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A novel liquid bridge model for estimating SWCC and permeability of granular material

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ABSTRACT

As traditional liquid bridge model based on Yang–Laplace theory fails to model behaviors of unsaturated granular materials when liquid bridges fuse with each other in funicular and capillary regimes, a method called "Redistribution of Air Volume and Reduction of Liquid Bridge Force" is proposed, and incorporated into the original discrete element method to resolve this issue. Both soil water characteristic curve and suction stress characteristic curve are worked out by the modified discrete element method, the results of which coincide with theoretical solutions for simple cubic packing and tetrahedral packing of granular materials. Furthermore, parameter study shows that soil water characteristic curve depends on effective particle diameter, particle size distribution and packing density. Typical soil water characteristic curves of sand and silt are obtained using the modified method, with a trend similar to that of experiment qualitatively. With the help of Mualem model and Kozeny–Carman equation, permeability is also predicated for granular materials. In particular, the air entry value coincides with or close to those of typical sand and silt in magnitude. Finally, a case study of SWCC prediction for sandy soil is implemented with acceptable results. We may conclude that the modified discrete element method is capable of predicting hydraulic properties of granular materials qualitatively and semi-quantitatively.

1. Introduction

There is vast expanse of arid and semi-arid areas on the earth surface where soil is mostly in an unsaturated state. Hence, people need to explore seepage flow in unsaturated soil for economy related to agriculture, forestry and husbandry. On the other hand, it is indispensable to have an in-depth understanding of terrestrial process for climate study, in which water and heat exchanges between land and atmosphere are remarkably important [1]. In particular, when the strategic plan of natural and human induced disasters was put on the agenda of International Council of Scientific Unions (ICSU), people have paid more attention to extreme hydro-meteorological hazards such as landslides and debris flows [2]. In order to reduce the risk in this regard, it is necessary for us to explore their mechanism by following the transient seepage process from unsaturated to saturated states in disaster evolution. During heavy rainfall, infiltration and runoff take place over a slope and the saturated zone gradually expands with a wet front moving downwards [3,4]. Fu and Li have also noticed that the strength degradation or softening of soil with the degree of saturation plays a decisive role to initiate landslides, and they have proposed three water-induced softening models [5]. Therefore, poor understanding in both mechanical and hydraulic behaviors of unsaturated granular materials motivated us to study this topic by discrete element method (DEM) based on micromechanics in this paper.

For unsaturated soil, we know that the soil matric suction may consist of matric or solute potentials etc. [6]. Soil water characteristic curve (SWCC) describing the relationship between suction and water content provides constitutive relationship, major parameters such as specific water capacity, relative permeability [7] and so on, are of great importance for unsaturated seepage. At the same time, SWCC plays a significant role in constitutive modeling of wet granular materials, which couple the hydraulic and mechanical behaviors, such as Li [8], Sheng [9] and Gens [10]. SWCC is usually obtained via numerical fitting of experimental data of soil moisture and suction tests by mathematical models, such as the Brooks and Corey (BC) model [11], van Genuchten (VG) model [12], and Fredlund and Xing (FX) model [13]. Although prediction of SWCC by using particle size distribution and capillary water state has progressed a lot [14–16], deep mechanism and coupling of capillary water and particles still need to be studied. Because the experimental measurements of permeability for unsaturated granular materials are hard and time consuming, permeability can also be easily worked out by integration of SWCC based on statistical methods including the Mualem model [17] and Burdine model [18].

Recently, DEM developed in 1979 by Cundall [19], has been extended to investigate behavior of unsaturated granular materials. Mechanical interaction between particles such as normal, shear and rolling

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interaction [20–23] has matured and already been incorporated into a few open source DEM code such as Yade [24]. In contrast, the work on physical–chemical interaction between particles is relatively fewer and only the works of Anandarajah [25,26] and Jiang [27] are representative. Furthermore, the study on influence of water content on physical–chemical process is especially lacking. Richefeu [28,29], Shamy [30] and Soulié [31] allowed liquid bridges to form in between separated but closing particles and calculated liquid bridge force by approximate formulae. Jiang [32] assumed that meniscus occurs in contacting particles then with liquid bridge force calculated explicitly by analytical formulae. Scholtès [33–35] worked out ten files recording both liquid bridge force and meniscus volume in dimensionless form and thus facilitate the calculation of liquid bridge force by interpolation. Liquid bridge model based on Yang–Laplace theory has been applied to investigate behavior of unsaturated granular materials. For instance, Richefeu [28] and Scholtès [33] studied the cohesion of three dimensional disperse granular materials in this way and found that cohesion increases with water content in pendular state. Scholtès [34] also produced SWCC in pendular state and analyzed hysteresis by ink-bottle mechanism.

All aforementioned scientists only restricted their research in the pendular state of unsaturated granular materials. Almost there is no research available to consider the interaction force and liquid volume of unsaturated soil in funicular and capillary regimes in the framework of DEM-liquid bridge coupling model. As an exception, only Jiang [32] preliminarily touched on the issue when he was concerned with effective stress of unsaturated granular materials.

