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A model of capillary cohesion for numerical simulations of 3D polydisperse granular media

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SUMMARY

We present a 3D discrete-element approach for numerical investigation of wet granular media. This approach relies on the basic laws of contact and Coulomb friction enriched by a capillary force law between particles. We show that the latter can be expressed as a simple explicit function of the gap and volume of the liquid bridge connecting a pair of spherical particles. The length scales involved in this expression are analyzed by comparing with direct integration of the Laplace–Young equation. We illustrate and validate this approach by application to direct shear and simple compression loadings. The shear and compression strengths obtained from simulations reproduce well the experimental measurements under similar material and boundary conditions. Our findings clearly show that the number density of liquid bonds in the bulk is a decisive parameter for the overall cohesion of wet granular materials. A homogeneous distribution of the liquid within the bridge debonding distance, even at low volume contents, leads to the highest cohesion. The latter is independent of the liquid content as far as the liquid remains in the pendular state and the number density of liquid bonds remains constant. Copyright © 2007 John Wiley & Sons, Ltd.

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KEY WORDS: capillary cohesion; discrete-element approach; shear strength; compression strength

1. INTRODUCTION

Granular materials are composed of well-defined particles with specific kinematics locally dictated by steric constraints and unilateral interactions that are responsible for the rich behavior of these materials at the macroscopic scale. These materials can thus be modeled at the particle scale, and various particle properties (shape, size, etc.) and contact interactions (friction, adhesion, etc.) can be quite naturally introduced in discrete-element numerical simulations of the material. In the same way, external and environmental factors such as moisture and temperature may be included

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in the description through dependence of local parameters with respect to such factors. In spite of drawbacks, mainly related to unavoidable simplification of the local description and the number of particles limited by computational efficiency, this approach with the corresponding numerical developments provides new scopes for a better understanding of the behavior of complex materials from their rich microstructural properties. Discrete-element method (DEM) for the simulation of dry granular media, first popularized by the pioneering work of Cundall and Strack [1], has evolved into a mature technique during the two last decades [2–5]. The focus is now mostly directed towards the inclusion of new ingredients such as cohesion due to cementation or capillary bonding as in unsaturated soils [6–9].

This paper is concerned with the mechanical behavior of wet granular materials investigated both by a discrete-element approach and experiments. Wet granular materials are of primary interest to various fields of science of engineering such as the mechanics of granular soils and wet processing of powders [10, 11]. Capillary cohesion is negligibly small for coarse soils or at high confining stresses. On the other hand, the moisture and the resulting cohesion are important for fine surface soils. For example, when plowing a wet granular soil, large cohesive aggregates are formed. The largest capillary cohesion force for millimeter-size sand grains is about 4×10^{-4} N independent of the volume of the capillary bond. This force is nearly four times the grain weight, allowing thus for the formation of cohesive aggregates. Transformations involving primary particle agglomeration into coherent granules are of special interest in many applications in a wide range of industries such as pharmaceuticals, agronomic products and detergents [10, 11].

Recently, several simulations of wet granular media have been reported [12–14]. Mikami *et al.* [15] used this type of simulation together with a regression expression for the liquid bridge force as a function of liquid bridge volume and separation distance between particles. They mainly studied bubbling behavior and agglomerate formation in a fluidized bed and they found realistic results. Dense agglomerates were simulated by Gröger *et al.* [16] using a cohesive DEM. They found a good agreement with experimental data for the yield stress at all confining pressures down to the value of the tensile stress. Shear strength behavior of unsaturated granulates was also studied numerically by Jiang *et al.* [17] as a function of suction (pressure difference between liquid and gas).

From the experimental point of view, the point is that classical testing machines employed in soil mechanics are designed to work at high levels of confinement and they involve massive elements that induce high inertia. For these reasons, they are not adapted for wet granular materials. Direct measurements of tensile strength by means of appropriate experimental setups have been reported recently [18–20]. In granular media, it is generally much more difficult to access local information such as contact forces or liquid bonds. Few investigations have recently been reported to visualize liquid bonds by means of the index matching technique [21, 22].

