Engineering Geology 181 (2014) 190–201

Contents lists available at ScienceDirect

Engineering Geology

journal homepage: www.elsevier.com/locate/enggeo

An elastoplastic model of bentonite free swelling

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ARTICLE INFO

Article history:
Received 20 February 2014
Received in revised form 24 June 2014
Accepted 20 July 2014
Available online 31 July 2014

Keywords:
Expansive soils
Bentonite free swelling
Plasticity
Partial saturation
Soil fabric/structure

ABSTRACT

This article proposes a new plastification mechanism to model bentonite free swelling processes by using an elastoplastic approach. The formulation is based on an interaction function that defines the plastic macrostructural strains induced by microstructural effects. This term is defined as a function of the microstructural void ratio, and it establishes a direct connection between the destructuration of the micro- and macrostructures of the bentonite during the free swelling processes. The formulation proposed also includes a new approach to the calculation of the microstructural void ratio as well as a new method to describe the kinetic mass exchange between micro- and macrostructural water, considering that there may not be equilibrium between the two types of water. The model was used to analyse several free swelling tests and was found to yield satisfactory results.

1. Introduction

Because of the physical and chemical properties of bentonite clays, they have been considered in several countries for use as buffer and backfill materials in spent nuclear fuel repositories. Specifically, in the KBS-3 disposal concept (developed by the Swedish nuclear fuel and waste management administration, SKB, 1999, and by Posiva, 2006, the Finnish expert organisation responsible for the spent nuclear fuel repository), dry Na-bentonite of the Wyoming type (called "MX-80"; see Karnland et al., 2005; Dueck and Nilsson, 2010) is considered for placement around high level radioactive waste (HLW) canisters in a highly compacted state. A reliable model of the behaviour of these bentonites is needed to assess the safety performance of the barrier. For this purpose, the model should characterise the bentonite free swelling (FS) associated with erosion (see, for instance, Birgersson et al., 2009; Moreno et al., 2010), a process of special interest in the field of designing HLW repositories.

Some authors have proposed sol–gel transition models to describe the soil behaviour close to this extreme situation (Liu et al., 2009). However, despite their value, at the present time these models are not able to describe the entire swelling process of bentonite, from an initial unsaturated (with values of suction on the order of tens to hundreds of MPa) and well structured (both micro and macrostructurally) state to the release of soil particles when it becomes a sol.

This study proposes an elastoplastic formulation that contributes to the characterisation of the saturated and unsaturated FS of bentonites. First, a review of its basic concepts will be presented. Afterwards, an analysis of its application to the simulation of FS is illustrated by several examples.

2. Theory (1): basis

Since the seminal work of Collins and McGown (1974) and Collins (1984), a number of researchers have observed the existence of two structural levels in compacted clays (Pusch, 1982; Romero et al., 1999; Pusch and Moreno, 2001; Lloret et al., 2003; Romero and Simms, 2008). Thus, the structure of the bentonites analysed in this paper is idealised into two structural levels: macro and micro structures. The microstructural level is associated with both intersheet voids and intra-aggregate pores (see Figure 1a, adapted from Pusch, 1987). The pores between the aggregates, inter-aggregate pores or macropores (Romero et al., 2011), define the macrostructural level.

Like the formulations derived from Gens and Alonso (1992), the one presented here foregoes the characterisation of the internal topology of the aggregates. Although it is reasonable to assume that at least two different hierarchical levels exist, interlamellar voids and interstack voids (following the notation in Neretnieks et al., 2009), only one macroscopic variable, the microstructural void ratio e_m ($e_m =$ volume of voids in the microstructure per volume of mineral), has been considered for characterising the intra-aggregate porosity (microporosity). The aggregate has been adopted as the support scale (according to Pachepsky et al., 2006) of the microstructure, performing an abstraction of its internal complexity.

Abbreviations: BBM, Barcelona Basic Model; BExM, Barcelona Expansive Model; FS, free swelling; HLW, high level radioactive waste.

