

An Elasto-Plastic Framework for the Chemo-Mechanical Behavior of Low to Medium Activity Clays

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Abstract. Pore fluid composition strongly influences the mechanical behavior of clays, impacting both on their volumetric and shear response. Accounting for this aspect is crucial for engineering applications where changes of the chemical composition of the pore fluid are anticipated, such as transport through engineered barriers for the containment of pollutants, or slope stability of natural formations rich of clay minerals subjected to freshwater infiltration. In this work, a chemo-mechanical model capable of reproducing the response of medium to low activity clays under both mechanical and chemical loading paths is presented. The model is developed starting from the interpretation of experimental evidences in an elastic-plastic framework. Chemo-mechanical coupling is introduced both in terms of stress variables and hardening law. In particular, the formulation is specialized to variations of salt concentration, introducing osmotic suction as a chemical stress variable. The model was implemented in a constitutive driver for the integration at the REV level of the incremental constitutive equations, thus allowing for its validation against literature data.

Keywords: Clay \cdot Elasto-plasticity \cdot Pore fluid chemistry \cdot Compression curve \cdot Osmotic suction

1 Introduction

Changes in the chemical composition and concentration of the pore fluid of saturated soils occur in many natural and engineering contexts, i.e. due to infiltration and evaporation processes or because of the underground transport of miscible or immiscible contaminants. Although irrelevant for most soils, pore fluid chemistry changes can have a significant impact on the hydro-mechanical behaviour of clays, as it is also for water content changes (e.g. Di Maio 1996; Musso et al. 2008; Gens 2010; Della Vecchia et al. 2015). This effect is related to the electro-chemical interaction forces acting at the particle level between the liquid and the solid phases, and thus linked with clay mineralogy. For clays, both transport properties and mechanical response are affected. For instance, active clays behave as semi-permeable membranes (e.g. Mitchell and Soga 2005), whose efficiency is concentration dependent (e.g. Della Vecchia

and Musso 2016). From the mechanical point of view, changes in pore fluid chemistry may induce relevant volumetric strains and changes in clay stiffness.

The chemo-mechanical behaviour of clays at the macroscopic level has been generally reproduced in the framework of hardening elasto-plasticity, as in Hueckel (1997), Loret et al. (2002), Guimaraes et al. (2013), Witteveen et al. (2013), Yan (2018). However, most of the models have been formulated for high activity clays, sharing the assumption of preconsolidation stress decrease for increasing concentration of chemical species in the pore fluid. This work aims at defining an elasto-plastic framework for low to medium activity clays, such as illites, kaolinites or natural mixed clayey soils found in many sites. A versatile mathematical function is used to define preconsolidation stress evolution with osmotic suction, thus allowing evaluating the effects of both its increase and its decrease with pore fluid concentration.

2 Chemo-Mechanical Model

The framework is formulated in the context of the theory of elasto-plasticity with generalized hardening (e.g., Tamagnini and Ciantia 2016), adopting as static variables the Terzaghi effective stress tensor σ' and the osmotic suction π , which depends on the composition and ionic concentration of the pore fluid. For compounds with low molar concentrations *c*, the van't Hoff equation holds:

$$\pi = icRT \tag{1}$$

where *i* is the number of dissolved species (e.g. 2 for NaCl and 3 for CaCl₂), *R* is the universal gas constant (8.31 J mol⁻¹ K⁻¹) and *T* is the absolute temperature.

