DEM simulations of unsaturated soils interpreted in a thermodynamic framework.

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ABSTRACT

This work deals with the study of the behaviour of unsaturated soils at the grain scale. A solid and verified thermodynamic framework that allows to fill the gap between thermodynamics and the DEM modelling is introduced. The study reduces as a start to a simple system of two particles of different radii connected by a microscopic pendular incompressible liquid bridge in perfect wetting conditions. The energy supplied to the system is determined and 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. The internal energies were also calculated. The results obtained from the first law of thermodynamics show that the interfaces between the different phases present in the medium have significant importance in the macro formulation of energies and must be taken into account.

INTRODUCTION

The macro behavior of unsaturated soils is dictated by the interactions between particles subjected to capillary effects which makes their study in the framework of continuum mechanics no longer sufficient. A micromechanical study where new features due to capillary forces in the medium must be taken into account to better describe how these materials behave is then required.

A micromechanical thermodynamic framework is introduced in the following work. The advantage of such study is that at the level of the microstructure of the soil, it is accounted for all the elements present in the medium, including the interfaces that separates the different phases in the medium.

One of the first to highlight the importance of the interfaces in the formulation of free energy and their influence on the effective stress tensor was Coussy (Dangla & Coussy (2002)).

Other studies also following a thermodynamic approach such as Gray et al. (2002) and Nikooee et al.(2013) have introduced balance laws for interfaces.

Nikooee et al. (2013) proposed a new formulation for the effective stress tensor assuming that the deformation in the soil can result 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. Solid-wetting and solid-non wetting interfaces were neglected in the case of rigid grains.

The main purpose is to test the importance of these interfaces and the energy that must be associated to, 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.

PENDULAR REGIME : NUMERICAL MODEL

At low water content, water bridges are formed between neighboring particles and the regime to which this study is limited is called pendular because in this case the capillary force resultant from the presence of these meniscii can be linked to the geometry of the grains and to the capillary pressure inside the medium by the capillary theory. At higher saturation, things become more complex.

The DEM model for the pendular regime model is inspired by the work of Scholtès et. al. (2012). The grains are rigid spherical grains connected by liquid bridge in perfect wetting conditions.

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

The shape of the liquid bridge is given by Laplace equation that is the exact numerical solution and gives a relationship between the curvature of the bridge and the matric suction in the medium.

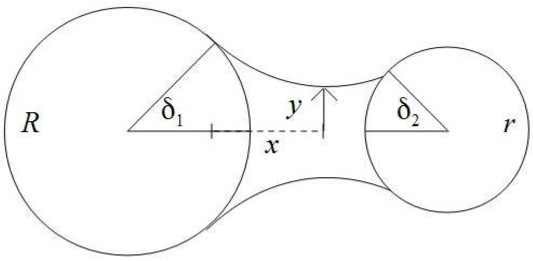

Figure 1. **Illustration of a liquid bridge between 2 spherical particles.**

Solving Laplace equation allows to calculate the capillary force and the geometric properties of the meniscus (volume and interfaces).

The capillary force is calculated at the gorge:

$$F_{cap} = \Pi s y_0^2 + 2 \Pi \gamma y_0 \tag{2}$$

The volume of the bridge is:

$$V = \int \Pi y^2(x) dx - V_1 - V_2 \tag{3}$$

V1 and V2 are the volumes of the spherical caps covered by both filling angles.

$$A_{wn} = \int 2 \Pi y(x) \sqrt{1 + y'^2(x)} dx$$

The wetting-non wetting interface is:

(4)

The solid-wetting interface is:

$$A_{sw} = 2 \Pi R^2 (1 - \cos \delta_1) + 2 \Pi r^2 (1 - \cos \delta_2)$$

(5)

The solid-non wetting interface is:

$$A_{sn} = 2 \Pi R^2 (1 + \cos \delta_1) + 2 \Pi r^2 (1 + \cos \delta_2) \tag{6}$$

The bridge breaks when no physical solution is possible.

ENERGY BALANCE OF A WATER BRIDGE

It is important for any model to verify the laws of thermodynamics that control the interaction between the elements of the system. In this section, the energy balance for a two spheres system connected by a bridge is examined, assuming a linear contact law between the grains and using the pendular bridge model presented in the section above.

We consider a model system of solid, wetted by water in the presence of gaz at atmospheric pressure. The system is inspired by the work of Morrow (1970) (Fig. 2). The solid phase is represented by 2 spherical grains of equal or different sizes. Water can leave or enter the bridge through a passage into one of the particles. The change in the volume of water and surface areas is assumed to be reversible. The walls of the piston have no contribution to the energy of the interfaces and the movement of pistons occurs in a way to keep equilibrium in the sample.

