

GENERALIZED PLASTICITY FOR GEOMATERIALS WITH DOUBLE STRUCTURE

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Abstract. The paper presents a double structure constitutive model based on a generalized plasticity formalism. The behaviour of macrostructure, microstructure and their interactions are described. A coupled hydromechanical formulation is then presented that assumes no hydraulic equilibrium between structural levels. Constitutive law and formulation are applied to the simulation of the behaviour during hydration of a heterogeneous mixture of bentonite powder and bentonite pellets. A satisfactory reproduction of observed behaviour is achieved.

1 INTRODUCTION

The behaviour of swelling clays is better understood if the effect of the pore size structure on their hydromechanical behaviour is taken into account. In compacted (and therefore unsaturated) swelling clays, the pore size structure is set up during compaction but it may change significantly in response to various actions such as loading and hydration. Although the distribution of pore sizes is of course continuous, useful insights can be obtained by considering only two structural levels: microstructural and macrostructural as well as their interactions. This dual material aspect is reinforced when the material is composed of a mixture of powder and highly compacted pellets. This mixture is an attractive sealing material in radioactive waste disposal schemes because, even when only modest compaction efforts are applied, a sufficiently high density value is achieved after hydration has taken place. However, the heterogeneity of the material gives rise to a complex hydromechanical behaviour that must be well understood if a sufficient degree of confidence in the performance of the seal is to be achieved.

The generalized plasticity model adopted for the description of the behaviour of the double structure material is presented first followed by the formulation of the hydromechanical problem. Constitutive law and formulation are then applied to description of a number of swelling pressure tests of a mixture of bentonite powder and highly compacted bentonite pellets being studied as a potential sealing material for a deep geological repository for high level nuclear waste.

2 GENERALIZED PLASTICITY CONSTITUTIVE MODEL

In strongly swelling clays, there are plastic mechanisms giving rise to irreversible behaviour in addition to those observed in non-swelling materials. Those additional mechanisms can often be attributed to the interaction between the macrostructure and the microstructure. This kind of irreversible behaviour generally appears at any value of applied suction and it is difficult to determine the initiation of the yielding. Those facts encourage the use of the generalized plasticity theory to describe these plastic mechanisms. In a generalized plasticity model the yield function is not defined or it is not defined in an explicit way [1]. The advantages in using the generalized plasticity theory to model the plastic mechanisms ascribed to the interaction between structures are presented in detail in [2].

The model is defined in terms of the three stress invariants (p , J , Θ) and suction (s). To formulate the double structure model is necessary to define laws for: i) the macrostructural level, ii) the microstructural level, and iii) the interaction between both structural levels.

2.1 Macrostructural level

The inclusion of this structural level in the analysis allows the consideration of phenomena that affect the skeleton of the material, for instance deformations due to loading and/or collapse of the macrostructure. The *BBM* (Barcelona Basic Model) has been adopted to describe the macrostructural behaviour [3]. The *BBM* considers two stress variables to model the unsaturated behaviour: the net stress (σ) computed as the excess of the total stresses over the gas pressure, and the matric suction (s), computed as the difference between gas pressure and liquid pressure ($p_g - p_l$). The *BBM* yield surface (F_{LC}) is defined as follows:

$$F_{LC} = 3J^2 - \left[\frac{g(\theta)}{g(-30^\circ)} \right]^2 M^2 (p + p_s)(p_o - p) = 0 \quad (1)$$

where M is the slope of the critical state, p_o is the apparent unsaturated isotropic pre-consolidation pressure at a specific value of suction, and p_s considers the dependence of shear strength on suction. To complete the definition of the yield surface as set out in (1), it is possible, in principle, to adopt any suitable Lode's angle function, $g(\theta)$.

The trace of the yield function on the isotropic p - s plane is called *LC* (Loading-Collapse) yield curve because it represents the locus of activation of irreversible deformations due to loading increments or to hydration collapse. The position of the *LC* curve is given by the pre-consolidation yield stress of the saturated state, p_o^* (hardening variable) that varies with plastic volumetric strain according to the following hardening law:

$$\dot{p}_o^* = p_o^* \frac{(1+e)}{(\lambda_{(0)} - \kappa)} \dot{\varepsilon}_v^p \quad (2)$$

where e is the void ratio, ε_v^p is the volumetric plastic strain, κ is the elastic compression index for changes in p and $\lambda_{(0)}$ is the stiffness parameter for changes in p for virgin states of the soil in saturated condition.

