Computational multiphysics modeling of long-term problems in geotechnical engineering

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ABSTRACT

Multiphysical coupling – the interactions among different physical phenomena such as solid deformation, fluid flow, and chemical reactions – often triggers long-term problems in geotechnical engineering. Examples range from long-term settlement of clayey grounds to weathering degradation of rocks. These problems are very challenging to address, because they require the characterization and prediction of multiphysical processes in geomaterials over a very long time period. This paper describes some computational models recently developed for addressing coupled multiphysical processes in long-term problems in geotechnical engineering. Specifically, we present two models: (1) a multiscale hydro-mechanical model of fluid-induced secondary compression and (2) a chemo-hydro-mechanical model of salt weathering damage. For these models, we outline the key aspects of the formulations and briefly present representative numerical examples. The results of these examples demonstrate that the models can simulate complex multiphysical processes in long-term geotechnical problems based on physical principles.

Keywords: long-term problems, coupled multiphysics, numerical modeling, secondary compression, weathering degradation

1 INTRODUCTION

Multiphysical coupling – the interactions among different physical phenomena such as solid deformation, fluid flow, and chemical reactions – is central to many long-term problems in geotechnical engineering. Examples range from long-term settlement in clays due to the delayed drainage of pore water, to degradation of rocks due to chemical weathering.

A common and major challenge for addressing these long-term problems is that it is extremely difficult to predict multiphysical processes taking place over a very long period of time. Two major reasons are as follows. First, it is very challenging to characterize a long-term process during the entire time scale of the problem – which may be up to dozens and hundreds of years. Second, environmental conditions of the problem will continuously evolve during the problem time scale. As such, empirical approaches based on limited data in the past environment may not work well for problems in the future environment.

A promising approach to the prediction of long-term problems is to construct a computational model that can emulate physical processes in the real underground and continuously adapt to new measurement data. If such a model is available, it can be used to predict a long-term process without limitation of time scale. Furthermore, if the model is based on sound physical principles, it can remain valid even as environmental conditions change continuously.

With this motivation, we have been developing physics-based computational models for long-term problems in geotechnical engineering. In this paper, we describe two types of such computational models: (1) a multiscale hydro-mechanical model of fluid-induced secondary compression in structured geomaterials, and (2) a chemo-hydro-mechanical model of weathering damage from salt crystallization. In what follows, we outline the key aspects of the model formulations and briefly present representative numerical examples.

2 MULTISCALE HYDRO-MECHANICAL MODELING OF LONG-TERM SETTLEMENTS

Firstly, we describe a multiscale model of coupled deformation and fluid flow in structured geomaterials such as natural clay and compacted soils. Structured geomaterials have distinct internal structures due to particle aggregation, fissures, and others. These internal structures give rise to the co-existence of two distinct pore systems at different scales, which are often referred to as macropores and micropores. For aggregated soils, the macropores correspond to inter-aggregate pores, and the micropores correspond to intra-aggregate pores.

The macropore and micropore systems exhibit highly contrasting fluid flow and deformation responses. As for fluid flow, the macropores serve as primary pathways for preferential flow due to their far larger pore sizes, while the micropores provide the majority of the fluid storage space. As for solid deformation, the macropore structure is much more compressible than the micropore structure. Also, the macropore deformation is totally irreversible whereas the micropore deformation includes recoverable elastic deformation (Koliji et al. 2010).

Thus, one should distinguish between the macropores and micropores to accurately model hydro-mechanical processes in structured geomaterials. In subsurface hydrology and petroleum reservoir engineering, a widely used approach for this purpose is the double-porosity modeling, which views that the two pore systems are overlapped and interacting within the overall medium. Fig. 1 schematically shows a double-porosity medium in the context of aggregated soils.

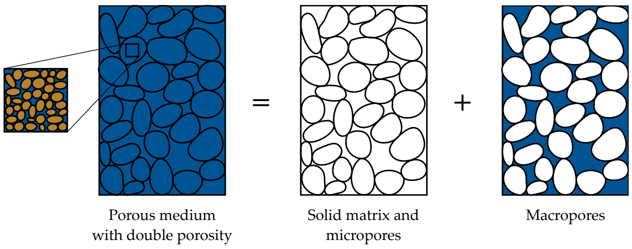

Fig. 1. Schematic illustration of a double-porosity medium. From from Choo (2016).

2.1 Model description

Building on the concept of double porosity, we have developed a novel constitutive framework for coupled hydro-mechanical modeling of structured soils (Borja and Choo 2016; Choo 2016). For the first time, it can simulate separate deformations in the macropores and micropores without any assumption of linear kinematics. In a nutshell, it decomposes the effective stress into the macro- and micro-effective stresses as follows:

$$\boldsymbol{\sigma}' = \psi^M(\boldsymbol{\sigma} - p_M\mathbf{1}) + \psi^m(\boldsymbol{\sigma} - p_m\mathbf{1}) = \psi^M\boldsymbol{\sigma}'_M + \psi^m\boldsymbol{\sigma}'_m \quad (1)$$

Here, $\boldsymbol{\sigma}$ and $\boldsymbol{\sigma}'$ are the total and effective stress tensors, respectively, p is the pore water pressure, ψ is the volume fraction of the macro/micro-pore system with respect to the total pore volume. The indices M and m denote quantities pertaining to the macropores and the micropores, respectively.

