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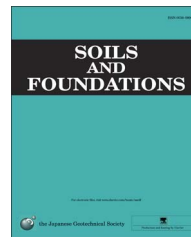


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# Some remarks on single- and double-porosity modeling of coupled chemo-hydro-mechanical processes in clays

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## Abstract

Active clays are known to possess an aggregated structure, which justifies the use of double-porosity models to reproduce their behavior. Simulation of chemo-mechanical processes requires instead the introduction of a relevant number of coupled mechanical and transport laws. It follows that double porosity models for coupled chemo-hydro-mechanical require a relevant number of parameters, which are twice those needed by single porosity models. The aim of this work is to evaluate the consequences of using single- and double-porosity frameworks to simulate the transient chemo-mechanical processes in active clays, showing how models based on simple microstructural considerations can help in performing simulations which are a reasonable trade-off between simplicity and accuracy. In particular with single porosity models, it might be necessary introducing parameters having a doubtful meaning to describe adsorption–desorption processes. This type of assumption is not required by double porosity models. While for compacted clays these conclusions are corroborated with microstructural observations, the same hold also when reproducing the behavior of an active clay at a remolded condition. In this latter case the delay of swelling with respect to desalinization, typical of remolded conditions, was satisfactorily reproduced only with double porosity models.

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**Keywords:** Bentonites; Active clays; Coupled processes; Double-porosity models; Single-porosity models; Ionic diffusion

## 1. Introduction

The mineralogy of active clays is characterized by an electrical imbalance which causes, together with the high specific surface, a chemistry-dependent behavior, since forces exchanged at the particle scale are influenced by electro-chemical interactions. Significant macroscopic effects descend; both volume changes and shear strength depend on the chemical composition of the pore fluid (dielectric constant,

electrolyte type and electrolyte concentration). As for conduction processes, active clays behave as semi-permeable membranes, allowing the onset of an osmotic flow (i.e., the flow of water under salt concentration gradients) which is typically not relevant in other types of porous materials. Moreover, the phenomenological response of active clays depends not only on the composition of the constituents, but also on the fabric, which in turn may change with the chemistry of the pore fluid (e.g., Hueckel et al., 1997). In several engineering applications where active clays are of concern, such impermeable barriers for waste disposal or shale formations sustained with different muds during drilling, transport and mechanical processes are coupled. As a consequence of chemically induced fabric changes, both volume and conduction properties evolve during

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the transient processes, increasing the complexity of the phenomena and the challenges for engineers.

Different levels of complexities have to be faced, for which justified rational assumptions must be put forward. The first level of complexity concerns the choice of a suitable approach to reproduce the response of the porous medium, i.e., whether adopting a standard equivalent continuum approach would be sufficiently accurate or, if introducing different scales (e.g., through double porosity, double permeability or fractured models) would be relevant. The second level of complexity is related to the number of couplings required to adequately reproduce the investigated processes: coupled fluxes and mutual influence between mechanical and transport processes could be introduced, with the definition of appropriate constitutive laws. The third level of complexity is related to the calibration of the parameters of the adopted model: a relevant number of parameters is normally required and it is not always possible to evaluate all of them through direct measurements.

A standard continuum approach assumes that a single scale is sufficient for reproducing the chemo-hydro-mechanical behavior of the material and thus, just a single set of state variables is introduced. The evaluation of model parameters in this case is solely based on external observations at the macroscopic scale, i.e., the scale of the standard laboratory specimens. In the following, models based on this assumption will be called 'single-porosity models'. 'Double-porosity models' assume instead that two scales are relevant. The existence of two scales implies effects on both the hydraulic-transport processes (since mass can be exchanged between the two structural levels) and the mechanical behavior (since the overall observed deformation depends on the mechanical behavior at the two scales and on the interaction between them). Double-porosity models require the definition of two sets of state variables, and thus a higher number of parameters, which can be obtained either through a back analysis of the experimental tests or a direct investigation of the micro-fabric of the material.

The aim of this note is to evaluate the consequences of using single- and double-porosity frameworks to simulate the transient chemo-mechanical processes in active clays, showing how models based on simple microstructural considerations can help in performing simulations which are a reasonable trade-off between simplicity and accuracy.

## 2. Physical processes related to concentration changes and concentration gradients in active clays

Clay particles, due to their small size, crystal structure and platy shape, have very large specific surfaces and are especially influenced by unbalanced force fields at the interface between soil and water. These fields cause interactions between small soil particles, water and dissolved ions, with a significant effect on the hydro-mechanical response of the material (Mitchell and Soga, 2005). For instance, both changes in the chemical concentration of the pore fluid and cation exchange phenomena can induce volumetric strains.

Around a charged colloidal clay particle suspended in a water solution, a double layer develops. Within the double

layer, the concentration of counterions (ions having an electrical charge whose sign is opposite to that of suspended solids) is greater than that of the co-ions (ions having an electrical charge whose sign is the same as that of suspended solids). Within the double layer, the electrical potential is also different from zero. According to the Gouy–Chapman theory, the electrical potential exponentially decreases with the distance from the charged particle. The distance at which the electrical potential is equal to 1/2.718 of the value at the solid-to-liquid interface is called the 'thickness' of the double layer,  $\vartheta$ :

$$\vartheta = \sqrt{\frac{\varepsilon_0 \kappa' RT}{2F^2 c_0 z^2}} \quad (1)$$

where  $\varepsilon_0$  is the permittivity of the free space ( $8.85 \times 10^{-12}$  F/m),  $\kappa'$  is the real relative permittivity of the fluid,  $F$  is Faraday's constant ( $9.6485 \times 10^4$  C/mol),  $R$  is the universal gas constant ( $R=8.314$  J mol $^{-1}$  K $^{-1}$ ),  $T$  is temperature (K),  $c_0$  is the bulk electrolyte concentration (mol/L) and  $z$  is the valence of the ionic species in the solution, supposed to be the same for cations and anions.

The overlapping of double layers causes electrostatic repulsion. The repulsion force  $R_{DL}$  between two platy particles is

$$R_{DL} = 64RTc_0 e^{-\frac{x}{\vartheta}} \quad (2)$$

where  $x$  is the distance between the particles. The same particles are attracted one to the other by the van der Waals attraction force,  $Att$ , as follows:

$$Att = -\frac{A_h}{6\pi x^3} \quad (3)$$

where  $A_h$  is the Hamaker constant, which depends on the compositions of the mineral specie and of the wetting fluid.

According to the DLVO theory (e.g., van Olphen, 1977), the net force exchanged by two parallel platy particles is given by the sum of  $R_{DL}$  and  $Att$  (e.g., Santamarina et al., 2001). The equilibrium between repulsive and attractive forces determines the distance between particles suspended in a fluid having a given dielectric constant and electrolyte concentration. Increasing values of bulk electrolyte concentration lead to smaller values of  $\vartheta$ ; thus,  $R_{DL}$  decreases and so does the distance between particles at equilibrium, and vice versa.

Although the fabric of real soils (both remolded and structured) is very different from that of colloidal suspensions, electrostatic repulsion and van der Waals attraction forces have been combined with total stress and water pressure in a number of formulations to provide a definition of effective stress that is different from that of Terzaghi (e.g., Bolt, 1956; Lambe, 1960). Bolt (1956) and others after him also tried to reproduce the macroscopic volumetric behavior of active monomineral soils exposed to stress and concentration changes starting from the DLVO theory. These models assume that the pores within a saturated soil mass under a given combination of total stress, water pressure and salt concentration have a uniform size.

Clay mineralogy also has important effects on the transport of water mass and charged species. Close to the particle surface, within the range of influence of the electrical field

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