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DEM SIMULATIONS OF UNSATURATED SOILS INTERPRETED IN A THERMODYNAMIC FRAMEWORK

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Abstract. The behavior of granular materials (e.g. soils) strongly depends on the interactions between particles at the grain scale. In addition, in multiphase systems, the presence of water and interfaces between different phases in the soil adds complexity to the study [1,2,5]. The main purpose of this work is to introduce some concepts that are able to fill the gap between discrete element method simulations [3,4] and thermodynamics in order to develop constitutive laws able to better describe the behavior of unsaturated granular medium. The problem is studied in a thermodynamic framework where energies are calculated at low water content for a simple system of two particles of different sizes connected by a liquid bridge. The effect of gravity is considered to be negligible in this study. The energy supplied to the simple system is divided into two parts: a) the energy due to the change of the matric suction in the system and b) the energy resulting from the movement of the particles with respect to each other. Comparisions with the first law of thermodynamics show that there are some features that have significant importance in the macro formulation of energies. These features may be related to the interfacial areas in the medium.

1 INTRODUCTION

The study of the mechanical behavior of unsaturated granular materials is important in many applications in geomechanics, chemical and petroleum engineering. However, the macro behavior of these materials depends strongly on the interactions between particles subjected to capillary effects, which makes their study in the framework of continuum mechanics difficult. A micromechanical study is proposed where new features due to capillary forces in the medium must be taken into account to better describe how these materials behave.

The effect of the capillary forces depends on the degree of saturation of the medium. At low water content, the water phase is discontinuous, water bridges are formed between neighboring particles and the regime is called pendular (Fig.1). The capillary force resultant from the presence of these disconnected bridges can be linked to the geometry of the grains and to the capillary pressure inside the medium by the capillary theory. At higher water

content, this assumption is not efficient. The present study of the unsaturated state is limited to the pendular regime.

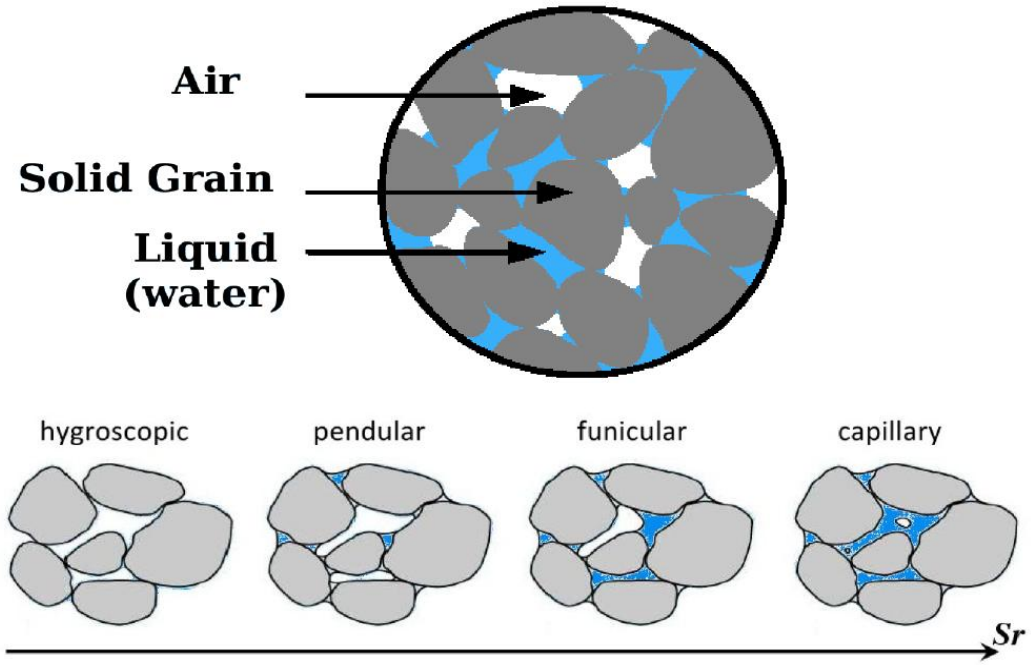

Figure 1: The different unsaturated states of granular medium that vary with the degree of saturation