This work extends the work of Morrow (1970) to moving particles. In the 2 grains system presented here, one of the particles is fixed and the other can be either fixed or moving at a given velocity *v*.

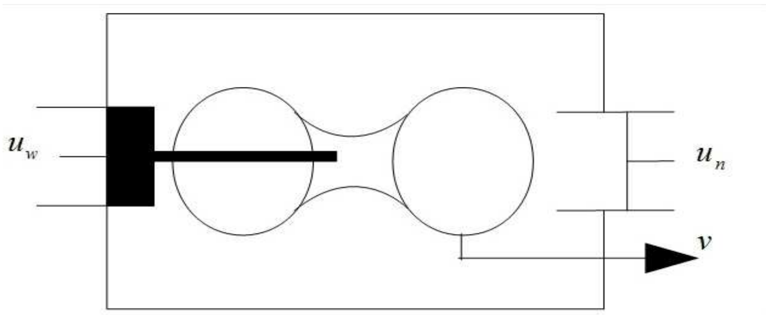

Figure 2. **Idealized system inspired by the work of Morrow (1970)**

The conservation of energy is checked for the system. For the first law of thermodynamic to be verified, the sum of all the internal energies of the components of the system must be equal to the external work supplied to the system.

$$W_{ext} = \Delta E_i \tag{7}$$

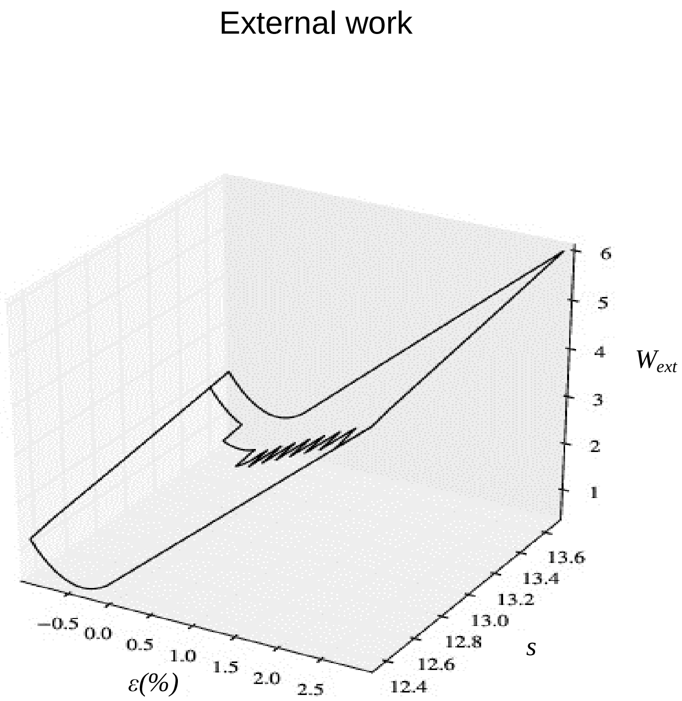

Figure 3. **The paths of external work supplied to the system.**

Different paths of external work are applied either by applying an incremental relative displacement to the particles (keeping the suction constant) or by changing the matric suction s in the medium (keeping both grains fixed) or by changing both together at time.

Figure 3 shows the plot of the external work per volume as function of the suction and the strain, and the different paths applied to the system. It is noticed that the total energy supply

to move the system from a state to another is path independent. Therefore it must be possible to define a formulation for the stored energy depending only on the current configuration.

External work is calculated as the sum of 2 components: a part related to the work done on the system by moving the piston connected to the bridge to provoke a change in the volume of water -dV and one related to the movement of grains.

$$W_{ext} = \int (F_{el} + F_{cap})\, d\alpha - \int s\, dV \qquad (8)$$

W_{ext} is the total external work, s is the matric suction, V is volume of meniscus, F_{el} is the contact force , F_{cap} the capillary force and α is the relative displacement between the grains.

Internal energy

The change in the total internal energy of the system is divided into 4 components, the change in the energies of the three phases present in the system and the change of the energy of the interfaces.

$$\Delta E_i = \Delta E_s + \Delta E_w + \Delta E_n + \Sigma \Delta E_{A_j} \qquad (9)$$

w denotes for wetting, n for non wetting and s for solid. A_j denotes for the three interfaces present in the system.