2.2 Microstructural level

The microstructure is the seat of the basic physico-chemical phenomena occurring at clay particle level. The strains arising from microstructural phenomena are considered nonlinear

elastic and volumetric. The microstructural strains are proportional to the microstructural effective stress (\hat{p}) through a microstructural bulk modulus according to:

$$\hat{p} = p + \chi s \quad (3)$$

$$\dot{\varepsilon}_{v_m} = \frac{\dot{\hat{p}}}{K_m} = \frac{\dot{p}}{K_m} + \chi \frac{\dot{s}}{K_m} \quad (4)$$

where the subscript m refers to the microstructural level, the subscript v refers to the volumetric component of the strains, K_m is the microstructural bulk modulus and χ is a parameter dependent on the degree of saturation of the microstructure. The parameter χ is included only to account for the possibility that the microstructure may become unsaturated. However, generally a constant value of $\chi = 1$ is adopted since the micro-structural level, associated with the behaviour of expansive clay particles, is very likely to be saturated. In very active expansive clays this assumption can be supported by the high affinity of the active clay minerals by water, which maintain the interlayer space and micro-pores saturated even at relatively high suction. Under this condition mean effective stress controls the mechanical behaviour at microstructural level.

The concept of a Neutral Line (NL) is introduced corresponding to constant \hat{p} and no microstructural deformation (Fig. 1). The NL divides the p - s plane into two parts, defining two main generalized stress paths, which are identified as: MC (microstructural contraction) when there is an increase in \hat{p} and MS (microstructural swelling) in the opposite case.

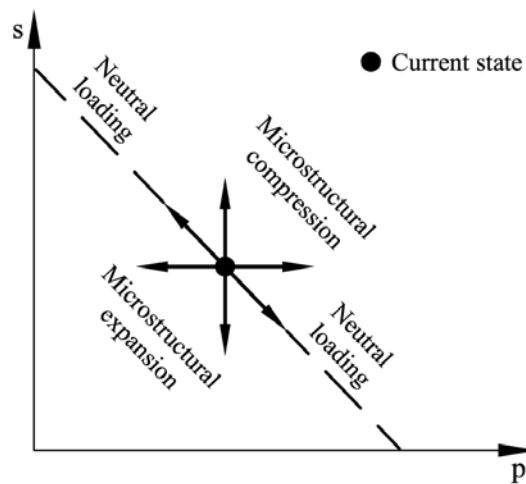


Figure 1: Neutral line and load directions in the microstructural model.

2.3 Interaction between microstructural and macrostructural levels

Based on experimental evidence, it is assumed that the macrostructure is affected by microstructural deformations generally in an irreversible way [4]. A hypothesis of the model is that the plastic deformations of the macrostructure (ε_{vM}^p) induced by microstructural effects are proportional to the microstructural strains (ε_{vm}) according to interaction functions f [2].

The total plastic macrostructural strains (i.e. the sum of the plastic strains induced by the yielding of the macrostructure, $\dot{\varepsilon}_{rLC}^p$, plus that induced by the microstructure, $\dot{\varepsilon}_{rM \rightarrow m}^p$) are evaluated using:

$$\dot{\varepsilon}_{rM}^p = \dot{\varepsilon}_{rLC}^p + \dot{\varepsilon}_{rM \rightarrow m}^p = \dot{\varepsilon}_{rLC}^p + f \dot{\varepsilon}_{r_m}^p \quad (5)$$

Two interaction functions f are defined: f_c for MC paths and f_s for MS paths. The interaction functions depend on the ratio p/p_o (Fig. 2). The ratio p/p_o is a measure of the degree of openness of the macrostructure relative to the applied stress state. When this ratio is low, it implies a dense packing of the material and it is expected that, under this condition (dense macrostructure), the microstructural swelling (MS path) affects strongly the global arrangements of clay aggregates, inducing large macrostructural plastic strains. In this case the microstructure effects induce a more open macrostructure, which implies a macrostructural softening. On the other hand, when the microstructure contracts (MC path) the induced macrostructural plastic strains are larger with open macrostructures, that is, for values of p/p_o close to 1. Under this path the clay tends towards a more dense state, which implies a hardening of the macrostructure. The result of the coupling between macro and micro levels is reflected in the value of p_o^* , the hardening variable of the macrostructure. In this way the effect of microstructural processes on the global arrangements of aggregates is taken into account.