Under the small strain assumption, the total strain increment $\dot{\varepsilon}$ is additively decomposed into an elastic, $\dot{\varepsilon}^e$, and a plastic, $\dot{\varepsilon}^p$, contribution. The elastic strain increment is in turn expressed as a sum of two contributions, one induced by mechanical loading and the other induced by osmotic suction changes. Consistently with microstructural evidences (e.g. Musso et al. 2013), an increase in π is assumed to cause compressive (positive) volume changes. In axi-symmetric conditions, the volumetric and deviatoric elastic strain increments are thus evaluated as:

$$\dot{\varepsilon}^{e}_{vol,mec} + \dot{\varepsilon}^{e}_{vol,ch} = \frac{\kappa}{\nu_0} \frac{\dot{p}'}{p'} + \frac{\kappa_\pi}{\nu_0} \frac{\dot{\pi}}{\pi + p_{atm}},\tag{2}$$

$$\dot{\varepsilon}^{e}_{dev,mec} = \frac{1}{3G}\dot{q} \tag{3}$$

where p' is the effective mean pressure, q the deviator stress, κ the mechanical elastic logarithmic compressibility, v_0 the initial specific volume, κ_{π} the chemical compressibility and G the elastic shear modulus. Null deviatoric elastic strains induced by chemical solicitations are assumed.

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The yield surface expression (f = 0) stems from the Modified Cam Clay Model, introducing the dependence of the internal variable p'_c (i.e. the preconsolidation pressure) on osmotic suction:

$$f(q, p', p_c') = \frac{q^2}{M^2} + p'(p' - p_c') = 0$$
(4)

with

$$p_c' = p_0' \mathbf{X}(\pi) = p_0' \left[1 - \gamma_\pi \ln \left(1 + \frac{\pi}{\pi_{ref}} \right)^\beta \right]$$
(5)

where *M* is the slope of the critical state line in p' - q plane and p'_0 is the preconsolidation pressure at null osmotic suction. The function $X(\pi)$, describing the evolution of the preconsolidation pressure p'_c with osmotic suction, is set to depend on two material parameters, namely γ_{π} and β . The increase or decrease of preconsolidation pressure with osmotic suction is ruled by the sign of parameter γ_{π} , as shown in Fig. 1 for $\beta = 2.3$. With increasing osmotic suction, the yield surface size reduces for positive values of γ_{π} , whereas its size increases for negative values of γ_{π} .

The hardening law reads:

$$\dot{\varepsilon}_{vol}^{pl} = \frac{\lambda - \kappa \dot{p}_0}{v_0 p_0'},\tag{6}$$

where λ is the elastic-plastic mechanical compressibility. Associativity of the flow rule is finally assumed. The hardening law thus states that any change of p'_0 is associated to the development of plastic volumetric strains, that can be induced by both mechanical



Fig. 1. Normalized evolution of preconsolidation stress varying the parameter γ_{π}

and chemical solicitations. The curve $p'_c(\pi)$ thus plays the role of the Loading Collapse (LC) curve of the BBM model (Alonso et al. 1990).

3 The Role of Yield Surface Evolution with Osmotic Suction

In order to investigate the role of the yield surface evolution with osmotic suction, the model was preliminary used to simulate the behaviour of two ideal materials (Material A and Material B) along two different loading paths (LPI and LPII). The two materials have the same parameters, except for γ_{π} , which is negative for Material A and positive for Material B (Table 1). The preconsolidation pressure in distilled water condition p'_0 has been set equal to 10 kPa

Material κ (-) λ (-)G(MPa)M (-) κ_{π} (-) γ_{π} (-)A0.0060.058670.980.0016-0.002

67

0.98

0.0016 +0.002

0.006 0.058

В

LPI is sketched in Fig. 2a and 3a (continuous line). The first stage (AB) consists in an isotropic compression with distilled water as saturating fluid from $p'_A = 1$ kPa to $p'_B = 50$ kPa. The response in the compression plane is elastic up to $p'_0 = 10$ kPa and then elasto-plastic (Fig. 2b and Fig. 3b). An increase in osmotic suction (BC) from $\pi = 0$ kPa to $\pi = 13800$ kPa is then imposed at constant $p'_B = p'_C = 50$ kPa, followed by a further isotropic compression (CD) at constant osmotic suction up to $p'_D = 1050$ kPa. The dotted line in Fig. 2a shows the values of p'_c corresponding to the osmotic suction increase for Material A. The yield surface size increases with osmotic suction, i.e. $p'_c > p'_0$ for any π , and thus the constant p' salinization path BC is purely elastic (i.e. the preconsolidation stress at null salinity p'_0 is not changing). Consistently, the mechanical response along the initial stages of the following mechanical compression path CD is elastic. Plastic strains start to develop just when $p' = p'_c$ again.

