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Jean-Michel Pereira. Effects of microstructure on THM behaviour of geomaterials. 8th International Conference on Unsaturated Soils (UNSAT 2023), May 2023, Ile de Milos, Greece. pp.11001, 10.1051/e3sconf/202338211001 . hal-04392938

HAL Id: hal-04392938

<https://hal.science/hal-04392938>

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Effects of microstructure on THM behaviour of geomaterials

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Abstract. In this paper, we discuss the thermo-hydro-mechanical behaviour of geomaterials at the light of their microstructure and its changes induced by multiphysics loading. After recalling the strong links between the microstructure and the water retention properties of unsaturated soils, the relation between the microstructure and the physical properties ruling heat and mass transfers are discussed. The mechanical behaviour of unsaturated soils is then discussed focussing on the definition of an effective stress based on a microstructure description. The experimental determination of this microstructurally-based effective stress is presented, including recent advances to identify the stress coefficient from Mercury Intrusion Porosimetry data. Opening remarks towards macroscopic modelling of unsaturated geomaterials accounting for their microstructure and its changes is finally discussed.

1 Introduction

Many geotechnical engineering applications require proper knowledge of the multiphysics properties of the involved geomaterials. Energy geotechnics, seen in a broad sense [1], is a typical example where a proper understanding of multiphysics processes taking place within these fluids-filled porous materials is necessary for an efficient design. Indeed, an improved understanding of the physics occurring at the various pore scales of geomaterials necessarily leads to more robust macroscopic models. A difficulty to overcome lies in the experimental characterization of this physics at various scales in materials that are inherently heterogeneous, and also in the upscaling process required to transfer this knowledge to the macroscopic scale, which is the scale of interest in engineering applications. Fig. 1 shows the time evolution of publications in geotechnical journals mentioning microstructure in their title, abstract or keywords. A fast-increasing rate is observed over the past twenty years.

In this work, microstructure and its effects on the overall behaviour of geomaterials are investigated and discussed. Microstructure involves complex concepts. In the first order, the microstructure of soils is measured by their porosity (or equivalently void ratio). Of course, this is a rather limited estimation. To go further, we will consider here the pore size distribution, which will be seen as a proxy for the soil's microstructure.

This paper is organized into three main sections, respectively focusing on water retention properties, thermal effects and mechanical behaviour of (unsaturated) soils. In each of these sections, typical couplings between the different physics are

described. Finally, a general discussion and closing remarks are proposed.

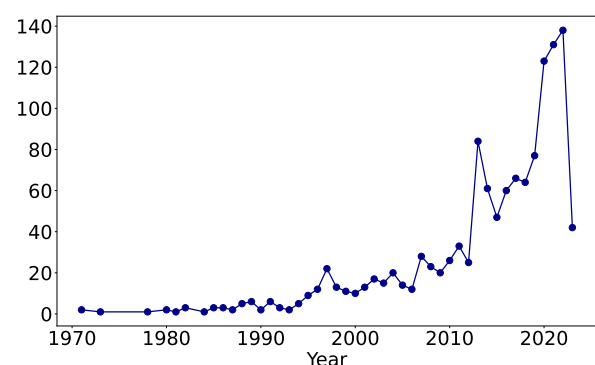


Fig. 1. Evolution of articles published in geotechnical engineering journals including "microstructure" in their title, abstract or keywords. Scopus query, performed on 2023/04/04: (TITLE-ABS-KEY (microstructure) AND SRCTITLE (geotech* OR geomech*)) AND (LIMIT-TO (DOCTYPE , "ar") OR LIMIT-TO (DOCTYPE , "re") OR LIMIT-TO (DOCTYPE , "no")).

2 Water retention properties

2.1 Definition

Knowledge of water retention properties is essential to the understanding and modelling of the thermo-hydro-mechanical behaviour of geomaterials. Central to the mechanics of unsaturated soil, the water retention properties greatly affect the overall mechanical behaviour of soils but also the thermal and fluid transport properties of porous materials.