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http://dx.doi.org/10.1016/j.enggeo.2014.07.014
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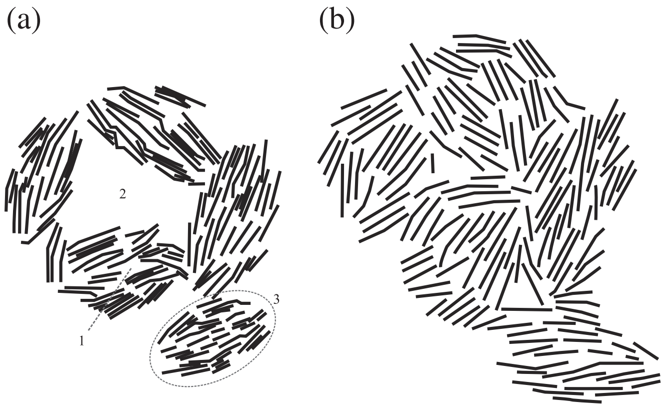

Fig. 1. (a) Schematic particle arrangement in a highly compacted Na-bentonite; 1, intra-aggregate space; 2, interaggregate space; and 3, aggregate. (b) State after swelling and saturation. Adapted from Pusch (1987).

In accordance with Gens and Alonso (1992), the microstructural void ratio variation is assumed to be associated with the variation of the intra-aggregate water content. According also to these authors and to Hueckel (1992) and Quirk (1994), the microstructure deformation is assumed to be fully reversible and unaffected by the macrostructure deformation. However, when considering the deformation of the aggregates, it must be taken into account that their swelling (micro-swelling) can occlude the macropores to different extents (Mašín, 2013). Given their random arrangement (Quirk, 1994), each aggregate (microdomain) swells in a different direction, and micro deformations induce macro deformations (Villar and Lloret, 2001; Cui et al., 2002; Khalili et al., 2010). This coupling causes a complex array of behavioural trends (Koliji et al., 2010; Sun and Sun, 2012; Della Vecchia et al., 2013), which are adequately described by the "Barcelona Expansive Model" (BExM; Alonso et al., 1999) for compacted bentonites (see Lloret et al., 2003). To achieve this description, the BExM introduces two interaction functions (Alonso et al., 1999): f_C, when microstructural compression is produced (i.e., e_m decreases), and f_S for microstructural swelling (i.e., e_m increases). The shape of these interaction functions is depicted in Fig. 2. The value of f_C and f_S depends on the degree of openness of the macrostructure relative to the applied stress state (Sánchez et al., 2005). The degree of openness is determined by the p/p_O ratio in isotropic stress states, where p is the net mean stress ($p = p_{TOT} - P_G$, where p_{TOT} is the mean stress and P_G is the gas pressure) and p_O is the net mean yield stress at the current suction (see Figure 3). If a deviatoric stress exists, the openness is determined by p_R/p_O (Sánchez et al., 2005), where the reference stress p_R is defined in Fig. 3. Once f_α is defined (α = "C" if $de_m < 0$ and α = "S" if $de_m > 0$, where de_m is the increment of the microstructural void ratio), the macrostructural plastic volumetric strains induced by microstructural effects, $d\varepsilon^{p}_{MV,m}$, can be expressed as:

$$d\varepsilon_{MV,m}{}^{p} = f_\alpha \cdot d\varepsilon_{mV} \quad (1)$$

where $d\varepsilon_{mV}$ is the microstructural volumetric strain, which is supposed to be elastic. Therefore, it is assumed that irreversible macrostructural plastic strains are induced whenever microstructural deformations occur.

