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Microstructural Modeling of Granular Materials with Inner Forces

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Summary. In this paper, we present a method to take into account the existence of inner forces between grains and their influence upon the mechanical behavior of granular assemblies. Two examples were retained. The first one concerns unsaturated granular materials for which we have considered capillary forces depending on the degree of saturation. The second one concerns extraterrestrial soils for which surface energy forces, such as Van der Waals forces, cannot be neglected due to tiny atmospheric pressure.

Keywords: granular materials, capillary forces, surface energy forces, homogenization.

1 Introduction

Macroscopic properties of granular materials are governed by the properties of inter-particle contacts. A homogenization technique has been developed to obtain an elastoplastic stress-strain relationship for these types of materials using a static approach. This approach is based on a technique consisting of a localization operator relating the macro stresses to the local contact forces and a homogenization operator relating the grain displacements to the macro strains. Local forces and displacements are related through a constitutive law at the contact level.

2 Dry Unbounded Granular Materials

For dry unbounded granular materials under common environmental conditions, the inter-particle forces are solely related to the applied external stresses. Detailed expressions of the homogenization and localization operators, and of the local constitutive law, are given in Chang and Hicher [1]. Comparisons of experimental results and numerical simulations have demonstrated the ability of this model to reproduce accurately the overall mechanical behavior of granular media and to account for the influence of key parameters such as void ratio and mean stress.

3 Unsaturated Granular Materials

When a certain amount of water is added to the grain assembly, significant changes, such as an increase in stiffness and strength, can be observed. These changes can be explained by the formation of water menisci between neighboring particles, which creates capillary forces. The amplitude of these capillary forces depends upon the degree of saturation and the morphology at particle level (grain and pore sizes). For modeling the behavior of unsaturated granular materials, capillary forces at the grain contacts are, therefore, added to the contact forces created by an external load. They are calculated as a function of the degree of saturation, depending on the grain size distribution and on the void ratio of the granular assembly. Numerical simulations show that the model is capable of reproducing the major trends of a partially saturated granular assembly under various stress and water content conditions.

In this study, we retained the following expression

$$f_n^{cap} = f_{\max} e^{-c\left(\frac{d}{R}\right)} \quad (1)$$

where f_{cap} is the capillary force between two neighboring grains, not necessarily in contact, $f_{\max}$ is the value of f_{cap} for two grains in contact, and R is the mean grain radius, d represents the distance between two grains and is equal to $l - 2R$, l being the branch length given as a distribution function of the grain size and the void ratio, c is a material parameter, dependent on the grain morphology and on the water content, $f_{\max}$ depends on the capillary pressure defined as the pressure jump across the liquid-air interface, on the liquid-air interface surface tension, as well as on the geometry of the menisci governed by the solid-liquid contact angle and the filling angle. In this study, a simplified approach was developed that considers an empirical relation between $f_{\max}$ and the degree of saturation S_r , without taking into account the hysteresis along drying and wetting paths

$$\begin{aligned} f_{\max} &= f_0 \frac{S_r}{S_0} & \text{for } 0 < S_r < S_0 \\ f_{\max} &= f_0 \frac{S_0(1-S_r)}{S_r(1-S_0)} & \text{for } S_0 < S_r < 1 \end{aligned} \quad (2)$$

where f_0 and S_0 are material parameters. f_0 depends on the grain size distribution, S_0 represents the degree of saturation at which any further drying of the specimen will cause substantial breaking of the menisci in the pendular domain. S_0 depends on the nature of the granular material. The following empirical expression was proposed by Wu *et al.* [4] for compacted granular materials:

$$(S_r)_{opt} = (-0.65 \log(d_{10}) + 1.5) / 100 \quad (3)$$

in which $(S_r)_{opt}$ is equivalent to S_0 in Eq. 5, d_{10} is the effective grain size in mm.

Figure 1 presents numerical simulations of water constant triaxial tests on a silty sand at various degrees of saturation. An overall good agreement with experimental results could be reached, particularly the evolution of the maximum strength as a function of the degree of saturation was well obtained by the model.

Fig. 1. Influence of the degree of saturation on constant water content triaxial tests on silty sand

4 Granular Materials with Surface Energy Forces

Environmental conditions can also modify the behavior of granular media. All materials, with or without a net surface charge, exhibit surface energy forces which act at a very short range. But whereas these forces are negligible for common sand or silty sand on Earth, they play a significant role under tiny atmospheric pressure. The mechanical behavior of the subsurface soil on Moon and Mars is, therefore, expected to be significantly different from that on Earth. The model is then extended to include Van der Waals forces in order to describe the possible behavior of these extraterrestrial soils. Van der Waals forces acting between two particles can be considered as the sum of two terms, one due to the interaction between two flat surfaces of area $S = \pi a^2$ and one along the remaining surface of the two spheres. Using the Derjaguin approximation for the second term, we obtain the expression of the Van der Waals force between two particles:

$$f = \frac{A}{6D^3} a^2 + \frac{AR}{12D^2} \quad (4)$$

where A = Hamaker coefficient; D thickness of molecules layer between two particles; R = the radius of particles. Hamaker constant A was estimated to be 4.3

$\times 10^{-20}$ J. for lunar soil and 1.5×10^{-20} J. for terrestrial quartz sand (Perko et al. [3]). The thickness of molecules layer between two particles D is highly dependent on the atmospheric pressure and composition. On the Moon, the atmospheric pressure is nearly zero, which can lead to a very thin layer of molecules between two particles compared to that under terrestrial environment. Therefore, according to Eq. (4), it is reasonable to expect that the surface energy forces between particles are much higher than those between particles under terrestrial environment. Under these conditions and in accordance with the observations made on the Moon's surface, the model shows that lunar soil has an additional component of shear strength described by a cohesion, c , higher than the one which could be found on Earth. Besides, because the radius a of the contact area in Eq. (4) increases with confining stress of a specimen, the surface energy force also increases with confining stress, which indicates that the surface energy force will contribute to the shear strength not only on the cohesive component but also on the frictional component. Figure 2 shows the influence of the distance D between the particles on the shear strength for soil specimens under 20 kPa confining stress, where q_0 represents the shear strength for soil without surface energy forces and q represents the shear strength with the effect of surface energy forces.

Fig. 2. Effect of distance between particles on shear strength

Predictions of the model indicate that the soil under extremely low atmospheric pressure has an increase of shear strength by several kPa higher than the one which would be present under the atmospheric pressure of the Earth's. This result is in accordance with the general trend observed in situ. The magnitude is in the same order as the measured increase of shear strength for lunar soil simulants tested under the usual atmospheric pressure and under a chamber with ultrahigh vacuum.

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