Water retention properties of soils correspond to the relationship between their water content and the

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water potential, which characterises the thermodynamic state of the water contained in the soil. The physics involved in this property fundamentally depends on the microstructure, and notably on the spread of the pore size distribution. In coarse granular soils, capillary phenomena are dominant and almost exclusive. For soils with larger fines content, physical interactions between the water phase and the solid particles might become significant, depending on the nature of the solid particles, the soil specific surface and the size of the smallest pores. In particular, water adsorption on solid surfaces significantly contributes to the water retention [2]. Depending on the situation, the chemical composition of the liquid phase could also play a key role.

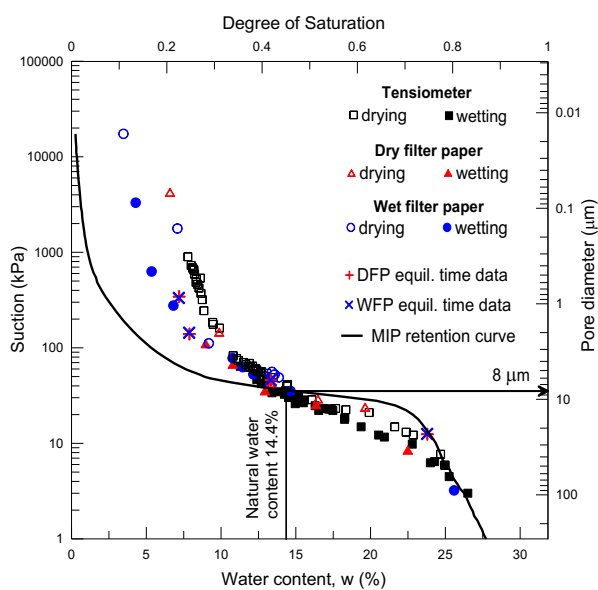


Fig. 2. Water retention curve of intact loess from northern France (adapted from [3]).

In Fig. 2, the water retention curve of an intact loess from northern France obtained using various experimental techniques [4,5] is plotted and compared to the intrusion curve obtained from mercury intrusion porosimetry (MIP), the latter being estimated assuming purely capillary effects [3]. The MIP curve, which corresponds to a drying branch, has been adjusted to match the water content at the saturated state (assuming that mercury intrusion catches all large pores within the material). Whereas the various techniques agree at low suctions, a strong discrepancy between the MIP curve and the drying branch of the WRC clearly appears at large suctions (corresponding to water contents smaller than c.a. 10%). This difference might be attributed to physical interactions between the water phase and the solid surfaces, but given the relatively small specific surface of loess soils, adsorption alone is not enough to explain such differences. Another explanation might be found in the experimental protocols themselves. Indeed, the loess WRC was obtained by letting the soil sample

dry freely. Such a procedure induces shrinkage of the material which decreases the size of pores that still contain liquid water at the corresponding suction. This phenomenon tends to shift the drying branch towards larger water contents. This is not the case for MIP curves since freeze-dried specimens are tested, after a processing preserving their microstructure [6].

2.2 Mechanical couplings

What is interesting about the retention properties is that they straightforwardly give access to the microstructure of the studied geomaterials. Or reversely, they reflect the microstructure of the material. As seen previously, the retention properties are also affected by changes in microstructure. Apart from drying-induced changes in pore size distribution, mechanical deformation induced by soil compaction affects the WRC of soils. This observation is of great importance for compacted soils [7].

Fig. 3 shows the electrical resistivity of the same loess from northern France taken at two different depths corresponding to two distinct void ratios. It is interesting to note that the curves collapse (no hysteresis between filled symbols (wetting branch) and empty symbols (drying branch)) when electrical resistivity is plotted as a function of (volumetric) water content or degree of saturation (not shown). The figure also clearly shows the influence of the microstructure (void ratio and pore size distribution) and mineral composition of the soil between these two loess soils taken from two different depths at the same location.