The profile of the water bridge is given by Young-Laplace equation which represents the exact numerical solution. The equation describes the capillary pressure difference Δu sustained across the interface between two static fluids (air and water), due to the phenomenon of surface tension γ.

$$\Delta u = \gamma C \tag{1}$$

If the water bridges are considered to be axisymmetric, this equation can be written in the following form:

$$\Delta u . y(x) + \gamma \frac{1+y'^2(x) - y(x).y''(x)}{(1+y'^2(x))^{3/2}} = 0 \tag{2}$$

The integration of this equation gives a simple first order differential equation where the constant is equal to the capillary force.

$$\pi . \Delta u . y^2(x) + \frac{2.\pi.y(x).\gamma}{\sqrt{(1+y'^2(x))}} = F \tag{3}$$

$$F = 2\pi y_0 \gamma + \pi {y_0}^2 \Delta u \tag{4}$$

The resolution of Young-Laplace equation allows the determination of all the geometric properties of the bridge (volume, intergranular distance,..)

In the following, a simple system of two particles connected by a water bridge is examined from an energetical point of view. The results show a contradiction with the first law of thermodynamics. Finally, capillary features that must be taken into account are discussed.

2 THE TWO SPHERE PROBLEM – ENERGETICAL ANALYSIS

Let us consider a system of two deformable grains of different sizes. One of the grains is fixed. The two grains are connected to each other by a pendular water bridge (Fig.2). Energy balance is examined in this simple system, assuming a linear contact law between the grains [9], and using a pendulat bridge model inspired by the work of Scholtès [3,4] and reimplemented by the first author of the present paper.

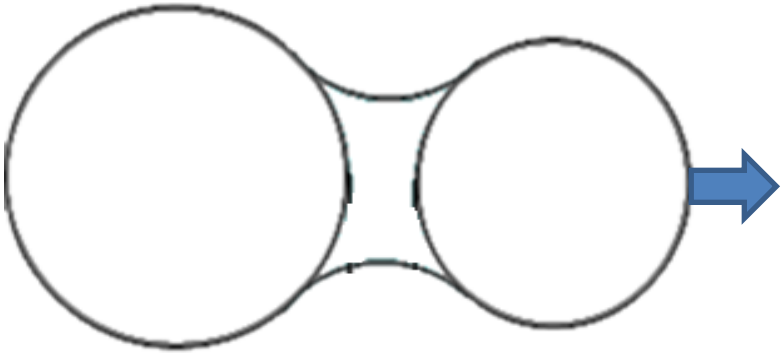

Figure 2: Two grains connected by a pendular water meniscus.

An external work is applied to the system either by moving the second particle by imposing an incremental displacement *d* or by changing the matric suction *s* in the system. The grains are mainly in contact. At the first stage, the grains are kept fixed and the suction is increased in the system up to a certain value. After, an incremental negative displacement was applied while the suction is kept constant in the system. The suction is then decreased followed by a positive incremental displacement to close the cycle. And the total energy E_{tot} is calculated.

Another path was also applied to the system by increasing suction and moving the sequentialy. The total energy input is calculated by integrating:

$$\dot{E}_{tot}=s\dot{V}+F\dot{d} \tag{5}$$

Where $\dot{V}$ is the rate of volume change of the liquid bridge and F is the total force on particle 2 (sum of the capillary force and contact force).

The results (Fig.3) indicate that the total energy supply to move the system from one state to another is path independant. This result is not trivial. The model itself is only based on Laplace's law, which gives no direct evidence of path independance in complex paths combining changes of suctions and movements of the particles. Therefore it must be possible to define an expression for the stored energy depending only on the current configuration.