Hence, both the numerical implementation of capillary interactions and the use of appropriate testing techniques are key aspects of the present work. In this paper, we present a new expression for the capillary force as an explicit function of the interparticle gap and local volume of the liquid. We show that this expression provides excellent fit for the capillary force between two particles of unequal sizes. This expression is used to perform DEM simulations of direct shear and simple compression tests, which are compared with experimental data obtained by means of an appropriate testing setup. In the following, we first present in Section 2 the numerical approach with focus on capillary cohesion. In Section 3, we apply the method to direct shearing of wet granular samples. The main characteristics of our experimental setup designed for low confining stress are described in this section. We compare the numerical and experimental data, and we analyze the effect of water

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content and the numerical density of capillary bonds. A similar approach is presented in Section 4 in the case of simple compression tests that confirm the good agreement between numerical and experimental data as to stress–strain behavior and the effect of liquid distribution. We conclude with a summary of the main results and perspectives of this work.

2. NUMERICAL METHOD

We used the DEM in the spirit of molecular dynamics with a velocity Verlet integration scheme [1, 23]. In DEM simulations, the equations of motion of the particles are integrated incrementally by taking into account the interactions between the particles according to an explicit molecular-dynamics-like scheme. The realism of such simulations is thus dependent on the underlying model of the interactions. For numerical stability, the time step was set to 10% below the elastic response time $\Delta t_c = \pi\sqrt{m/K_\mathrm{n}}$, where m is the smallest particle mass and K_n is the largest normal stiffness in the system [1, 23]. In quasi-static loadings, where the inertia plays no major role, the particle masses can be increased artificially, allowing thus for larger time steps. On the other hand, the damping rate v_n should be below the critical value $v_\mathrm{crit} = 2\sqrt{mK_\mathrm{n}}$. In this section, we first present the interaction laws that we used for elastic contact, Coulomb friction and capillary cohesion. We discuss in more detail a new analytical form that we propose for the capillary force as a function of the gap and local water volume. Then, we present the protocols for deriving the distribution of liquid in the bulk.

2.1. Normal repulsion force

The force laws involve normal repulsion, capillary cohesion, Coulomb friction and normal damping. The normal force f_n is modeled as a sum of three contributions:

$$f_\mathrm{n} = f_\mathrm{n}^\mathrm{e} + f_\mathrm{n}^\mathrm{d} + f_\mathrm{n}^\mathrm{c} \tag{1}$$

where f_n^e, f_n^d and f_n^c are the repulsive contact force, damping force and capillary force, respectively.

The repulsive force between two smooth elastic spheres is given by the Hertz approximation that expresses the repulsion force as a function of the distance between two spheres [24]. From a computational viewpoint, it is more common to use a linear approximation where f_n^e depends linearly on the normal distance δ_n between the particles (Figure 1(a)):

$$f_\mathrm{n}^\mathrm{e} = \begin{cases} -k_\mathrm{n}\delta_\mathrm{n} & \text{for } \delta_\mathrm{n} < 0 \\ 0 & \text{for } \delta_\mathrm{n} \geqslant 0 \end{cases} \tag{2}$$

where k_n is the normal stiffness.

The damping term f_n^d accounts for inelastic shock between particles. The simplest model of damping is a viscous force depending linearly on the normal velocity $\dot{\delta}_\mathrm{n}$:

$$f_\mathrm{n}^\mathrm{d} = \begin{cases} 2\alpha_\mathrm{n}\sqrt{mk_\mathrm{n}}\dot{\delta}_\mathrm{n} & \text{for } \delta_\mathrm{n} < 0 \\ 0 & \text{for } \delta_\mathrm{n} \geqslant 0 \end{cases} \tag{3}$$

where $m = m_i m_j/(m_i + m_j)$ is the reduced mass of the particles i and j, α_n is a damping rate varying in the range $[0, 1[$. The rate of normal dissipation or the restitution coefficient between particles can be expressed as a function of α_n [25].

