

A COUPLED CHEMO-MECHANICAL MODEL FOR CEMENTED SOILS, FROM THE MICRO- TO THE MACRO-SCALE

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Abstract

Chemical effects in the mechanical behavior of geomaterials have received increasing attention in recent years for a number of applications, ranging from the stability of slopes and coastal structures to geological CO₂ sequestration in carbonate rocks. Chemical processes result in either strengthening or weakening effects, the latter being particularly critical for safety assessment of applications in civil and energy engineering. In this work, coupling of chemical and mechanical processes in cemented soils and rocks is investigated by means of a micro-structure inspired model, consisting of an assembly of grains and bonds undergoing dissolution or deposition of mineral mass, affecting geometrical characteristics of the system and thus determining the evolution of specific surface area and of bond cross-sectional area at the micro-scale, and of porosity at the macro-scale, which become key variables linking the micro-scale and macro-scale mechanisms. At the macro-scale, a reactive chemo-plasticity model incorporating elasto-plastic coupling for bonded geomaterials is formulated. The resulting micro- to macro-scale model, schematically applicable to both materials with reactive grains and bonds and materials with only reacting bonds, is validated against the available experimental evidence, consisting of a number of different chemo-mechanical experiments on calcarenite. The model is thus shown to provide a flexible framework for consistent interpretation of experimental loading paths, and can be readily extended to more complex materials or to incorporate additional chemo-mechanical effects.

1. Introduction

Terzaghi (1950) in his paper on Mechanism of Landslide discusses the chemical weathering affecting rock of any kind which “weakens intergranular bonds” leading to decrease in cohesion, leading to a progressive decrease in Factor of Safety, due to chemical weathering. Also in the case of loess, water from external reservoirs is identified as responsible for removing soluble binders and destroying intergranular bond(s), with the same macroscopic effect of a decreasing cohesion. In a more modern day context one needs to add that the dissolution of cementation bonds may be dramatically enhanced by an increase in acidity of the run-off water, namely from an acid rain (e.g. see Zhao et al. 2011).

Further, the recent interest in geological CO₂ sequestration in carbonate rocks brings challenges in predicting the effectiveness of injections since CO₂, upon being injected, dissolves into an in-situ brine and produces also a weak acid, which in turn reacts with the surrounding carbonate rock (e.g. see Andre et al. 2010). On the other hand, the technique of acid softening of rocks prior to hydraulic fracturing in unconventional gas and oil recovery or heat recovery from geothermal reservoirs poses interesting questions in ensuring the control of the process (Hu & Hueckel 2011).

The aim of this work is to investigate coupling of chemical and mechanical processes involved in weakening or strengthening of bonded geomaterials by means of a micro-structure inspired model.

The micro-scale model is calibrated on (but it is not limited to) a regular array of grains and bonds undergoing dissolution or deposition of mineral mass, which both affect geometrical characteristics of the system. Simple reactions of dissolution and deposition between pore fluid and solid minerals are considered, thus complex phenomena involving solid-solid mass exchange are neglected for the sake of simplicity. Variable geometrical characteristics are used to determine the evolving specific surface area and the bond resisting cross-sectional area at the micro-scale, and variable porosity at the macro-scale, which become key variables linking the micro-scale and macro-scale mechanisms. At the macro-scale, a reactive chemo-plasticity model (e.g. Loret et al. 2002) is combined with a model for bonded geomaterials (e.g. Gens & Nova 1993), while kinetic rate equations must be adapted for dissolution/precipitation accounting for their acidity sensitivity (e.g. Sjöberg 1976).

Schematically, based on the kinetics of dissolution/deposition reaction of different minerals, two main cases are discussed, namely the case of both reactive grains and reactive bonds (e.g. calcarenite, where both grains and bonds are made of calcium carbonate) and the case of non-reactive grains and reactive bonds (e.g. silicic sand with carbonate bonds). While in the former case the timescales of dissolution/deposition of grains and bonds are comparable, in the latter case the timescale of reaction of bonds is negligibly small compared to that of the grains. However, the proposed framework could be easily extended to situations involving the presence of different families of cementation bonds characterized by different strengths and chemical dissolution properties.

2. Model outline

Two types of information can be obtained from the existing literature: information on the material strength change and on stiffness change, due to mechanical loading and chemical dissolution - that is typically provided by macro-scale experiments; and information about the chemical processes of dissolution and precipitation of the key minerals, which is obtained from micro-scale information. Consequently, we construct a two-scale model, which includes: (i) a macro-scale chemo-elasto-plastic model, where both the apparent preconsolidation stress and the apparent isotropic tensile strength depend on the material microstructural features, and (ii) an integrated model for mass change of minerals, in the framework of an idealized evolving micro-scale structure of grains and bonds, subject to removal or addition of mineral mass, localized mechanical failure and chemical healing.