The upshot of the stress decomposition approach in Eq. (1) is it enables us to assign separate compressibility laws for the macropores and the micropores. Notably, this modification only adds two more parameters to the standard Cam Clay model: the plastic compressibility and the initial void ratio of the macro (or micro) pores. The two parameters can be obtained by carrying out standard oedometer tests on the soil of interest at its structured and reconstituted states. It is noted that performing two tests on structured and reconstituted states is commonly required by other constitutive models for structured geomaterials. As such, the new model does not require any new parameter or laboratory test than existing models for structured geomaterials.

2.2 Representative numerical examples

For this model, we present two examples: a stress-point simulation of drained triaxial compression tests, and an initial boundary value problem simulation of 1D consolidation. The former is intended to validate the constitutive framework, and the latter is to demonstrate the capability of the modeling framework for capturing long-term settlement (secondary compression) due to the delayed drainage of fluids in the micropores.

The first example considers the triaxial test results of Anagnostopoulos et al. (1991) on the Corinth Canal marl. These experimental results are selected because they have been simulated by existing constitutive models of structured soils, e.g. Liu and Carter (2002) and Koliji et al. (2010). We calibrate the parameters from the same oedometer test results provided in the paper.

Fig. 2 presents the simulation results of the triaxial compression tests using our new constitutive model. Experimental data are plotted as open symbols. For the purpose of comparison, we also plot the simulation results of Liu and Carter (2002) obtained by their own model of structured geomaterials. The figure clearly shows our new model has superior accuracy to the model of Liu and Carter. The same conclusion was also made in comparison with the model of Koliji et al. (2010). We refer to Borja and Choo (2016) and Choo (2016) for more details about this comparison.

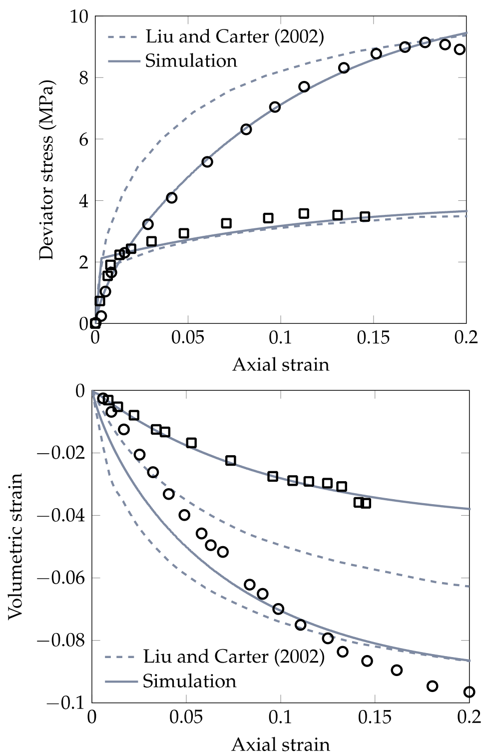

Fig. 2. Simulation results of the triaxial compression tests conducted by Anagnostopoulos et al. (1991) on the Corinth

Canal marl, using the new constitutive model. Open squares are for tests at confining pressure of 1.5 MPa, and open circles at 4 MPa. The results are also compared with the simulation results of another model proposed by Liu and Carter (2002). From Choo (2016).

The second example simulates the 1D consolidation behavior of a structured soil with double porosity. For this initial boundary value problem simulation, we insert the above-described constitutive model into the finite-deformation version of a continuum hydro-mechanical modeling framework for double-porosity media (Choo et al. 2016). As we explicitly consider separate fluid flows in the macropores and micropores, we assign different permeability values for the two pore systems. The pore fluid can migrate between the two pore systems via a constitutive law for mass transfer. More details of the formulation and parameters are referred to Borja and Choo (2016) and Choo (2016).

Fig. 3 shows a 1D consolidation curve simulated by the multiscale hydro-mechanical model. The most important feature herein is the presence of two S-shaped curves. Such a two-stage consolidation behavior is commonly observed from many natural clays. However, the latter consolidation stage – often called secondary compression in the literature – cannot be simulated by a classical hydro-mechanical model such as Terzaghi's consolidation theory.

The two-scale hydro-mechanical model can capture the secondary compression behavior because it explicitly distinguishes the drainage processes in the macropores and micropores and the associated structural evolutions of the two pore systems. In fact, fluid-induced secondary compression has been suggested and investigated by a number of researchers (e.g. Navarro and Alonso 2001; Cosenza and Korošak 2014). However, prior to our study, no mathematical model had been able to simulate fluid-induced secondary compression in general initial boundary value problems. Our modeling framework has made it possible by advancing and combining plasticity and poromechanics. Because secondary compression followed by primary consolidation is a major process responsible for long-term ground settlement, the new hydro-mechanical model enables us to simulate long-term settlement based on physical principles.