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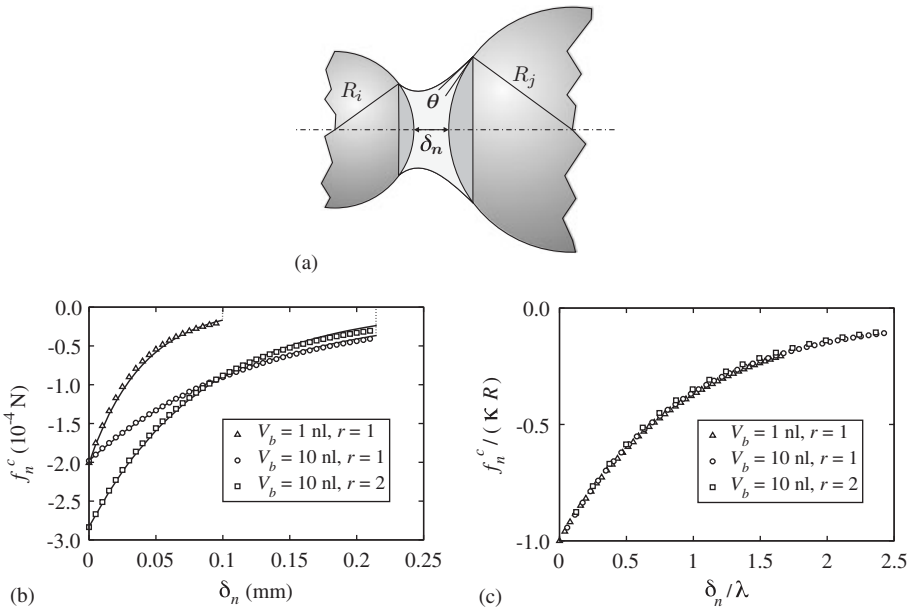

Figure 1. (a) Geometry of a capillary bridge; (b) capillary force f_n^c as a function of the gap δ_n between two particles for different values of the liquid volume V_b and size ratio r according to the model proposed in this paper (solid lines), and from direct integration of the Laplace–Young equation (open circles); and (c) scaled plot of the capillary force as a function of the gap from the direct data shown in (b).

The repulsion force f_n^e together with the viscous damping force f_n^d defines a spring-dashpot model commonly used for the simulation of dry granular media. Subtle changes to this framework allow for more realistic description of shock laws and nonlinear elastic regimes [25]. Since we are interested here in capillary interactions, we stay with this basic framework and focus on the capillary force f_n^c.

2.2. *Capillary force*

Capillary force f_n^c is a function of the liquid bond parameters, namely the gap δ_n, the liquid bond volume V_b, the liquid surface tension γ_s and the particle–liquid–gas contact angle θ. The capillary force can be obtained by integrating the Laplace–Young equation [15, 26–28]. However, for efficient DEM simulations, we need an explicit expression of f_n^c as a function of the liquid bond parameters. On the other hand, most authors have considered the capillary force for liquid bond between two spheres of the same diameter. When the diameters are different, the Derjaguin approximation is used. Recently, by means of experiments and fitting considerations, Soulié *et al.* [28] proposed an expression for the capillary force between two smooth spheres. Here, we propose a new expression for the capillary force that can be considered as a simplified and analytical writing of that expression. We show that this form is well fitted by the data from direct integration of the Laplace–Young equation both for monodisperse and polydisperse particles.

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The geometry of a capillary bridge between two spherical particles of unequal diameters is illustrated in Figure 1(a). At leading order, the capillary force f_0 at contact, i.e. for $\delta_n \leqslant 0$, is

$$f_0 = -\kappa R \tag{4}$$

where R is a length depending on the particle radii R_i and R_j, and κ is given by [29–31]

$$\kappa = 2\pi\gamma_s \cos\theta \tag{5}$$

Note that a negative value of δ_n corresponds to an overlap between the particles. The assumption is that the overlap is small compared with the particle diameters. The data obtained from direct integration of the Laplace–Young equation show that the geometric mean $R = \sqrt{R_i R_j}$ is more suited than the harmonic mean $2R_i R_j/(R_i + R_j)$ proposed by Derjaguin for polydisperse particles in the limit of small gaps (see below) [32]. We also note that f_0 in Equation (4) is independent of the bond liquid volume V_b.