The macro-scale, in the considered case, is described by continuum variables of (elastic and plastic) strain and stress tensors, continuum free energy, and compressive and tensile strength. Such variables all depend on a series of macro-scale variables, such as the mass change of the minerals, and on micro-structural quantities (as the geometry of bonds and grains). The macroscopic continuum variables depend through phenomenological functions on micro-structural variables.

The macroscopic constitutive model is developed assuming a yield function along the lines of an existing approach for bonded geomaterials (e.g. Gens & Nova 1993), in which an isotropic tensile strength function is included, as an extension of the modified Cam Clay model. An associated flow rule is adopted for the sake of simplicity. The expression of the yield locus includes two macroscopic quantities, p_{tens} and p_{comp} , representing the increase of tensile and compressive strength, compared to uncemented soil, due to the presence of cementation bonds (Gajo et al. 2015). Coupling with the micromechanical behavior is introduced by assuming that p_{tens} and p_{comp} depend on the mean specific cross section area a_b of all mechanically active cementing bonds (corresponding to unbroken bonds, thus ‘actively’ contributing to the macroscopic strength).

Further, a simplified hardening relationship similar to that of Cam Clay is adopted, assuming negligible elastic compressibility (Gajo et al. 2015). However, the proposed constitutive framework is not limited to the above outlined simple assumptions.

The macroscopic strain tensor is decomposed into additive elastic and plastic parts. The macroscopic elastic behavior of the material is described in the framework of hyperelasticity and elasto-plastic coupling (Hueckel 1976), and can thus be deduced upon defining a suitable elastic free energy density function. To account for the presence of both mechanically and chemically interacting bonds, the standard linear elasticity form of the free energy function of the uncemented solid skeleton (i.e. the

unbonded soil) $\varphi_g = \varphi_g(\boldsymbol{\varepsilon}_e)$ is modified, based on phenomenological interpretations, into a more general function:

$$\varphi = \varphi(\boldsymbol{\varepsilon}_e, \boldsymbol{\varepsilon}_p, m_b). \quad (1)$$

A macroscopic variable m_b is the time-integrated mass change of all mechanically active cementing bonds per unit volume, from a reference configuration m_{b0} ($\Delta m_b > 0$ implies an increase of bond mass with respect to the reference configuration).

From the chemical point of view, for the case of only reacting bonds, during cement dissolution a fraction of cement bonds, which in a general situation carries a fraction of the overall stress, disappears, causing the reduction of a_b . This leads to a stress increase in the remaining fractions of the bonds, thus inducing strains at constant stress level. As a result, cement dissolution induces a decrease of soil stiffness with associated strains (if dissolution occurs at constant stress) or a decrease of soil stiffness with an associated decrease of applied stress (if dissolution occurs at constant strain). On the other hand, cement deposition induces an increase of material stiffness, at constant stress and strain. This behavior is taken into account with a step-wise form of the elastic energy (Gajo et al. 2015).

In the case of both reactive solid grains and bonds, the additional consideration must be made that if the number of cementing bonds is negligible, grain dissolution implies some macroscopic volumetric strain. In fact, in the limit of null active cementing bonds, grain dissolution is associated to volume compression (due to the decrease of grain volume). The volumetric effect of grain dissolution in uncemented soil is completely analogous to the volumetric effect of a decrease of temperature in the grain material, in contrast with the effect of deposition, which is assumed to produce no volumetric strain.

From the macroscopic point of view, the net mass change \dot{m} within the REV due to dissolution and/or deposition is controlled by chemical kinetics. The rate at which the minerals aggregate or dissociate is proportional to the specific reactive surface area a_r per unit volume of the reacting materials. The macroscopic quantity a_r (with units m^2/m^3) corresponds to the area per unit volume of all interfaces of the porous skeleton that are exposed to chemical interaction, i.e. the areas that are actually in contact with the pore fluid.

Further, a chemo-mechanical rate equation is defined via an empirical function, expressing the rate of change of mechanically active bonds per unit volume, N_{ba} , including the two mechanisms of destructuration and cement deposition, $\dot{N}_{ba} = f(\dot{m}_b, \dot{\boldsymbol{\varepsilon}}_p)$. As a result, in general cement dissolution/deposition \dot{m}_b affects soil's mechanical strength in two ways, namely (i) through the restoration of previously broken bonds and (ii) through the reduction/increase of the bond cross sections. In fact, in general cement dissolution/deposition is expected to affect both porosity and the thickness of bonds.