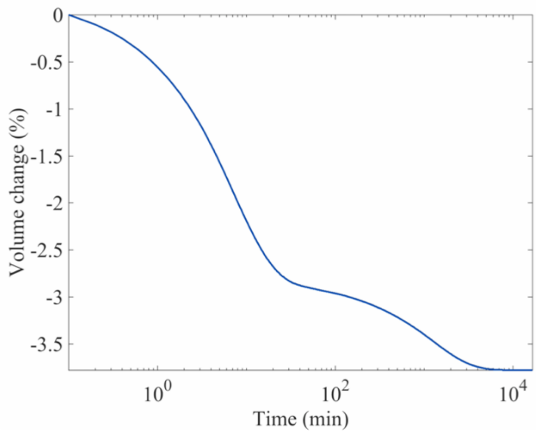

Fig. 3. A 1D consolidation curve simulated by the multiscale hydro-mechanical model. Note the secondary compression behavior, which cannot be captured by classical hydro-mechanical models (e.g. Terzaghi's 1D consolidation theory).

3 CHEMO-HYDRO-MECHANICAL MODELING OF SALT WEATHERING

The second model introduced in this paper is a chemo-hydro-mechanical model of damage in rocks from crystallization of salts in pores. This process is the central mechanism of salt weathering. Salt crystals can grow inside pores when the salinity of the pore fluid exceeds some threshold value. Growth of salt crystals then gives rise to crystallization pressure, which exerts tensile stress onto the pore wall (Scherer, 2004). As the crystallization pressure increases during crystal growth, it can in turn damage the overall material. Fig. 4 shows some examples of salt weathering caused in this way.

In the literature, a few models have been proposed for modeling this phenomenon, but they are restricted to 1D conditions. Numerical modeling of this phenomenon in multi-dimension is very challenging because it involves complicated interactions among chemical reaction, fluid flow, rock deformation, and (micro-)cracking. Moreover, cracks in salt weathering problems feature extremely complicated geometry, which adds another significant challenge for modelers.

Fig. 4. Examples of salt weathering damages in rocks. Modified from Flatt et al. (2004).

3.1 Model description

Recently, we have developed a coupled chemo-hydro-mechanical formulation for salt weathering problems based on mixture theory and continuum thermodynamics (Choo and Sun 2018b). An important contribution of our work is the derivation of a thermodynamically consistent effective stress in porous media containing growing crystals in pores. The effective stress can be written as

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma} - [(S^l + S^c)p_l + S^g p_g + S^c p_{cr}]\mathbf{1} \qquad (2)$$

where the indices l, g, and c denote the liquid, gas, and the crystal phases, respectively, S is the saturation ratio, and p_{cr} is the crystallization pressure. Observe that an increase in the crystallization pressure can lead to tensile effective stress, which can result in tensile cracking even under compressive total stress. Note that this effective stress was derived from continuum thermodynamics, rather than being assumed. We have also formulated conservation laws for the coupled processes of solid deformation, liquid and gas flows, and chemical reaction, and found the suitable forms of necessary constitutive relationships based on energy-conjugate pairs.

For modeling damage from crystallization-induced cracking, we adopt a phase-field approach to fracture, which can be regarded as a type of gradient damage model. The phase-field approach is useful because it can address complicated crack geometry without algorithm and it can also incorporate both of damage and fracture. Details of the derivation and performance of the phase-field model for geomaterials are presented in Choo and Sun (2018a,b).

3.2 Representative numerical examples

Using the new chemo-hydro-mechanical model, we simulate the salt damage in a laboratory-size specimen subjected to capillary rise from the bottom and drying in the upper part. Note that it is a typical laboratory setup for studying salt weathering. Fig. 5 shows various field variables at the moment of damage development. We see that the model can simulate the coupled chemo-hydro-mechanical processes leading to salt damage, and the shape of the damage zone agrees well with real-world observations.

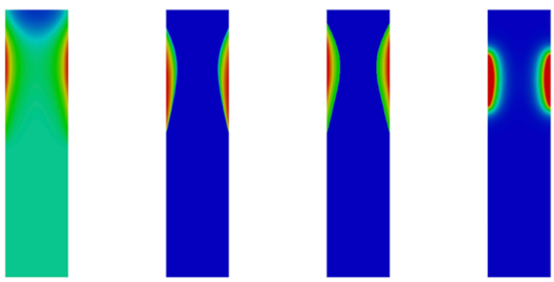

Fig. 5. Chemo-hydro-mechanical simulation of salt weathering.

4 CLOSING REMARKS

This paper has introduced two types of computational models of coupled multiphysical processes in long-term problems in geotechnical engineering. They have been shown to be capable of reproducing the key processes with physical principles. As such, they have the potential to be used for addressing long-term problems even for a very long time period in which environmental conditions may change significantly.

A crucial means for utilizing these models at the field scale is accurate and robust numerical methods. For this reason, we have also been advancing numerical methods for coupled multiphysics and multiscale problems (Choo and Borja, 2015; Sun et al. 2017; Choo and Lee 2018; Choo 2018). Addressing field-scale problems through a tighter combination of advanced models and numerical methods is our research objective in the coming years.

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