A method called "Redistribution of Air Volume and Reduction of Liquid Bridge Force" is proposed based on the work of Jiang [32] in this study to extend the original liquid bridge model by the Young–Laplace theory in DEM to funicular and capillary regimes. Section 2 describes DEM and "Redistribution of Air Volume and Reduction of Liquid Bridge Force" approach in detail. The verification of this new approach is implemented in Section 3 for simple cubic packing and tetrahedral packing. Section 4 further addresses the influences of particle size distribution, packing density, effective diameter and confining stress on SWCC and permeability by numerical simulation based on this modified DEM. A case study for the sandy soil is implemented in Section 5. Finally, we come to a few very useful conclusions.

2. DEM and modified DEM

Since the invention of DEM by Cundall and Strack [19], DEM has been widely applied to study fundamental behavior of both soil and rock, such as dilatancy of granular materials [23,36,37], behavior of rock and rock joint under uniaxial and triaxial compression etc. [38,39]. With inter-particle capillary force taken into account, DEM has been extended to examine the behavior of unsaturated granular materials including SWCC [32] and strength under bi/triaxial compression tests [32,33] in recent years. For instance, liquid bridge model based on Yang–Laplace theory has been broadly used and implemented in Yade [40]. However, the work of Scholtès [33–35] is only applicable in pendular regime, while the 2D approach of Jiang [32] is suitable for cases when liquid bridges exist between contacting particles. The method fails to model 3D granular material phenomena in funicular and capillary regimes due to the complicated water distribution in the packing.

Based on the works of both Jiang [32] and Scholtès [35], the "Redistribution of Air Volume and Reduction of Liquid Bridge Force" approach is proposed and implemented on the platform of the open source Yade [41].

2.1. Contact model

The interaction between two contacting particles is decomposed into a normal component F_n and a shear component F_s, where the normal part is modeled by a spring with stiffness k_n, and the shear part is modeled by a shear spring with stiffness k_s. The definitions of k_n and k_s are shown in Eqs. (1) and (2), in which E is contact modulus of particles, R_1 and R_2 are diameters of the two contacting particles, respectively. The objective of doing so is to keep macroscopic the Young's modulus of granular packing proportional to the contact modulus [33]. A Mohr–Coulomb friction is added into the shear part to simulate the frictional behavior as shown in Eq. (3), where μ and ϕ are friction coefficient and inter-particle friction angle, respectively. If not specially stated in the following passage, contact modulus E is assumed as 50 MPa, α as 0.4 and ϕ as a number of values until 30° corresponding to different initial porosities.

$$k_n = 2 \cdot \frac{E \cdot R_1 \cdot R_2}{(R_1 + R_2)} \tag{1}$$

$$k_t = \alpha \cdot k_n \tag{2}$$

$$\mu = \tan(\phi) \tag{3}$$

2.2. Calculation of liquid bridge force and volume

Water inside the pores of granular materials exhibits some kinds of morphologies, namely, pendular, funicular and capillary states. In the pendular regime when water saturation degree is as low as 15%, water exhibits a clear pattern and liquid bridges may occur in between independent particles. It is obvious that the surface of a liquid bridge can be formed by revolving an arc tangent to two spherical particles, as shown in Fig. 1. Based on Yang–Laplace theory, the relationship between suction Su and principal curvature radius r_1 and r_2 can be written in Eq. (4), where σ is the surface tension.

$$Su = \sigma\left(\frac{1}{r_2} - \frac{1}{r_1}\right) \tag{4}$$

If the liquid bridge force pulling the two particles towards each other is represented by F^{cap} [35], then F^{cap} and the bridge volume can be calculated via iteration of Eq. (4). All the work has been completed by Scholtès [33,35] and incorporated into Yade.

2.3. "Redistribution of air volume and reduction of liquid bridge force" approach

The above theory and numerical implementation have already been applied to investigate behavior of unsaturated granular materials including SWCC and triaxial compression behavior only in the pendular state. As water content is increasing, however, a liquid bridge is very possible getting closer to its neighboring bridges and then fusion of them may occur, as shown in Fig. 2. In particular, the pore space between them can soon be flooded by water when bridges become unstable. Then the granular material is in the funicular regime, in which slight reduction of pore pressure can result in apparent rise in water content. As water content continues to grow, wet granular material will be in its capillary regime, which is already very close to saturated regime and the granular materials are usually regarded as saturated soil.

If liquid bridge fusion happens, new physical theory and numerical algorithm for the calculation of force and water volume between particles should be developed. Nevertheless, there is no straightforward method available for capillary force and water volume in this regime thus far owing to the complicated reticulate morphologies of water in pores [2]. For this reason, a new approach as a simplification of the above fusion process is proposed. Liquid bridge model based on Yang–