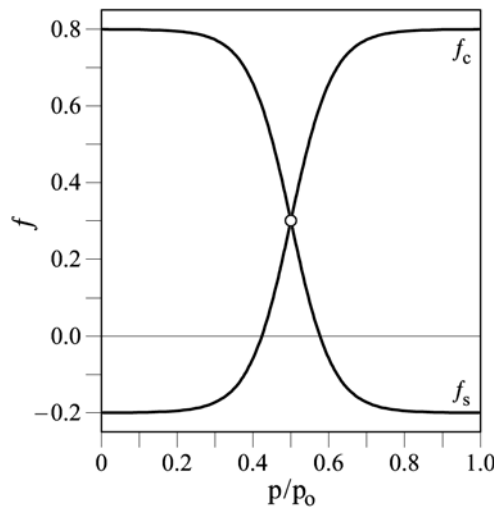


Figure 2: Interaction functions

To fully describe the soil behaviour, the definition of specific elasto-plastic laws for each domain is required according to the microstructural stress path followed (MC or MS). Generalized plasticity theory can deal with such conditions, allowing the consideration of two directions of different behaviour and the formulation of proper elasto-plastic laws for each region. Thus, a complete description of a generalized model includes the definition of the: i) loading and unloading direction, ii) plastic flow direction, and iii) a plastic modulus. Equivalent to loading/unloading directions in conventional stress/strain formulations, two

vectors may be defined at every point of the stress space. One vector indicates the *MC* direction and the other the *MS* direction. Given a generalized stress state and stress increment, the criterion to identify the microstructural stress path is illustrated in Figure 1.

2.4 Stress-strain relations

The constitutive model described contains two plastic mechanisms: i) a plastic mechanism associated with the yield of the macrostructure defined by a classical plasticity law, and ii) a plastic mechanism associated with the interaction between microstructure and macrostructure described by a generalized plasticity approach.

In classical plasticity theory, it is assumed that the material behaves either as an elastic or an elasto-plastic solid. The yield surface defines the transition from elasticity to plasticity, stress states inside the yield surface are considered as elastic ($F < 0$). In generalized plasticity theory, the state of the material is determined directly from the control variables: generalized stresses, strains and a finite number of internal variables. A process of loading is defined as elastic if the set of internal variables remains unchanged.

In the case of a purely (nonlinear) elastic loading, the stress increment is related to the increment of strains and suction by the following relationship:

$$\dot{\boldsymbol{\sigma}} = \mathbf{D}_e \cdot \dot{\boldsymbol{\varepsilon}}^e + \boldsymbol{\alpha}_s \dot{s} \quad (6)$$

where \mathbf{D}_e is the global elastic matrix that considers the elastic component of both structural levels. $\boldsymbol{\alpha}_s$ is the elastic vector associated to suction.

When a loading process is inelastic, the material behaviour is described by the elasto-plastic mechanisms that are activated during the loading process. A multidissipative approach [5] has been adopted to derive the general elasto-plastic relations that can be expressed as follows:

$$\dot{\boldsymbol{\sigma}} = \mathbf{D}_{ep} \cdot \dot{\boldsymbol{\varepsilon}} + \boldsymbol{\gamma}_s \dot{s} \quad (7)$$

where \mathbf{D}_{ep} is the global elasto-plastic matrix and $\boldsymbol{\gamma}_s$ is the elasto-plastic vector associated with suction. The expressions for the vectors and matrices in (6) and (7) together with the details of numerical implementation are presented in [6].

3 HYDROMECHANICAL FORMULATION

The overall media is assumed to consist of two overlapping but distinct continua. In the following, subscript *M* will stand for the macrostructure and subscript *m* for the microstructure. Accordingly, macroporosity and microporosity are denoted as ϕ_M and ϕ_m respectively. Macroporosity and microporosity are defined as the volume of macropores and micropores, respectively, divided by the total volume of the soil. Thus, total porosity ϕ equals $\phi_M + \phi_m$. The degree of saturation of the macroporosity, S_{wM} , is the volume of macropores occupied by water over the volume of the macropores; an equivalent definition holds for the microporosity degree of saturation, S_{wm} .