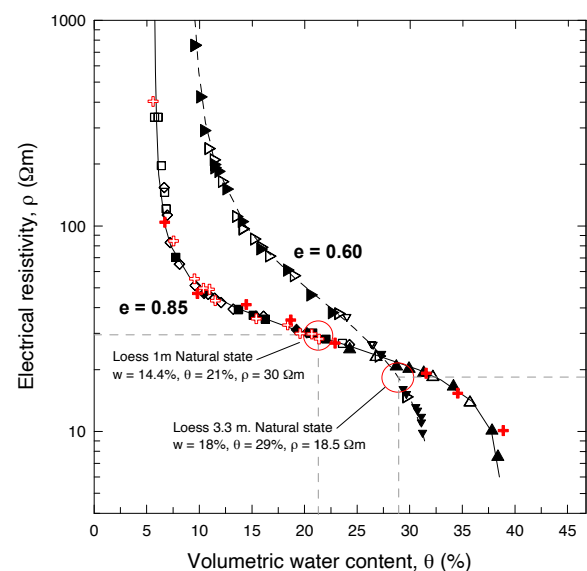


Fig. 3. Electrical resistivity of two intact loess soils from northern France (adapted from [8]).

2.3 Thermal couplings

Water retention properties are temperature dependent. In the capillary regime, this dependency is mainly due to the role played by temperature on

the surface tension. Osmotic and adsorptive components are also temperature dependent. However, in usual ranges of temperatures (let's say below 100 °C), these effects modestly translate into the water retention curve of geomaterials [9]. A recent work focusing on a larger temperature range reports appreciable effects of temperature on the water retention curves, suggesting that such effects should be considered in applications where field temperatures are significantly different from laboratory temperatures at which WRC is measured or where large temperature changes are expected [10].

3 Heat transfer

3.1 Models for thermal properties of unsaturated soils

Thermal properties are obviously key for applications where temperature changes are expected. One can cite energy geostructures (such as thermal piles) and also radioactive waste disposals, among others. Thermal properties are not often measured experimentally in the laboratory, and even less in situ.

In a first approach, heat capacity and thermal conductivity can be estimated from the properties of the soil constituents, provided the mineral composition and the porosity are known. However, it should be noted that thermal conductivity cannot be estimated as easily as volumetric heat capacity. While this latter is deduced from a volume average of the heat capacities of the soil constituents, including the fluids filling its porosity (since the volumetric heat capacity describes the amount of energy necessary to increase the temperature of a unit volume of soil by one degree), the thermal conductivity strongly depends on the soil fabric and cannot be estimated without knowing the soil microstructure.

Neglecting the contribution of the gaseous phase, the volumetric heat capacity C of an unsaturated soil is given by:

$$C = (1 - n)\rho_s c_s + nS_w \rho_w c_w \quad (1)$$

where ρ_s and ρ_w are the soil and water densities, c_s and c_w are specific heat capacities of the solid phase and liquid water, respectively and n is the soil porosity.

Several models have been proposed for the thermal conductivity of soils. A basic arithmetic weighted average (similar to equation (1)) is used in some studies. In other studies, Johansen's model (based on a weighted geometric average) [11] is used:

$$\lambda = \prod_{\alpha} (\lambda_{\alpha})^{f_{\alpha}} \quad (2)$$

where α represents the phase, λ is the thermal conductivity of the soil and λ_{α} is the thermal conductivity of the phase α . This formula is used for frozen soils for instance. However, in the case of unsaturated soils, Johansen proposed another complementary approach to track the influence of the degree of saturation of water instead of using equation (2):

$$\lambda(S_r) = (\lambda_{sat} - \lambda_{dry})k(S_r) + \lambda_{dry} \quad (3)$$

where $k(S_r)$ is a function of the degree of saturation to be determined experimentally.

As an illustration of experimental data that could be used to fit equation (3), Fig. 4 shows the thermal conductivity of the same intact loess from northern France (at a depth of 1 m) as a function of the degree of saturation. As in the case of electrical resistivity, it appears that the various drying/wetting paths collapse on a master curve. Furthermore, in the range of water contents reached during the experiments, the variation of the thermal conductivity is approximately linear.