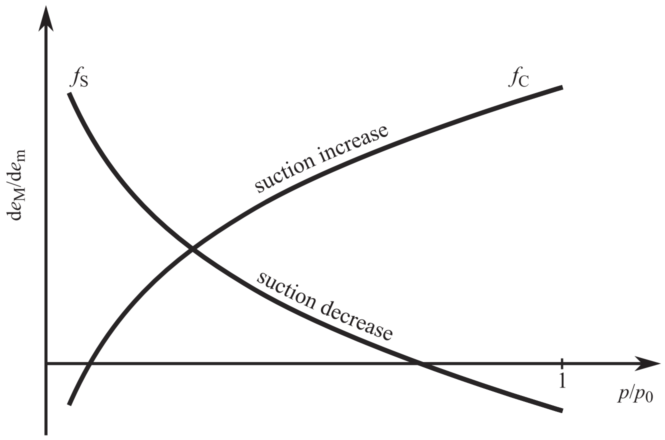

Fig. 2. Interaction functions between micro and macroporosity deformations. Adapted from Alonso (1998).

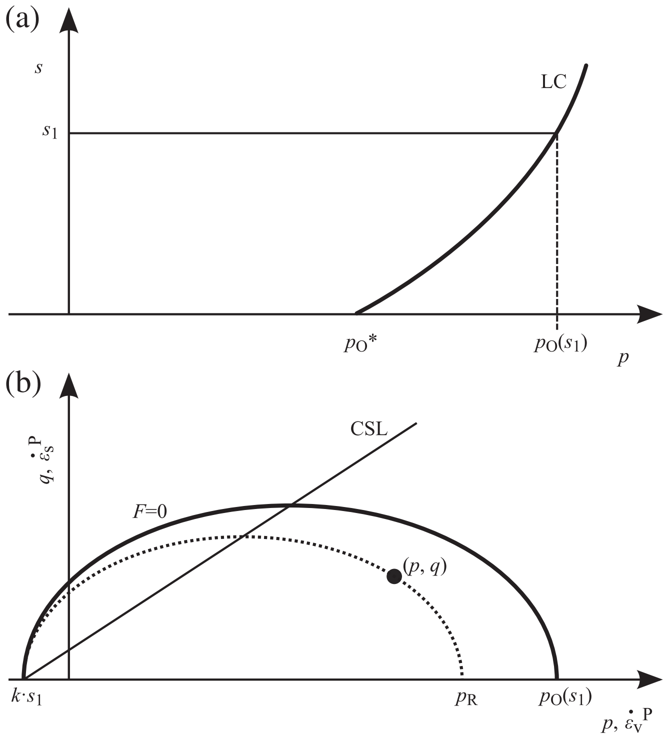

Fig. 3. (a) Representation of the "loading–collapse" (LC) yield surface in the p–s space. (b) Yield surface in the p–q space and definition of the reference pressure p_R; "CSL" defines the critical state line.

Functions f_α are constitutive terms. To define them, Alonso et al. (1999), Sánchez et al. (2005) and Gens et al. (2011) considered not only different parameters but also different "shapes" for different soils. Different ways of defining $d\varepsilon_{mV}$ have been considered (see, for instance, Romero et al., 2011; Mašín, 2013; Musso et al., 2013). Sánchez et al. (2005) take into account both exponential and logarithmic laws to define $d\varepsilon_{mV}$ in terms of the variation of the microstructural effective stress. In this paper, e_m is calculated by a one-to-one model based on the formulation by Zhang et al. (1995):

$$\frac{1}{e_m} = \frac{1}{e_{m0}} + \frac{1}{k_m} \cdot \mathrm{Ln}\left(1 + {}^{\pi}\!/_{P_{ATM}}\right) \quad (2)$$

where k_m is a micro deformability parameter and e_{m0} is the microstructural void ratio when the bentonite swelling pressure π is equal to 0, that is, when only the atmospheric pressure P_{ATM} is applied. Note that the swelling pressure is interpreted as the pressure exerted by the aggregates when swelling occurs in pure water, that is, when the vapour pressure is set only by the clay skeleton.

The analyses used by Zhang et al. (1995) to derive Eq. (2) were conducted with bentonites in which the void ratio reached high values (greater than 1). This formulation is valuable when simulating free swelling processes. However, this casts doubt on the validity of Eq. (2) for compacted bentonites in which the void ratio may be substantially