The adhesion force f_0 at contact is the highest level of the capillary force. The latter declines as the gap δ_n increases. The capillary bridge is stable as long as $\delta_n < \delta_n^{max}$, where δ_n^{max} is the debonding distance given by [13]

$$\delta_n^{max} = \left(1 + \frac{\theta}{2}\right) V_b^{1/3} \tag{6}$$

We note that the debonding distance depends only on the liquid volume V_b, whereas the adhesion force f_0 at contact is a function only of particle diameters through the geometric mean R.

Between these two limits, the capillary force falls off exponentially with δ_n:

$$f_n^c = f_0 e^{-\delta_n/\lambda} \tag{7}$$

where λ is a length scale that should be a function of V_b and the particle radii. The role of particle size is two-fold. On one hand, the liquid volume should be compared with a mean particle radius R', a function of R_i and R_j, but which can be different from R introduced in Equation (4) for the adhesion force. On the other hand, the asymmetry due to unequal particle sizes can be taken into account through a function of the ratio between particle radii. We set

$$r = \max\{R_i/R_j;\, R_j/R_i\} \tag{8}$$

Dimensionally, a plausible expression of λ is

$$\lambda = ch(r)\left(\frac{V_b}{R'}\right)^{1/2} \tag{9}$$

where c is a constant and h is a function only of r. When introduced in Equations (9) and (7), this form yields a nice fit for the capillary force obtained from direct integration of the Laplace–Young equation by setting $R' = 2R_i R_j/(R_i + R_j)$, $h(r) = r^{-1/2}$ and $c \simeq 0.9$.

Figure 1(b) shows the plots of Equation (7) for three different values of the liquid volume V_b and size ratio r together with the corresponding data from direct integration. We see that the fit is excellent at $\delta_n = 0$ (at contact) and for nearly all values of δ_n up to the debonding distance. Figure 1(c) shows the same plots of the direct data as in Figure 1(b), but the forces are normalized by κR and the lengths by λ. The data collapse on the same plot, indicating again that the force κR and the expression of λ in Equation (9) characterize correctly the behavior of the capillary bridge.

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In summary, the capillary cohesion can be expressed in the following form:

$$f_{\mathrm{n}}^{\mathrm{c}}=\begin{cases}-\kappa R & \text{for } \delta_{\mathrm{n}}<0\\ -\kappa R\mathrm{e}^{-\delta_{\mathrm{n}}/\lambda} & \text{for } 0\leqslant\delta_{\mathrm{n}}\leqslant\delta_{\mathrm{n}}^{\max}\\ 0 & \text{for } \delta_{\mathrm{n}}>\delta_{\mathrm{n}}^{\max}\end{cases} \tag{10}$$

with

$$\lambda=\frac{c}{\sqrt{2}}V_{\mathrm{b}}{}^{1/2}\{\max(R_i/R_j;R_j/R_i)\}^{-1/2}\left\{\frac{1}{R_i}+\frac{1}{R_j}\right\}^{1/2} \tag{11}$$

In the simulations, a capillary bridge is removed as soon as the debonding distance is reached, and the liquid is redistributed among the contacts belonging to the same particle in proportion to grain diameters [33]. We also assume that the particles are perfectly wettable, i.e. $\theta=0$. This is a good approximation for water and glass beads (GB).

2.3. Friction force

For the friction force $\mathbf{f}_{\mathrm{t}}$, we use the well-known viscous-regularized Coulomb law [25, 34, 35]

$$\mathbf{f}_{\mathrm{t}}=-\min\{\gamma_{\mathrm{t}}\|\dot{\boldsymbol{\delta}}_{\mathrm{t}}\|,\mu(f_{\mathrm{n}}-f_{\mathrm{n}}^{\mathrm{c}})\}\frac{\dot{\boldsymbol{\delta}}_{\mathrm{t}}}{\|\dot{\boldsymbol{\delta}}_{\mathrm{t}}\|} \tag{12}$$

where γ_{t} is a tangential viscosity parameter, μ is the coefficient of friction and $\dot{\boldsymbol{\delta}}_{\mathrm{t}}$ is the sliding velocity. In relaxation to equilibrium, $\dot{\boldsymbol{\delta}}_{\mathrm{t}}$ declines but never vanishes due to residual kinetic energy. The equilibrium state is practically reached as soon as we have $\gamma_{\mathrm{t}}\|\dot{\boldsymbol{\delta}}_{\mathrm{t}}\|<\mu(f_{\mathrm{n}}-f_{\mathrm{n}}^{\mathrm{c}})$ at all contacts, i.e. when the friction force is inside the Coulomb cone everywhere in the system.