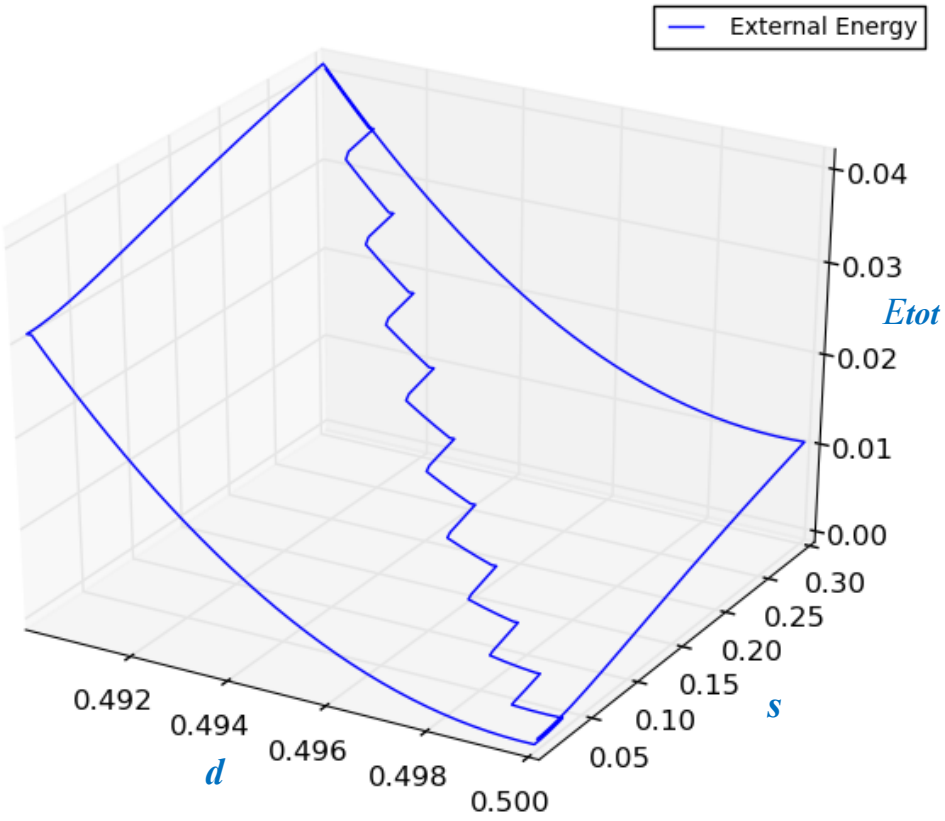

Figure 3: The plot of the total external energy ***Etot*** as function of the suction *s* in the system and the displacement *d* of the second grain

For the first law of thermodynamics to be verified, the internal (or "free") energy must be defined in such a way that its change is always equal to the external work applied on the system.

The pressure of the gaz in the system is considered to be equal to the atmospheric pressure which means that the potential of the gaz phase is negligible. The internal energy of the water is also null as it is an incompressible fluid.

If we don't take into account the energy of interfaces, the only energy left to calculate is the elastic energy of the solid phase determined by the contact law.

The external energy due to the change of bridge volume in the system E_s, the energy due to the movement of the grains E_d, the total external energy E_{tot}which is the sum of both previous energies, and the elastic energy of solid phases E_e are plotted as function of the suction in the system (Fig.4) and as function of the displacement of the second grain (Fig.5).