The constitutive concepts described above are based on two key macroscopic quantities, the cross section of active bonds a_b and the reactive surface area a_r , which must be defined in terms of microscopic variables. To relate the evolution of microscopic variables with the macroscopic chemo-mechanical description of the material, reference is made to a simplified microscopic geometry. As an example, in Figure 1a, a 2D schematic of the considered geometry at the microscopic scale inspired from microscope photographs of thin sections of calcareous rocks is shown, in the general case where grains might not be in direct contact, but they are linked by cementation bonds that are assumed to be isotropically distributed. In a large porosity configuration such as that illustrated in Figure 1, the geometry of bonds can be approximated with that of a cylinder, and the geometry of grains can be represented by that of a sphere. In Figure 1b, a 2D schematic is shown of the case where, regardless of the size of bonds, grains remain in direct contact, resulting in a simplification of the bonds' geometry.

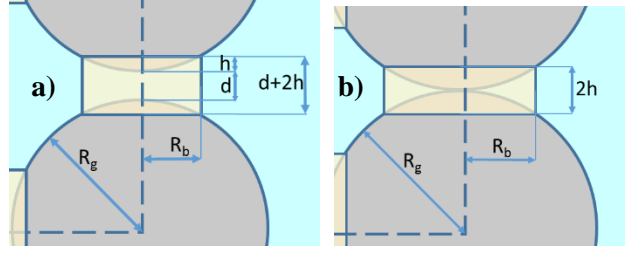


Figure 1. Schematic of the considered simplified geometry at large porosity, (a) in a general case where the spherical grains are not in direct contact, but they are linked by cylindrical bonds, and (b) in the case where the spherical grains are in direct contact, and bonded by cylindrical bonds.

The key cross-scale functions that are developed by considering the material microstructure are the expressions of $a_r = f(R_b, R_g, L_b, d, v_b, v_g, \epsilon)$ and $a_b = f(R_b, \epsilon_p, a_r)$, where R_b, R_g are the mean bond and grain radii, L_b the mean bond length, d the mean distance between grain edges, v_b, v_g the bond and grain specific volume and ϵ, ϵ_p the total and plastic strain tensor. The interested reader is referred to Gajo et al. (2015) for further details.

3. Model validation

The above described model was numerically integrated through a fully implicit, backward Euler integration scheme, showing adequate convergence.

The model capabilities to reproduce the experimental chemo-mechanical behavior of bonded geomaterials were tested by simulating a series of loading paths along the lines of experimental datapoints reported in the literature, after having deduced the relevant parameters as much as possible from published data.

As a first example, the model is tested by simulating unconfined compression tests on saturated calcarenite, by first reproducing an acid weathering phase and subsequently a mechanical loading phase, and comparing the simulations with the experimental data of Ciantia et al. (2014). In this context, a variable expressing the ‘degree of dissolution’ can be introduced as $\xi = M_{dis}/M_0$, where M_{dis} represents the dissolved mass and M_0 the initial mass of reacting solids, so that $\xi=0$ for the unweathered material and $\xi=1$ at complete dissolution of the reacting solids.

As discussed in section 2, the equivalent elastic modulus of the bonded material E depends on both the elastic properties of calcite cement and of the unbonded granular material, and is calculated upon taking the second derivative of the free elastic energy density with respect to elastic strain. Thus, we obtain an expression of the form

$$E = E_g (1 - a_b^\alpha) + E_b a_b^\alpha \quad (2)$$

where E_g and E_b the elastic moduli of uncemented solid skeleton and of completely cemented soil (which is approximated with that of pure calcite) respectively, and parameter $\alpha=1.8$. It should be noted that eqn. (2) is also consistent with mixture theory-based rules to obtain the equivalent parameters of a composite mass, typically employed in soil improvement calculations (e.g. see Ou et al. 1996). Moreover, eqn. (2) includes elasto-plastic coupling, because the cross section of active bonds a_b depends on plastic strains, which may induce damage of elastic stiffness.

In Figure 2a, simulations of stress-strain curves during unconfined compression tests are plotted at different values of ξ , together with analogous experimental data. To adequately reproduce experimental conditions, the simulation consisted of two steps, namely of a first step reproducing exposure to an acid solution up to the target value of ξ , and of a second step simulating the unconfined compression test in the weathered material. The reproduction of experimental data is especially accurate until the ultimate strength is attained. After the peak, simulations exhibit a smaller

amount of softening than experiments, overall showing a less markedly fragile behavior. Since the post-peak response is typically deeply affected by shear or compaction banding which leads the conventional behavior to be much different from that of a homogeneously deforming sample, additional ad-hoc constitutive assumptions were not introduced for more accurate reproduction of this phenomenon.

Further, oedometer tests on calcarenite samples previously subjected to different degrees of weathering (Ciantia et al. 2014) were reproduced. In Figure 2b, satisfactory oedometer test simulations are shown in terms of vertical strain versus vertical stress, at different degrees of dissolution. Experimental data from Ciantia et al. (2014) are also reported in the graph for comparison.