2.4. Distribution of liquid

The capillary force $f_{\mathrm{n}}^{\mathrm{c}}$, according to Equation (10), and the debonding distance $\delta_{\mathrm{n}}^{\max}$ in Equation (6) depend on the bond liquid volume V_{b}. It is thus important to use a convenient distribution rule for the allocation of the total volume, V_{ℓ}, of the liquid to contacts or adjacent particles within the debonding distance. To do so, the following conditions must be satisfied:

(i) The liquid is fully distributed in the form of capillary bonds (no liquid at the interstitial sites or pores), so that

$$V_{\ell}=\sum V_{\mathrm{b}} \tag{13}$$

(ii) The bond volume is dependent on the mean particle size. This is because the liquid retention capacity increases with particle size.
(iii) The particle pairs with a gap beyond the debonding distance are not eligible to receive liquid.

For a homogeneous distribution, the liquid is attributed to all eligible pairs. We assume that the bond volumes are proportional to the volumes of the pairs:

$$V_{\mathrm{b}}=\alpha R^3 \tag{14}$$

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where α is fixed by condition (13). The use of geometric mean $R \equiv \sqrt{R_i R_j}$ is a simple matter of choice. Any other mean can be used for the same purpose. When debonding occurs, the bond liquid volume is redistributed among neighboring bonds. This local redistribution can gradually lead to a globally inhomogeneous distribution. In order to ensure homogeneous distribution all along a simulation run, the liquid distribution should be updated regularly according to Equation (14). As a result, new eligible pairs appear and new liquid bonds are formed. Below, we will refer to this redistribution procedure as Protocol 1.

The distribution can be made more realistic by taking into account the 'loss' of liquid in the form of droplets at the surface of the particles or partial draining due to gravity. The liquid may also cluster in the interstitial pores [21, 22, 36]. However, most simulation results presented below are not sensitive to such refinements. This is because the deformations are not large enough for the liquid distribution to evolve significantly from the initial homogeneous distribution.

3. DIRECT SHEAR

3.1. Experiments

We designed an experimental setup which, in contrast to the standard Casagrande testing machine, allowed us to measure the shear strength at very low confining pressures (<1 kPa). Similar setups have been used by several authors in the past [37–40]. We present here the setup, the materials and the wetting protocol and our main experimental results.

3.1.1. Experimental setup. A sketch of the shearing setup is shown in Figure 2. Wetted grains are poured in a plexiglas cylindrical cell and confined by means of a circular lid of area S placed on the top of the material. The lid is equipped with a reservoir allowing to impose an overload by adding a desired amount of sand. The total vertical force N acting on the sample is the sum of the weights of lid and sand (A). A cell is composed of two disjoint parts kept together during sample preparation. The upper part can move horizontally with respect to the lower part by pulling on a rope attached to it and which supports a cupel through a pulley (B). The pulling force T can be increased by adding sand into the cupel. The friction force between the two parts of the cell is reduced by water lubricating the rims. In order to reduce the friction force exerted by the material along the walls, the thickness h of the upper part of the sample is taken to be below the diameter of the cell (46 mm). The heights of the upper and lower parts are about 10 and 15 mm, respectively.

The sample is sheared along the common section of the two parts of the cell. This shear plane is subjected to a tangential stress $\tau = T/S$ and a normal stress $\sigma = N/S + \rho g h$, where ρ is the bulk density and g the gravity. We gradually increase the shear stress τ for σ kept constant. Unstable failure occurs when τ reaches the shear strength τ_{m}. At this point, an infinitesimal stress increment causes a finite deformation of the sample manifesting itself as a sudden slide of the upper part of the sample. The upper part is stopped by collision with two bars located 5 mm away from the cell. We did not measure the displacements. We recorded τ_{m} for different values of σ in the range varying from 200 to 800 Pa, and for different values of water content.