An important feature of the formulation is that hydraulic equilibrium between the two continua is not assumed, i.e. at each point of the domain the water potentials in the two continua may be different leading to an exchange of water between them. For simplicity, a linear relationship is assumed (e.g. [7]) where water exchange is described by:

$$\Gamma^w = \gamma(\psi_M - \psi_m) \quad (8)$$

where Γ^w is the water exchange term, γ is a parameter (often called the leakage parameter) and ψ is the total water potential. It is assumed that only matric and gravitational potential contribute to the total potential of the macrostructure but an additional osmotic component may also contribute to the microstructural potential [8]. Here, potential is defined in pressure units. As the water exchange is local in space, the gravitational potential will be the same for the two media. Water exchange will therefore be driven by suction differences alone.

Using the concept of material derivative, the balance equation for the solid phase can be written, for the case of a single porosity medium, as:

$$\frac{D\phi}{Dt} = \frac{(1-\phi)}{\rho_s} \frac{D\rho_s}{Dt} + (1-\phi)\dot{\epsilon}_v \quad (9)$$

where $D(\cdot)/Dt$ denotes material derivative, ρ_s is the solid density, $\dot{\epsilon}_v$ is the volumetric strain increment and t is time. For the case of double porosity equation (9) becomes:

$$\frac{D\phi}{Dt} = \frac{D\phi_M}{Dt} + \frac{D\phi_m}{Dt} = \frac{(1-\phi)}{\rho_s} \frac{D\rho_s}{Dt} + (1-\phi_M - \phi_m)(\dot{\epsilon}_{vM} + \dot{\epsilon}_{vm}) \quad (10)$$

where it has been assumed that the total volumetric deformation is the sum of the volumetric deformations of each medium.

3.1 Balance equations

The water mass balance equation for the case of two overlapping flow media is:

$$\frac{\partial}{\partial t}(\rho_w S_{wj} \phi_j) + \nabla \cdot (\mathbf{j}_{wj}) \pm \Gamma^w = f_j^w \quad ; \quad j = M, m \quad (11)$$

where S_{wj} is the liquid saturation of medium j , \mathbf{j}_{wj} is the total mass fluxes of water in the liquid phase and f_j^w is the external mass supply of water per unit volume in medium j . The possible presence of dissolved air in the liquid phase is neglected for simplicity.

Finally, it is assumed that total stresses for the overall medium affect equally the macro and the microstructure. The equilibrium equation is:

$$\nabla \cdot \boldsymbol{\sigma} + \mathbf{b} = \mathbf{0} \quad (12)$$

where $\boldsymbol{\sigma}$ is the total stress tensor and \mathbf{b} is the vector of body forces. In contrast, the total deformation of the medium is obtained from the sum of the deformations of each domain.

3.2 Hydraulic relationships

Liquid flow is governed by Darcy's law:

$$\mathbf{q}_{wj} = -\mathbf{K}_{wj} (\nabla \psi_j) = -\mathbf{K}_{wj} (\nabla p_{wj} - \nabla \rho_{wj} \mathbf{g}) \quad ; \quad j = M, m \quad (13)$$

where \mathbf{q} is the mass liquid flow (with respect to the solid phase), \mathbf{K}_l is the liquid permeability tensor, p_l is the liquid pressure, ρ_l is the liquid density and \mathbf{g} is the gravity vector. The permeability tensor is expressed as

$$\mathbf{K}_{wj} = \mathbf{k}_j \frac{k_{rj}}{\mu_j} \quad ; \quad j = M, m \quad (14)$$

where \mathbf{k} is the intrinsic permeability and k_r is the relative permeability that expresses the effect of degree of saturation (or suction) on global permeability. Intrinsic permeability

depends on many factors such as pore size distribution, pore shape, tortuosity and porosity. Here a dependence of intrinsic permeability on porosity is adopted:

$$\mathbf{k}_j = k_o \exp\left(b(\phi_j - \phi_o)\right) ; j = M, m \quad (15)$$

where ϕ_o is a reference permeability for which the intrinsic permeability is k_o . Relative permeability and retention curves are also defined for the two porosity levels using standard relationships. .

