction). Consequently, according to Navarro et al. (2017), the chemical potential of the macrostructural water, μ_M, was equal to:

$$\mu_M = \mu_{VO}(T) - \frac{WMM}{\rho_W}\cdot s_{MO} \tag{1}$$

where μ_{VO} is the chemical potential of pure water at temperature T (absolute value), WMM is the molar mass of water, ρ_W is the density of free water, and s_{MO} is the macrostructural osmotic suction. The analysis of the system only includes chloride and sodium as dissolved species, because, as mentioned in Section 2, the tests were conducted with sodium-purified bentonite, and the salinity conditions are imposed using a NaCl aqueous solution. Consequently, the presence of calcium is disregarded (Appendix A describes how the formulation should be modified to consider it). Therefore, s_{MO} can be calculated as:

$$s_{MO} = R\cdot T\cdot \rho_W\cdot(c_{Cl,M} + c_{Na,M})\cdot \phi_M \tag{2}$$

where R is the universal gas constant, and φ_M is the macrostructural osmotic coefficient, which is assumed to be equal to 1 in this approach. Thus, the proposed formulation should be applied with caution under high salinity conditions.

The variables $c_{Cl,M}$ and $c_{Na,M}$ are the molal concentrations of the chloride and sodium ions, respectively, in the macrostructural solution. At equilibrium, the molar concentrations ($C_{Cl,M}$ and $C_{Na,M}$, respectively) are given by the values indicated in Fig. 1. In the "chemical loading steps", by increasing the boundary salinity, s_{MO} increased, and μ_M decreased. When μ_M became smaller than μ_m (the chemical potential of the microstructural water), the equilibrium between macro- and microstructural water was lost. A transient process occurred in which water passed from the microstructure to the macrostructure, which decreased e_m and increased e_M (macrostructural void ratio: volume of voids in the macrostructure per volume of mineral) until the new value of μ_m was equal to the value of μ_M. This transient process is not described in this paper. The analysis focuses on the stationary situation when μ_m was equal to μ_M, which was determined by the water salinity in contact with the sample boundaries.

The chemical potential of the microstructural water can be calculated as (Navarro et al., 2017):

$$\mu_m = \mu_{VO}(T) + \frac{WMM}{\rho_m}\cdot(p - s_{mS} - \Delta s_{mO}) \tag{3}$$

where ρ_m is the microstructural water density, p is the net mean stress (which under saturated conditions is equal to the Terzaghi effective mean stress), s_{mS} is the "structural" suction of the microstructure. This magnitude defines the affinity of water for the solid components of the soil-water system, and changes with the arrangement of the soil particles (Box and Taylor, 1962), which in the microstructure can be assumed to be characterised by e_m. If, starting from conditions in which the microstructure only includes the cations necessary to compensate the *CEC*, the soil salinity is increased maintaining e_m constant, although