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

The energy of the solid phase is equal to the elastic energy:

$$\Delta E_s = \Delta E_{el} = \Delta(0.5\, k_N\, x_N^2 + 0.5\, k_T\, x_T^2) \qquad (10)$$

k_N and k_T are relatively the normal and shear stiffnesses.

The change in the interfacial energy is calculated based on the work of Morrow(1970).

$$\Delta E_{cap} = \Sigma \gamma_i \Delta A_i \qquad (11)$$

In this case, the particles are dry, connected by a water bridge. Three types of interfaces is present in the system, the wetting- non wetting, the solid-wetting and the solid-non wetting interface.

$$\Delta E_{cap} = \gamma_{wn} \Delta A_{wn} + \gamma_{sw} \Delta A_{sw} + \gamma_{sn} \Delta A_{sn}$$

(12)

The equilibrium at contact line gives a relationship between γ_{sw}, γ_{sn} and γ_{wn}. In perfect wetting condition this relationship is:

$$\gamma_{wn}=\gamma_{sw}-\gamma_{sn} \quad (13)$$

For rigid particles $\Delta A_{sw}=-\Delta A_{sn}$; Replacing it in the previous equation, the total change in capillary energy is:

$$\Delta E_{cap}=\gamma_{wn}(\Delta A_{wn}-\Delta A_{sw}) \quad (14)$$

ΔA_{sw} , ΔA_{wn} and $\Delta A_{wn}-\Delta A_{sw}$ are plotted in figure 4 as function of strain and suction to evaluate how each of the interfaces contributes in the total interfacial free energy.

The plots show that the variation of ΔA_{sw} and ΔA_{wn} is of the same order of magnitude, and the difference $\Delta A_{wn}-\Delta A_{sw}$ that is proportionnal to the interfacial energy is much smaller than the value of the change of each individual interface. That means that all interfaces vary significantly with suction and deformation and neglecting the energy of one of the interfaces can lead to an overestimation of the free interfacial energy with a significant error.

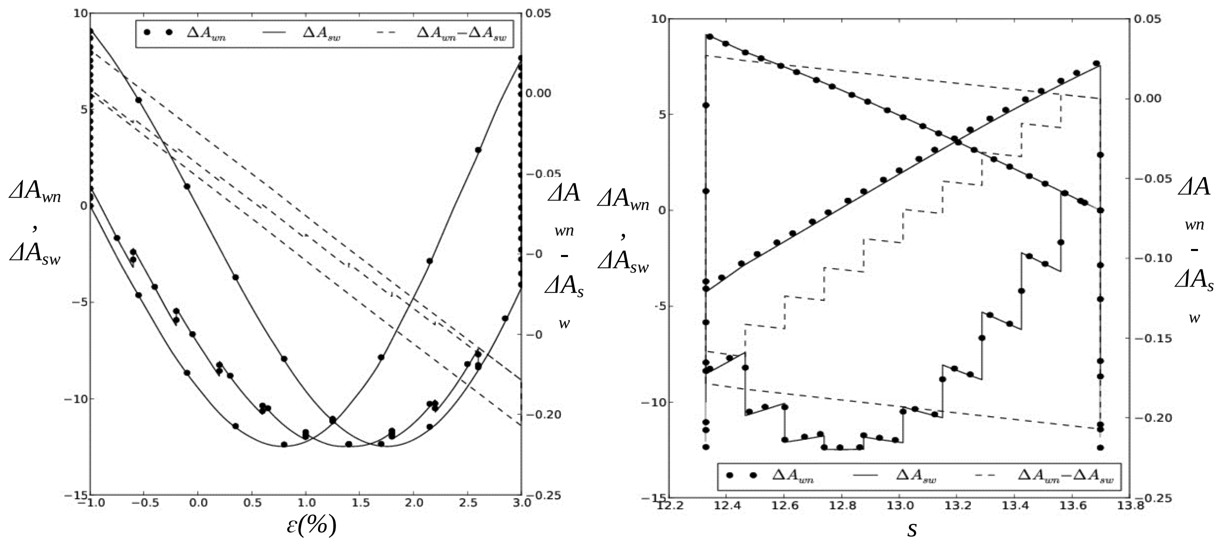

Figure 4. **The plots of the change of the interfaces ΔA_{sw} , ΔA_{wn} and $\Delta A_{wn}-\Delta A_{sw}$ with strain and suction**