4 APPLICATION

The double-structure constitutive law and hydromechanical formulation is applied to the modelling of the behaviour of a mixture of 50% bentonite powder and 50% bentonite pellets, by dry weight, during hydration as observed in a number of laboratory swelling pressure tests [9]. FoCa clay, a calcium bentonite from the Paris Basin has been selected for the study. The major component of the clay fraction is an interstratified clay mineral of 50% calcium beidellite and 50% kaolinite. Pellets are manufactured by dynamic compaction of the powder between two rotating wheels. The dimensions of the pellets are 25 x 25 x 15 mm and their average dry density is 1.89g/cm³. Compaction water content lies in the range of 4% to 5%.

In particular, three tests performed on samples with a dry density of 1.60 g/cm³ (RS2B, RS2E and RS2F) are considered. Their lengths are 5, 10 and 12 cm respectively. Computed evolutions of swelling pressures compared with the measured values are shown in Figures 3a, 3b and 3c. Testing times ranged from 150 to 500 days depending on specimen length. The model reproduces very satisfactorily the observed behaviour. The evolution of water intake is also well matched (Figures 3d, 3e and 3f), some discrepancies at the end of the test have been attributed to small leakages in some of the very long term tests.

The evolutions of macrostructural and microstructural suctions at three different points (bottom, middle and top of the specimen) of test RS2E obtained in the analysis are plotted in Figure 4. It can be observed that, at the bottom boundary, the macrostructural and microstructural suctions reduce rapidly but they differ at the beginning of the test because of the delay in water transfer between the two porosities. Eventually, however, they come together and remain in equilibrium for the remainder of the test. Interestingly, at the other two points the two porosities come into equilibrium before they are reached by the hydration front, i.e. before they exhibit any suction reduction. They also maintain this equilibrium condition throughout the rest of the test. The analysis suggests, therefore, that non-equilibrium between the two porosity levels is only likely to affect the early stages of the test.

The cause underlying the characteristic temporary drop in swelling pressure is the collapse of the macrostructure that, in the constitutive model, corresponds to reaching the LC yield surface in the BBM. This is illustrated in Figure 5, where the stress paths (in macrostructural suction – vertical net stress space) followed by the same three points of test RS2E are plotted. The initial position of the LC yield surface is also shown. In the section of the stress path that moves towards the LC surface, stress increase appears to be more significant than suction reduction. Once the LC yield surface is reached, the vertical stress drops to compensate the tendency of the macrostructure to collapse so that the sample length is kept constant. It can also be noted that the point of start of the collapse does not coincide exactly with the plotted LC; this is because, by then, the yield surface has moved slightly due to the interaction with

the microstructural strains (MS, microstructure swelling) that develop from the very start of the test.