The choice between these models of thermal conductivity relies on assumptions on how the heat flux circulates between the soil phases (series, parallel, etc.). These assumptions heavily rely on the soil microstructure, including how the liquid phase is distributed within the porosity in the case of unsaturated soils. Interested readers are referred to a critical review available in [12]. An interesting approach is proposed in [13], where a two-scale homogenisation is proposed for claystone due to its complex microstructure. Again, this demonstrates that the microstructure plays a key role in the thermal properties of geomaterials.

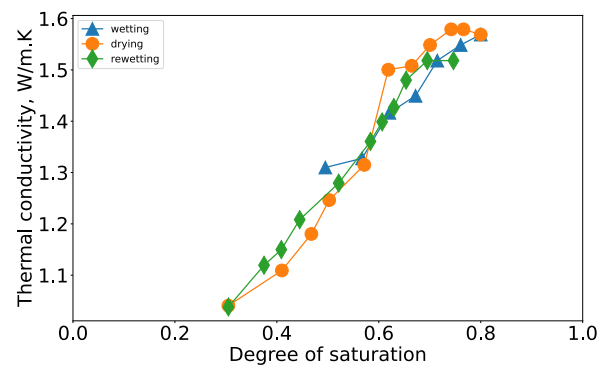


Fig. 4. Thermal conductivity of loess from northern France (adapted from [14]).

3.2 Other couplings

The case of couplings between the hydric state of the soil and its thermal properties has been included in the previous section. The effects of mechanical deformation on the thermal properties of soils have not been thoroughly studied. Such couplings are of second order and their effect might not be easy to determine experimentally.

In a first approach, it seems reasonable to use porosity changes as a proxy to account for these coupled effects on thermal properties and inject those changes into the models fitted for the soil at a reference (undeformed) state.

It is however evident that this would not be enough if accurate modelling of the evolution of thermal properties with mechanical deformation is sought. One can imagine the case of pure shear deformation of granular materials (at critical state, for instance). Such a mechanical loading affects the number of contacts within the soil mass and thus is expected to drastically affect the apparent thermal conductivity. In general, microstructure changes are likely to affect how heat flows through the representative volume element. In these conditions, a model suitable for a given microstructure might not be pertinent anymore if the microstructure significantly changes.

4 Mass transfer

4.1 Introduction

Fluid transfers in geomaterials are strongly dependent on the porous network and its structure. Furthermore, water transfers also depend on the thermodynamic state of the liquid water. Indeed, in small pores, the fraction of water bonded to the solid surfaces will remain quasi-immobile and thus does not participate in the liquid flow. This observation often leads to the definition of an effective degree of saturation :

$$\tilde{S}_w = \frac{S_w - S_{w,res}}{1 - S_{w,res}} \quad (4)$$

where $S_{w,res}$ is the residual degree of saturation. This value is generally estimated as the asymptotic value observed in the water retention curve at large suction values. This effective degree of saturation might then be used to compute the relative permeability coefficient k_{rel} , thus leading to an apparent permeability k_{app} writing as follows:

$$k_{app} = k_{sat} k_{rel}(\tilde{S}_w) \quad (5)$$

In very small pores, with dimensions comparable to the fluid molecule size, corrections to the Darcy law are necessary because molecules cannot travel along their free mean paths without colliding with the pore walls. This is known as the Klinkenberg effect (see e.g. [15]). This effect will not be further discussed here.

4.2 Coupling effects

The saturated permeability is usually corrected for mechanical deformation using the Kozeny-Carman equation. This relation has been developed to predict the (saturated) permeability in granular media, with

a given porosity [16]. However, its use to estimate permeability changes induced by porosity changes is quasi-generalised in numerical modelling at the continuum scale. In this case, Kozeny-Carman equation writes as follows:

$$\frac{k}{k_0} = \left(\frac{n}{n_0}\right)^3 \left(\frac{1-n_0}{1-n}\right)^2 \quad (6)$$

In the absence of any other data, this relation is also used in the context of reactive transport modelling, where chemical reactions induce dissolution-precipitation reactions. However, this relation does not seem appropriate in the case of porosity changes induced by chemical reactions. This is confirmed by experimental and numerical studies of permeability changes induced by dissolution of the solid matrix [17–19].