The dotted line in Fig. 3a shows the evolution of p'_{c} during the osmotic suction increase path BC for Material B. In this case, the yield surface size is supposed to shrink with osmotic suction, i.e. $p'_{c} < p'_{0}$ for any π . However, upon salinization the consistency condition forces the stress state to lay on the yield surface, and thus p'_{c} coincides with p'. This causes an increase of p'_{0} in light of Eq. (5), and thus, according to Eq. (6) the development of plastic strains upon salinization. Consistently, the response is elasto-plastic from the beginning during the following mechanical compression CD (Fig. 3b).

Loading path LPII is sketched in Fig. 4a. Samples are prepared with a saline solution and the initial osmotic suction is different from zero ($\pi_A = 13627$ kPa, which according to Eq. 1 corresponds to a NaCl molar concentration c = 3 mol/l). They are then mechanically compressed up to $p_B' = 50$ kPa (path AB): the response is firstly



Fig. 2. (a) Loading path LPI and preconsolidation pressure p'_c evolution with osmotic suction for Material A (b) Predicted volumetric response.



Fig. 3. (a) Loading path LPI and preconsolidation pressure p'_c evolution with osmotic suction for Material B (b) Predicted volumetric response.

elastic and then elasto-plastic. The osmotic suction is then decreased up to 0 kPa (path BC) at constant stress ($p'_B = p'_C = 50$ kPa). Finally, a further mechanical compression is imposed (path CD). When the yield surface is assumed to increase with osmotic suction (Material A, Fig. 4b), the net effect of the desalinization path BC (i.e. a decrease in π) is a plastic collapse and the internal variable variation coincides with the evolution of p' (Fig. 4a). Accordingly, the following mechanical loading (CD) is elasto-plastic from the beginning. When the yield surface is assumed to decrease with osmotic suction (Material B, Fig. 5b), a desalinization (decrease in π) only causes elastic strains: consequently, the material swells in the compression plane and the volume increases. The following mechanical loading predicts initially an elastic response until the yield surface is met again.



Fig. 4. (a) Loading path LPII and preconsolidation pressure p'_c evolution with osmotic suction for Material A (b) Predicted volumetric response.



Fig. 5. (a) Loading path LPII and preconsolidation pressure p'_c evolution with osmotic suction for Material B (b) Predicted volumetric response.

4 Comparison with Experimental Data

The capabilities of the model are evaluated against the experimental results obtained by Witteveen et al. (2013) for compacted samples of an illitic clay. A loading history very similar to Loading path LPI was applied, with the only difference that mechanical path occurred under oedometric, and not isotropic, conditions. Model parameters, reported in Table 2, and the initial value of the preconsolidation pressure p'_0 (set equal to 45 kPa) were calibrated to provide the best fit to test results. Model predictions agree very well with the experiments data (Fig. 6) if a negative value of γ_{π} is imposed. The reproduction of the experimental results is remarkably good even with a limited number of material parameters and without introducing any dependence of these parameters on the concentration of the pore fluid.



Fig. 6. Simulation of two experimental tests presented in Witteveen et al. 2013

Table 2. Model parameters used in the simulation of the oedometer test on an illitic clay from Witteveen et al. (2013)

κ	λ	G	М	κ_{π}	γ_{π}	β
0.006	0.058	67	0.98	0.0016	-0.002	2.3

5 Conclusions

A simple framework to reproduce the chemo-mechanical response of medium to low activity clays subject to changes in pore fluid chemical composition has been presented. The constitutive model has been validated against experimental data reported in the literature. A limited number of parameters is sufficient to model the chemo-mechanical response of these materials, due to the limited effect of chemical solicitations on material microstructure. The model appears to provide realistic results if it is assumed that the yield surface size is larger for larger pore fluid concentration.

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