3.1.2. Materials and wetting protocol. Four types of materials were tested: (1) a sand 'S' composed of angular grains with diameters ranging from 0.1 to 0.4 mm, (2) 'tightly graded' polydisperse

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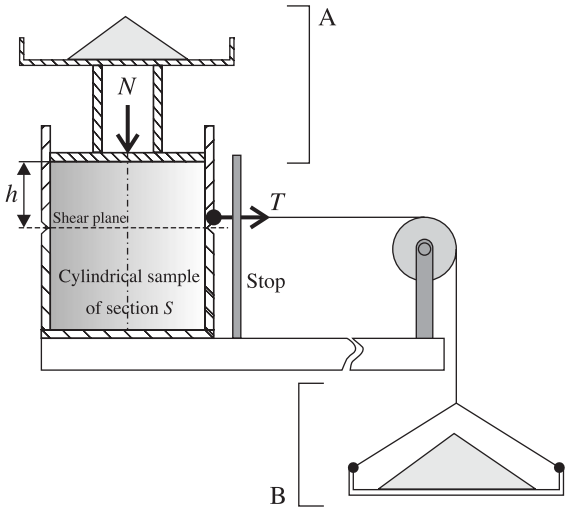

Figure 2. Testing cell and shearing setup.

GB 'GB45' with diameters from 0.4 to 0.5 mm, (3) 'well-graded' polydisperse GB 'GB48' with diameters from 0.4 to 0.8 mm, and (4) monodisperse GB 'GB1' of diameter 1 mm.

The grains were wetted by adding distilled water to dry material placed in a vessel and shaking energetically until all visible water clusters disappear. The vessel used for mixing is transparent allowing us to check visually the state of the material. After mixing, the wetted material is poured into the testing cell. The water content is evaluated by comparing the masses of a sample of the material before and after testing by means of a heat chamber used for drying the sample at 105°C. The water content is given by $w = m_{\mathrm{w}}/m_{\mathrm{s}}$, where m_{w} and m_{s} are the masses of water and grains, respectively. The wet materials were tested for water contents below 5% corresponding to the pendular state for our materials. The experiments were performed at ambient conditions. Each experiment lasted a few minutes. The loss of liquid was always below 2%. This loss is not only due to evaporation but also due to partial wetting of the internal walls of the cell. But it is low enough to assume a constant liquid volume (as in simulations, see below).

3.1.3. Results. Several tests were carried out with the four materials at our disposal (S, GB45, GB48 and GB1) for different values of water content w and normal stress σ. Figure 3 shows the yield loci τ–σ. Within experimental precision, the data are well fitted by a straight line for each material, in agreement with the Mohr–Coulomb model

$$\tau = (\tan\varphi)\sigma + c \tag{15}$$

where $\tan\varphi$ is the internal coefficient of friction and c is the Coulomb cohesion. We also observe that the angle of internal friction φ is independent of w as the Coulomb lines are nearly parallel.

Using a similar experimental setup, Schellart found that the yield loci are curved down as the normal stress tends to zero [38]. In dry granular media, the shear stress vanishes naturally at zero normal stress. However, in the wet case according to Figure 3, there is a finite cohesion c corresponding to the intersection point of the Coulomb line with the axis $\sigma = 0$. Figure 4 displays