In the context of CO₂ geological storage, and to account for permeability changes within the wellbore cement induced by cement carbonation, [20,21] used a permeability-porosity relation obtained experimentally by [22] for cementitious materials. This relation has been fitted on experimental data linking porosity changes induced by mechanical deformation and permeability. This relation, specific to the studied material, was more appropriate than Kozeny-Carman equation. However, chemical reactions are likely to affect the porous network and thus the microstructure of the materials differently than mechanical deformation for a given porosity change. It is therefore essential to obtain experimentally or estimate numerically permeability – porosity relations. It is obvious here that porosity alone would not be sufficient and should be understood as a representation of the porous network (or material microstructure). So, one should at least pursue a permeability – pore size distribution relationship.

4.3 Modelling approaches

Following on this idea of numerical modelling to estimate this permeability – pore size distribution relationship, it appears that modelling approaches at the pore scale are an interesting research path to follow. The example of [18] has already been cited. The authors use the lattice Boltzmann method in simplified two-dimensional pore network geometries.

In [23], the authors plugged a damage model to a microstructural description of the porous volume of geomaterials. Elastic deformations were related to changes in a “natural” pore size distribution and damage-induced cracks to the creation of another family of pores through compatibility relations between macroscopic strains and statistical descriptors of the pore size distributions. Using the Hagen–Poiseuille equation at the pore scale (bundle of tubes hypothesis) and Darcy’s law, it was then possible to estimate the macroscopic permeability of the materials. This procedure allows us to relate

deformations and permeability through a straightforward micro-macro approach. Fig. 5 shows an example of the modelling approach validation.

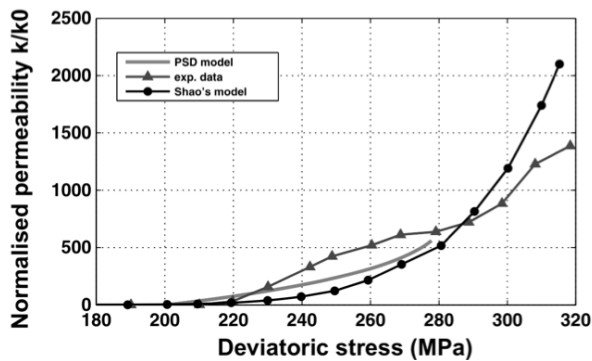


Fig. 5. Permeability evolution during a triaxial compression test: results from the micro-macro approach (“PSD model”) compared to experimental data on a brittle rock and another numerical approach due to Shao et al. [24] based on crack connectivity (figure adapted from [23]).

This work has been extended [25] to unsaturated geomaterials. Indeed, the knowledge of the evolution of the pore size distribution at various states of mechanical loading allows quite straightforwardly to estimate the water retention curve (similar to the procedure that allows determining the WRC from MIP data) and the relative permeability of the material, using the Hagen–Poiseuille equation (considered only those pore sizes filled by liquid water) and Darcy’s law extended to unsaturated states.

The simplicity of this approach, in terms of micro-macro approach and also in terms of microscopic descriptors, can be extended to more realistic microstructures using numerical upscaling approaches such as FEMx FEM, FEMx DEM or FFTx FEM approaches (see among [26,27] others). Such methods benefit from the improvement in three-dimensional imaging of geomaterials in situ during multiphysics loading [28–32]. These techniques are computationally expensive but various strategies might significantly improve their efficiency in the future [33].

5 Mechanical behaviour

5.1 Mechanically effective degree of saturation

In this part, we will not cover the topic of the choice of an effective stress for unsaturated soils. We will however discuss how the microstructure is taken into account in a specific proposition for such an effective stress. The definition of the stress proposed by Alonso et al. [34] is considered.

This proposal is based on the introduction of a so-called microstructural degree of saturation used to rescale the (total) degree of saturation. A Bishop-like stress coefficient is then used in the effective stress:

$$\chi(S_w) = S_w^{\text{eff}} = \frac{\langle S_w - S_{w,m} \rangle}{1 - S_{w,m}} \quad (7)$$

where $\langle x \rangle$ stands for the positive part of x . This stress coefficient corresponds to an effective degree of saturation, but in the mechanical sense now. Despite the obvious analogy observed between equations (6) and (7), the two effective degrees of saturation have no reason to be equal. In [34], the authors have back-analysed the evolution of mechanical properties (shear strength and/or elastic properties) with soil suction to fit this microstructural degree of saturation. In the case of Boom clay, $S_{w,m}$ has been found close to a “quasi-immobile” water content identified in a completely distinct manner from MIP data by Romero [35].