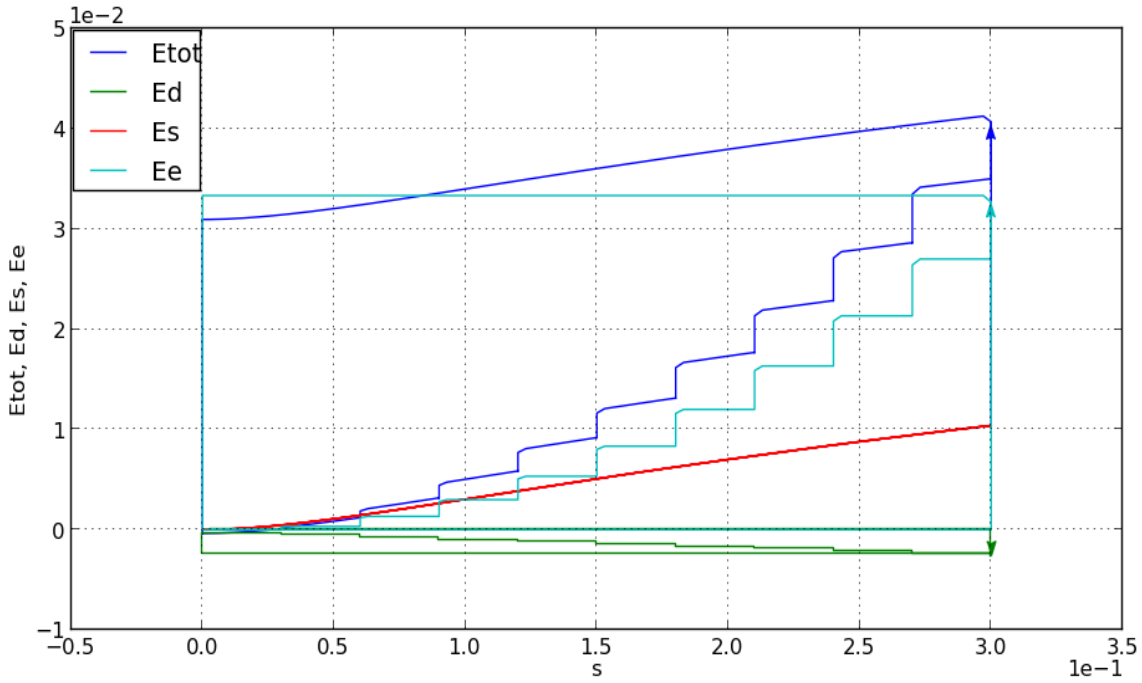

Figure 4: The plot of external and internal energies as function of the matric suction in the system. E_s: energy due to the change of matric suction, E_d: energy due to the movement of particles, E_{tot}: the total external work applied to the system, E_e:: internal elastic energy of solid phase.

