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DEM and experimental analysis of the water retention curve in polydisperse granular media

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ABSTRACT

We investigate the water distribution and the link between suction and water content in granular media. Firstly, we examine the effect of suction on the shape and the volume of the liquid bridge by four different methods. Method I is based on the local expression of the capillary force coupled with the gorge method and Method II is based on the Laplace law. These two methods use the toroidal approximation. Methods III and IV are based on the integration of the differential equation that defines the liquid bridge shape (established from the Laplace law). This local behaviour is then used in a discrete element study of a sample composed of several thousands of grains. We focus our study on the pendular state. A liquid film around the grains involving the continuity of the liquid phase is assumed. The water distribution and the water content associated with a given suction are calculated. Then retention curves of the granular media are built. A parametric study is made to bring to light the effect of macroscopic parameters (grain-size distribution) and physical parameters (liquid/air surface tension and contact angle) on the water retention curve. Finally, numerical data are compared to experimental results.

1. Introduction

A realistic description of the physical phenomena at the grain scale is necessary to understand better the overall behaviour of a granular material. The macroscopic behaviour can then be predicted by including such local interactions in numerical simulations by the discrete element method (DEM) [1]. This numerical analysis technique, based on the discretization of the domain into a set of particles, uses basic constitutive laws to define inter-particle contacts and interactions between grains in order to provide the macroscopic behaviour of the entire sample. This method is very useful and can even predict quantitatively the macroscopic behaviour of a granular material [2,3]. In this paper, we focus on the capillary interaction at the local scale with the study of the relation between the suction and the properties of a liquid bridge.

Water in granular media and powders can strongly affect their texture and rheology. Due to their fine grain-size distribution and high density, these media can have large hygroscopic domain (water forms thin adsorption layers on the grain surface) and pendular domain (water form liquid bridges between grains in contact or close to be in contact). In the pendular domain, the water distribution creates attractive forces between particles, due to the surface tension and the pressure difference $\Delta p = p_a - p_w$ between the air pressure (p_a) and the liquid pressure (p_w) across the liquid bridge interface. This difference is called capillary pressure or suction s at the local scale. Capillary forces are sufficient to ensure the mechanical stability of a soil even without external stress confinement (sand castles). Former works on capillary forces in a granular media—using DEM—underlined the effect of capillary interactions on the macroscopic cohesion [2,3]. Two points have been underlined: the number of liquid bridges per grain is a key point to ensure macroscopic strength [3], whereas the liquid bridge volume doesn't have strong effect on strength. In these studies, the liquid bridge volume was obtained using geometrical configuration such as grain radius and inter-particle distance.

Polydispersity is a generic feature of granular materials. Commonly, granular media (soils and powders) involve a broad range of particle sizes produced by fragmentation and aggregation processes. The pore space characteristics of granular media directly depend on the polydispersity. It has been shown [4] that the macroscopic cohesion of a wet granular material increases with polydispersity and that the water retention curve depends on the polydispersity [5] (slope of the water retention curve and air entry value). Some authors have yet calculated water retention curves of monodisperse granular media [6,7]. Recently, water retention of polydisperse granular media was calculated [8]—coupling DEM and an interpolation scheme on a set of discrete solutions of the Laplace law to calculate the water content for a given suction—but without comparison to real samples.

Literature provides few experimental data on water retention curves in model media. An original experimental device to study this point is made. The water retention curves obtained for two different samples (different grain-size distribution) of spherical glass beads are presented.

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The following study presents 4 approaches to have an accurate estimation of the liquid bridge volume between the grains as a function of the suction. Then, the relation between suction and water content also called water retention curve is studied numerically. The purpose of this paper is to give a numerical approach to model water retention curves for polydisperse granular media and to compare the results with experimental water retention curves.

2. Water retention at the local scale

We study the liquid bridge between two spherical grains. We call "grain-pair" the assembly of two grains linked by a liquid bridge. For given geometrical characteristics (grain radius and inter-particle distance) of the grain-pair, and given physical characteristics (contact angles and liquid/air surface tensions), we examine the effect of suction on the shape and the liquid bridge volume by four different methods. Methods I and II are based on the toroidal approximation, in which the meridional profile of the liquid is assumed to be an arc of circle (Fig. 1). This approximation doesn't respect the Laplace law in the whole liquid bridge since the liquid pressure is not constant in every part of the liquid bridge (the outer radius is constant). Nevertheless, the toroidal approximation leads to good results comparing with experimental data [9]. Methods III and IV are based on the integration of the differential equation that defines the liquid bridge shape. The liquid bridge volume is given by:

$$V = \pi\int_{x_{c1}}^{x_{c2}} y^2(x)dx - V_1 - V_2 \tag{1}$$

$y(x)$ defines the meridional profile of the liquid which is an arc of circle in the toroidal approximation. For Method IIIs and IV, it is the solution of the differential equation (Eq. (6)) that defines the shape of the liquid bridge. x_{c1} and x_{c2} are respectively the x-positions of the contact line with grains 1 and 2. V_1 and V_2 are respectively the dimensionless volumes of portions of grains 1 and 2 which are recovered by the liquid bridge.