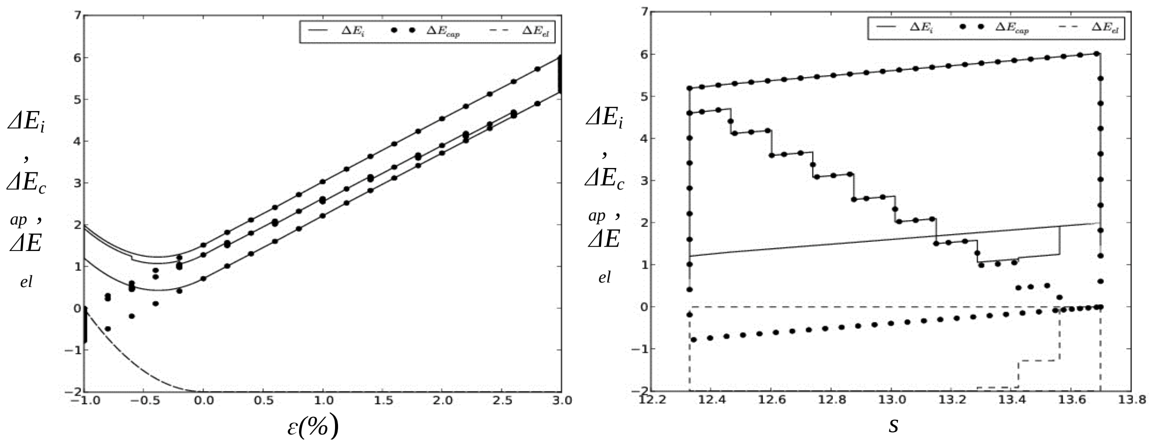

Figure 5. **The plots of the elastic and interfacial energies and the total internal energy stored in the system as function of strain and suction**

The change in internal free energy components and the total free energy that is the sum of both previous components are represented in figure 5 as function of strain and displacement.

FIRST LAW OF THERMODYNAMIC

The external work supplied to the system and total internal energy are plotted as function of strain and suction in figure 6 taking into account the energy of interfaces. The external work is equal to the internal energy stored in the system and the numerical error doesn't exceed 2 percent.

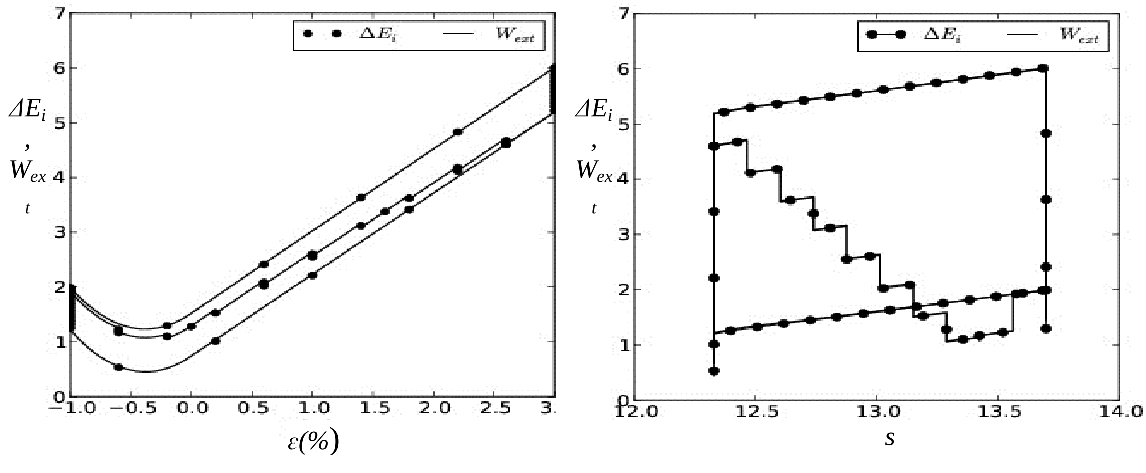

Figure 6. **The plots of the external work and the total internal energy stored in the system as function of strain and suction**

Figure 5. shows also that the interfacial energy may be significant. When the grains for example are distant, the elastic energy is equal to zero while the external work is not null since the grains are moving. If only the elastic energy was taken into account, the energy balance of the system is not verified and there are obviously missing terms that must be taken into account. These terms are equal to the energy of the interfaces in the system.

CONCLUSION

The energy balance for 2 grains connected by water bridge was verified in this work. It has been shown that the energy balanced is not verified without the energy of interfaces that play an important role in the behaviour of unsaturated soil and their energy must be taken into account. The variation of each of the interfaces was also checked and it has been shown that all interfaces must be taken into account to estimate correctly the total interfacial energy in the system.

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