Finally, in Figure 3 the stress path of Castellanza and Nova (2004)'s oedometer test on calcarenite in the (p, q) plane is simulated, and fittingly compared to experimental data. The path A-B represents the mechanical loading phase. Upon reaching point B, the vertical load is kept constant and the acid weathering phase starts, gradually causing an increase of radial stress, revealing as a linear decrease of deviatoric stress with increasing mean stress (path B-C).

In all of the above described examples, satisfactory agreement between the model prediction and the experimental data is obtained, after adequate parameter calibration (Gajo et al. 2015), suggesting that the presented model provides a powerful and flexible framework for adequately reproducing different experimental chemo-mechanical loading paths.

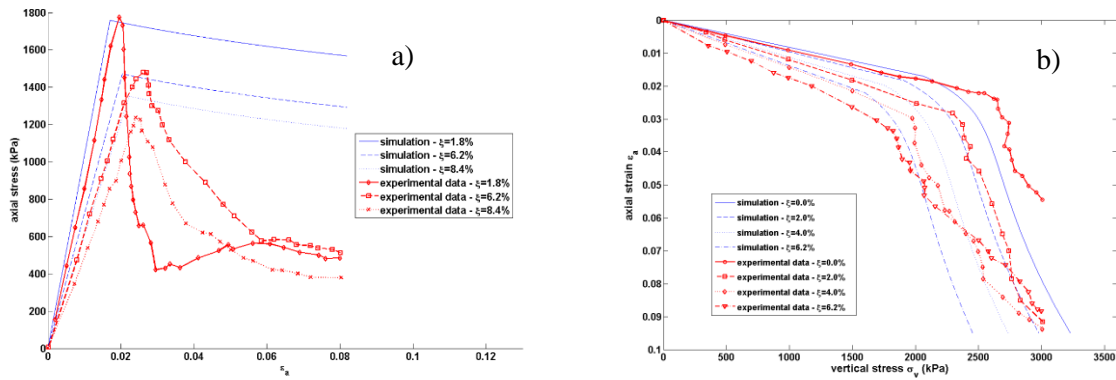


Figure 2. Comparison of simulations and experimental data in terms of (a) deviatoric (axial) stress versus axial strain in unconfined compression tests on calcarenite, (b) axial strain versus vertical stress in oedometer tests on calcarenite, carried out after weathering up to different values of degree of dissolution.

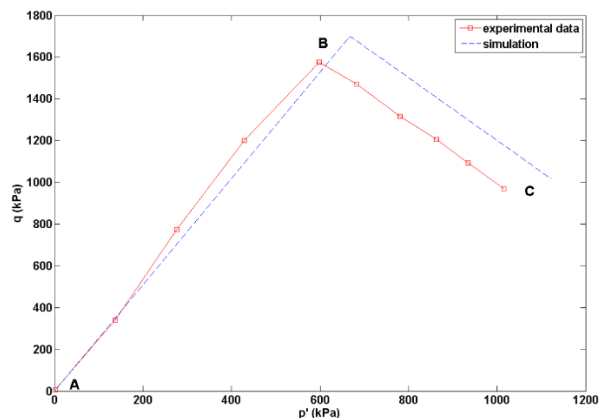


Figure 3. Comparison of simulations and experimental data in terms of deviatoric stress versus mean effective stress in an oedometer test on calcarenite. Path A-B represents the loading phase in unweathered conditions, path B-C represents the acid weathering phase at constant applied load.

4. Conclusions

In this work an innovative, general two-scale modelling framework able to account for the key aspects of the coupled chemo-mechanical behavior of bonded granular materials is presented, and validated against experimental evidence. The proposed framework includes an integrated model for mass change of minerals, in the frame of an idealized evolving micro-scale structure of grains and bonds, subject to removal or addition of mineral mass, localized mechanical failure and chemical healing, and a macro-scale chemo-elasto-plastic model, where both the yield stress under isotropic compression and the isotropic tensile strength depend on the material microstructural features, incorporating elasto-plastic coupling to describe the degradation of elastic properties due to mechanically induced debonding.

For the sake of simplicity, the distribution of bonds and their cross sections are assumed isotropic and the model presentation is based on simple linear isotropic elasticity and Cam Clay yield function. The proposed constitutive framework is not however limited to these simple assumptions and could be straightforwardly applied to more complex elasticity models and yield functions. Moreover, the proposed framework could be easily extended to situations involving the presence of different families of cementation bonds characterized by different strengths and chemical dissolution properties, such as those experimentally observed by Ciantia et al. (2014) on calcarenite.

It can be concluded that the presented model provides a powerful and flexible framework for adequately reproducing different experimental chemo-mechanical loading paths. It is worth remarking that the model is to be intended as an open framework rather than being specialized on a particular material type. Different additional effects, such as mechanical anisotropy, could easily be incorporated depending on modeling needs.

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