2.1. Method I: use of the Laplace law

The Laplace law postulates that the pressure difference $\Delta p = p_a - p_w$ (suction s) between the gas phase (p_a) and the liquid phase (p_w) across the interface between two fluids is equal to the product of the surface tension σ and the mean curvature of the liquid bridge $C = \frac{1}{\rho_{int}} + \frac{1}{\rho_{ext}}$, where ρ_{int} and ρ_{ext} are the algebraic curvature radii of the surface. $\rho_{int} = -h$ and $\rho_{ext} = \rho$ because the suction is calculated at the center of the meniscus and the liquid bridge shape presents inversed curvature. So the Laplace expression is defined by:

$$\Delta p = s = \sigma\left(\frac{1}{\rho} - \frac{1}{h}\right) \tag{2}$$

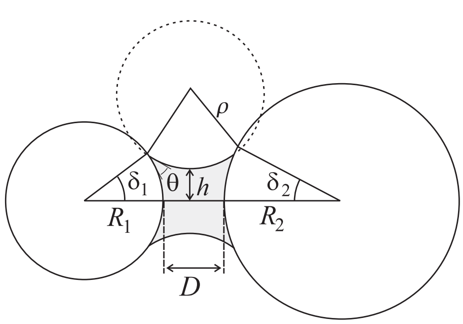

Fig. 1. Geometrical model of the toroidal approximation of liquid bridge between two grains of different sizes: ρ is the liquid bridge outer radius, h is the gorge radius, D is the inter-particle distance, δ_1 and δ_2 are the filling angles, θ is the contact angle and R_1,R_2 the grain radii with $R_1 \leq R_2$.

ρ and h are functions of $\delta_1, \theta, R_1, R_2$ and D. It is thus possible to find the filling angle δ_1 for given geometrical configuration and suction and then to calculate the appropriate liquid bridge volume using Eq. (1).

2.2. Method II: local expression of the capillary force and the "gorge method"

The capillary force F_{cap} due to the liquid bridge is directly linked to its geometry. Using the "gorge method" [10], it is assumed that the capillary force depends on the contribution of the surface tension σ and the suction s. The capillary force is calculated at the gorge of the liquid bridge and its expression is given by:

$$F_{cap} = 2\pi h\sigma + \pi h^2 s. \tag{3}$$

Using dimensionless numbers $F^*_{cap} = \frac{F_{cap}}{2\pi\sigma R_2}$ and $h^* = \frac{h}{R_2}$, it is possible to express the suction s as:

$$s = 2\frac{\left(F^*_{cap} - h^*\right)\sigma}{(h^*)^2 R_2}. \tag{4}$$

The relation between the capillary force and configuration of the grain-pair is described by a system of coupled non-linear equations. This system is numerically solved for several configurations of the grain-pair. An appropriate fitting form for this set of numerical solutions is [2]:

$$F^*_{cap} = \frac{\sqrt{r}}{2}\left(c + \exp\left(aD^* + b\right)\right). \tag{5}$$

Where $D^* = \frac{D}{R_2}$ and $r = \frac{R_1}{R_2}$.

The coefficients a,b and c are functions of the liquid bridge volume V, the contact angle θ and R_2. The proposed fitting form (Eq. (5)) is consistent with experimental results reported both by Willet et al. [11] and Soulié et al. [2]. Using Eqs. (1), (4), (5) and geometrical considerations, the calculation of the liquid bridge volume V is done for a given suction.

2.3. Methods III and IV: integration of the differential equation

The shape of the liquid bridge (Fig. 2) is described by a differential equation [12]:

$$Hy^*(x^*) + \sigma\frac{1 + \dot{y}^{*^2}(x^*) - y^*(x^*)\ddot{y}^*(x^*)}{\left(1 + \dot{y}^{*^2}(x^*)\right)^{\frac{3}{2}}} = 0. \tag{6}$$

Where $x^* = \frac{x}{R_2}$, $y^* = \frac{y}{R_2}$ and $H = \frac{sR_2}{\sigma}$.

This equation can be established from the Laplace law. Using the boundary conditions at the gorge as well as at the contact line, we numerically solve Eq. (6) looking for a polynomial solution (Method III) or using the numerical method based on a trapezoidal rule[1] (Method IV). The polynomial approximation is only composed of pair powers. Then, it is possible to calculate the liquid bridge volume V for given suction s, geometrical and physical parameters (R_1, R_2, D, σ, θ).

2.4. Result of the local study

For given $R_1, R_2, D, \sigma, \theta$ and s, it is possible to determine the volume of the liquid bridge. Fig. 3 presents the relation between the liquid bridge volume and the inter-particle distance for given suctions using the four methods. Method IV, which gives the more exact solution,

[1] Function ode23t in Matlab in this case.