Actually, this concept of microstructural degree of saturation is comparable to the concept of active porosity introduced by Ghabezloo [36], which is defined in terms of the poromechanical behaviour of cement pastes. Interestingly, Ghabezloo proposes to identify this active porosity to the porosity accessed during MIP tests, as opposed to the total porosity of cementitious materials. Readers interested in a discussion on how to satisfactorily obtain this total porosity from various drying techniques are referred to [37].

5.2 Microstructural degree of saturation

An interesting outcome of [34] is that the microstructural degree of saturation depends on the nature of the soil. Specifically, it was shown that $S_{w,m}$ is close to zero in sandy soils and increases as the fines content increases. It also increases with the plasticity index of soils.

However, the determination of $S_{w,m}$ remains challenging. Indeed, fitting this parameter as done in [34] requires conducting various mechanical tests at various water contents together with the knowledge of the water retention curve. This is time consuming.

Recently, Vaunat and Casini [38] have demonstrated that the Bishop coefficient can theoretically and directly be determined from the knowledge of the pore size distribution at two different deformation states. This procedure thus requires two MIP tests at two values of porosity. The Bishop stress coefficient is then computed from the difference between the two curves. Niu et al. [39] have adapted this procedure by rescaling the porosity considering the fraction of pores that are not affected by the mechanical compression, thus separating micro- and macro-porosities. This approach is illustrated in Fig. 6. It should be noted that the distinction between these two classes of pores based on their size (and susceptibility to mechanical loading) is considered by many authors (see e.g. [40]). The micro-pore size distribution is often considered mostly independent of macroscopic porosity changes.

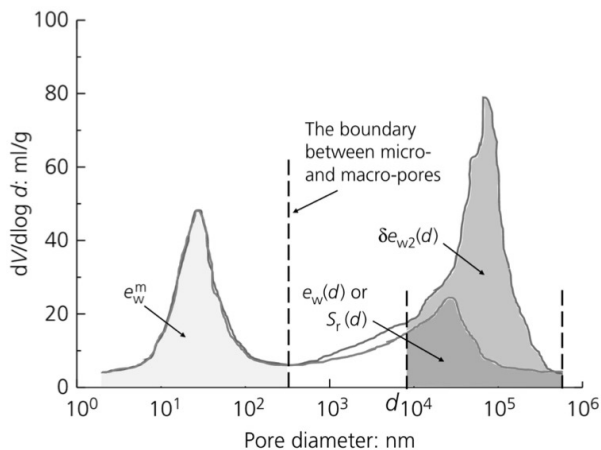


Fig. 6. Illustration of the methodology proposed by [38] and adapted by [39], the porosity value used to rescale the Bishop stress coefficient is marked as the boundary between micro- and macro-pores (adapted from [39]).

6 Concluding remarks

In this paper, we have discussed how microstructural features (mainly the pore size distribution) translate into various components of the overall thermo-hydro-mechanical behaviour of unsaturated soils.

The water retention properties of soils are central to the THM behaviour of unsaturated soils and closely related to their microstructure. Since the water retention curve defines the water content in soils, which itself significantly affects heat and mass transfer properties and the mechanical behaviour of unsaturated soils, the microstructure of soils and its changes appear as a key property that has to be properly understood, characterised and modelled in order to build a complete picture of the THM behaviour of soils.

We have provided a few illustrations of the links between a soil microstructure and heat and mass transfer properties, including the consideration of multiphysics couplings. An integrated approach accounting for micro-macro interactions has been presented as an illustration of a modelling approach to account for geomaterials microstructure when modelling the macroscopic behaviour. The recourse to multiscale numerical approaches is a possible path to pursue this idea, provided the computational efficiency of these numerical methods is improved.

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