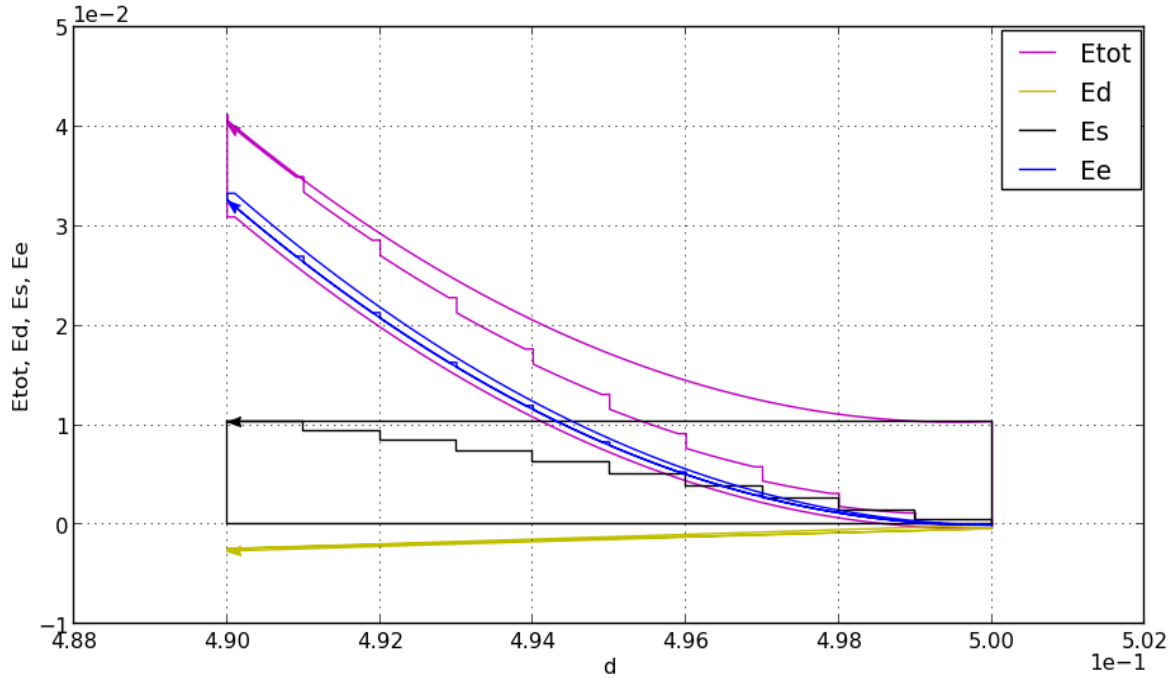

Figure 5: The plot of external and internal energies as function of the displacement of the grains.

3 RESULTS

The curves show that the elastic energy of the solid phase, which is equal to the internal energy of the system is not equal to the total external work applied to the system, and therefore, the first law of thermodynamics is not verified.

The difference between the total external work and the elastic energy means that there are some terms that must be taken into account in the formulation of internal energies. And as the graphs show, this difference is significant, which means that the interfaces in unsaturated medium may add a considerable complexity to the study and should be taken into account.

4 DISCUSSION

The main purpose of this work is to test the importance of the interfaces in the study of unsaturated granular medium, in order develop new micro-macro constitutive relations suitable to better describe the mechanical behavior of these materials and fill the gap between the thermodynamics and the DEM modeling. Our current work, not reported here, concerns the proper definition of the missing energetical term in internal free energy.

Some researchers following a micromechanical approach in the study of unsaturated granular materials have already included the effect of interfaces in the formulation of the effective stress from a thermodynamic point of view.

Coussy and Dangla (2002) considered important terms in the formulation of the free energy to take into account the presence of interfacial areas and its influence on the effective stress tensor but they did not introduce any balance laws for the interfaces.

That was done by Gray et. al (2002) where they introduced the conservation equations for all phases, interfaces and common lines in a multiphase system.

Nikooee et al. (2012) proposed a new formulation for the effective stress tensor assuming that the deformation in the soil can result in a change in the curvature of fluid-fluid interfaces and alter their free energies. This assumption leads to a separate term in the formulation of the effective stress tensor, taking into account the amount of wetting non-wetting interfaces and dependent on the derivative of the Helmholtz free energies on the Lagrangian strain tensor.

However, the choice of the interfaces that must be taken into account and the energy that must be associated to, remains a question to answer.

Nikooee et al. (2012) considered that for rigid grains the air-water interface is the only interface that must be included in the formulation of effective stress.

Another way to introduce these interfaces and their energies is Morrow's work [8]. Morrow applied the first law of thermodynamics and sets the change in free energy inside this system equal to the amount of external work, and expressed the interfacial internal energies in the medium as the sum of the energies of interfaces considering the oil to be the wetting liquid and the water as the non-wetting fluid. He also considered the grains to be rigid and neglected the internal energy of the solid phase. Similarly to what Morrow did, we introduce the internal energies in the medium where water in the wetting fluid and air is the non-wetting phase.

$$dWext = \sum_{k=1}^{3} \gamma_k dA_k \tag{6}$$

dWext is the total supplied energy, A_k the surface of k phase and γ_k the surface tension .

Hence, as the above equation suggests, the change of internal energy due to interfaces may be defined as the surface tension of interfaces multiplied by the change of respective area.

All the articles cited here insist on the importance of micro behavior of unsaturated granular materials and show how small changes in the interfaces at micro scale can affect significantly the macro formulations of stress and energies.

In the next steps of our work, the assumption of Morrow and the other papers accounting for the interfaces will be tested using DEM simulations, and the results will be used to

enhance the constitutive quations defining mechanical behavior of unsaturated materials through additional terms reflecting capillary effects.

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