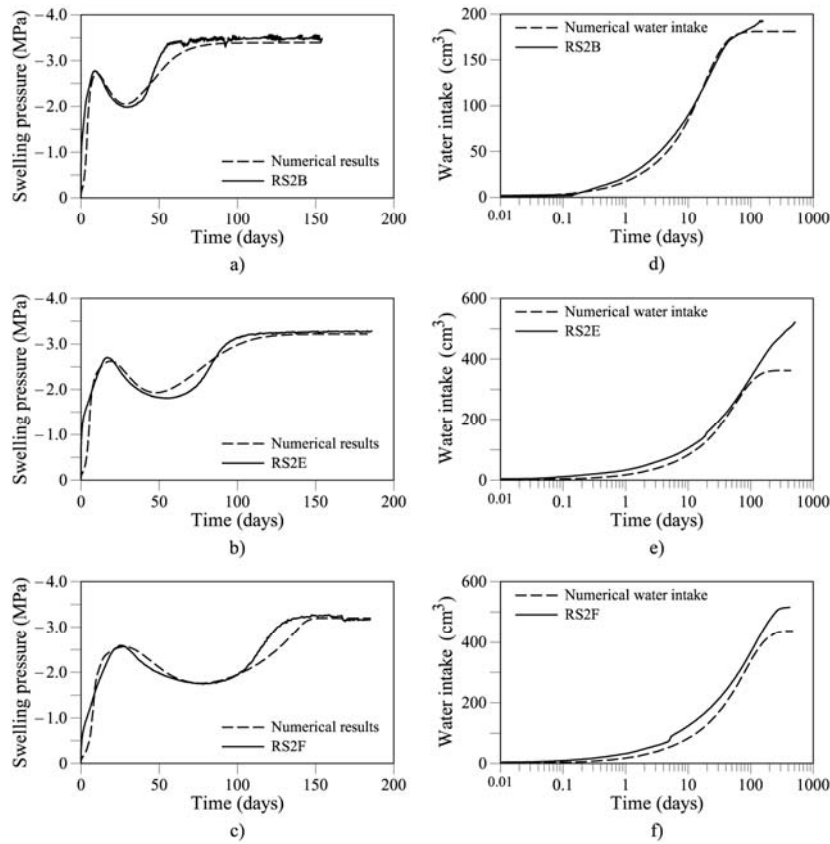


Figure 3: Observations vs. computed results for tests on samples of 1.60 g/cm^3 dry density. a), b) and c) Swelling pressure evolution for tests RS2B, RS2E and RS2F. d), e) and f) Evolution of accumulated water intake for tests RS2B, RS2E and RS2F.

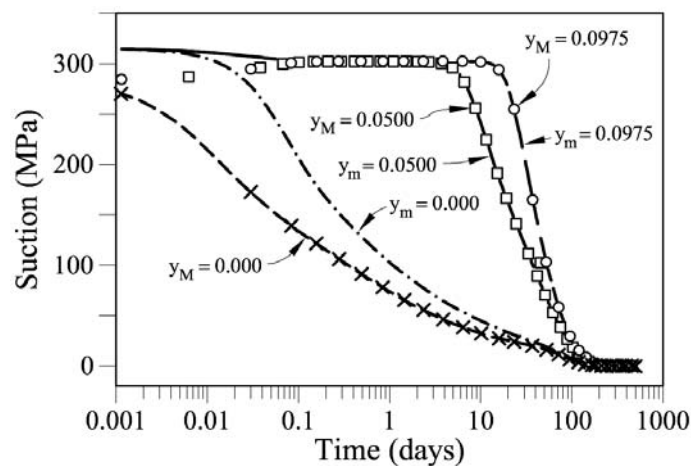


Figure 4: Computed evolution of macrostructural and microstructural suctions at three different points of test RS2E.

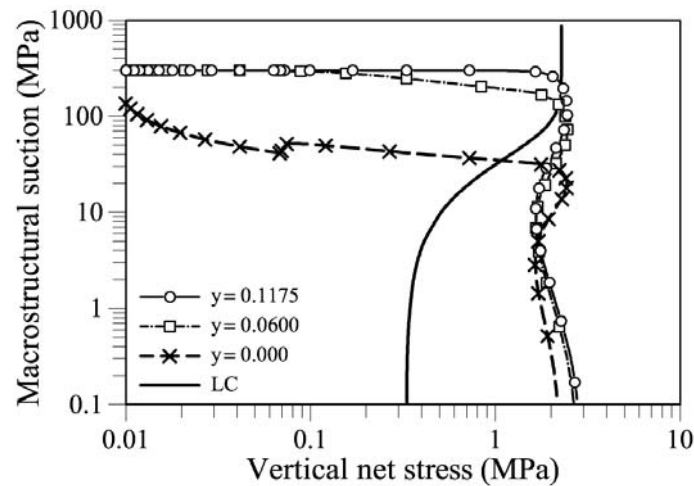


Figure 5: Computed stress path (macrostructural suction – vertical stress) for three different points of sample RS2E.

5 CONCLUSIONS

A double-porosity numerical formulation and a constitutive model have been developed to deal with the coupled hydromechanical behaviour of swelling clays exhibiting two levels of structure. The formulation is especially appropriate to reproduce the behaviour of mixtures of bentonite pellets and powder; a material that is receiving much attention as a potential component of sealing systems. It has been shown that the formulation results in a close quantitative reproduction of a number of swelling pressure tests performed on samples of different lengths. In addition, a detailed examination of the computational results provides valuable insights and understanding of the basic processes that underlie the observed macroscopic behaviour. The formulation is thus validated for use in analysis of field problems [10]

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