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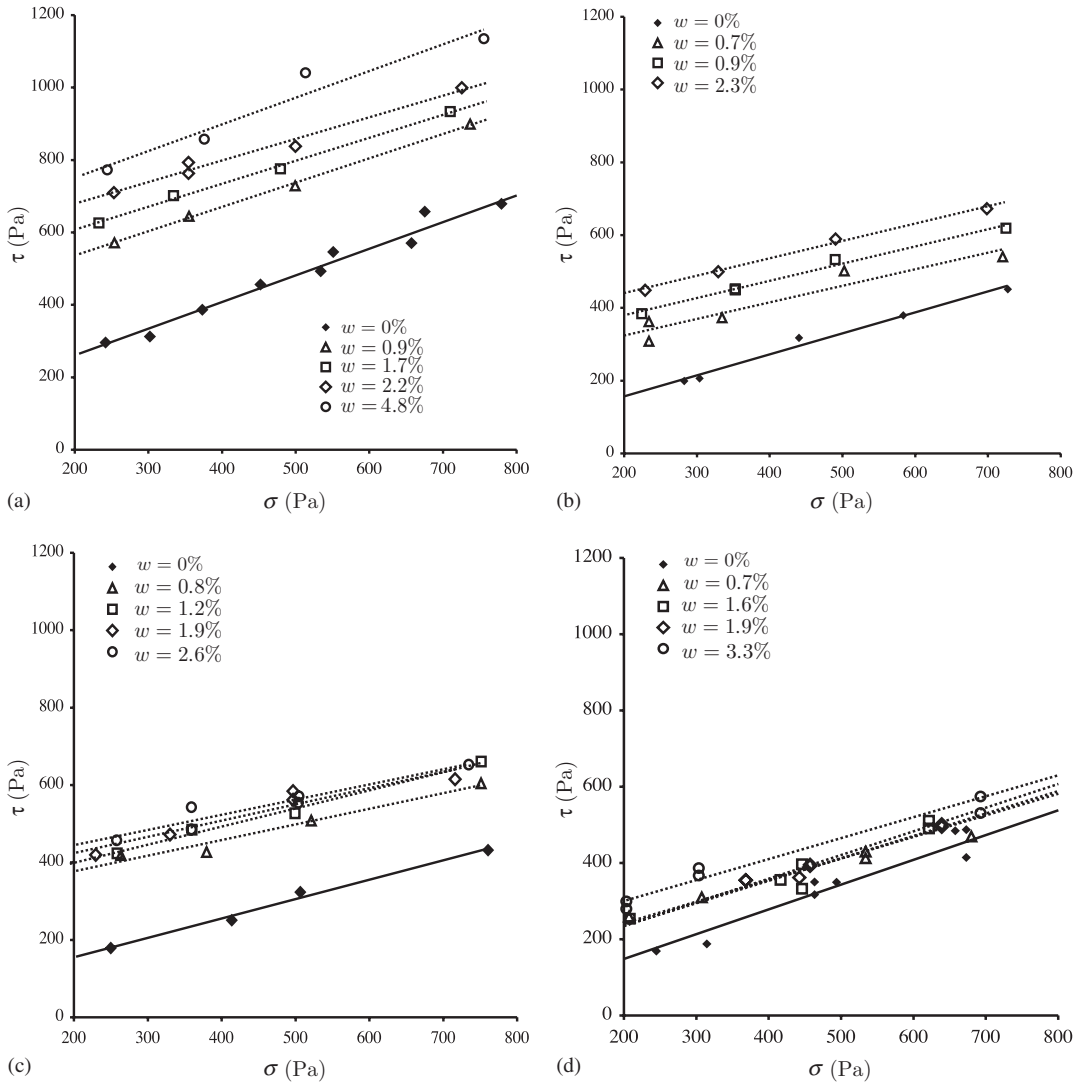

Figure 3. Yield loci, fitted by straight lines, for our experimental granular materials: (a) S; (b) GB45; (c) GB48; and (d) GB1.

the evolution of c as a function of w for the four materials. The evolution of c is strongly nonlinear and saturates at a level $c = c_{\mathrm{m}}$ for a water content $w = w_{\mathrm{m}}$, both depending on the material. The experimental estimations of c_{m} and w_{m}, as well as the internal angle of friction for our materials, are given in Table I.

The experimental data at different levels of water content show larger fluctuations for GB than for sand. These fluctuations stem certainly from the lower level of cohesion for GB and also from their tighter particle size distribution. The differences in the values of c_{m} can be attributed to differences in the mean particles sizes in different materials. In the case of sand, the nonspherical

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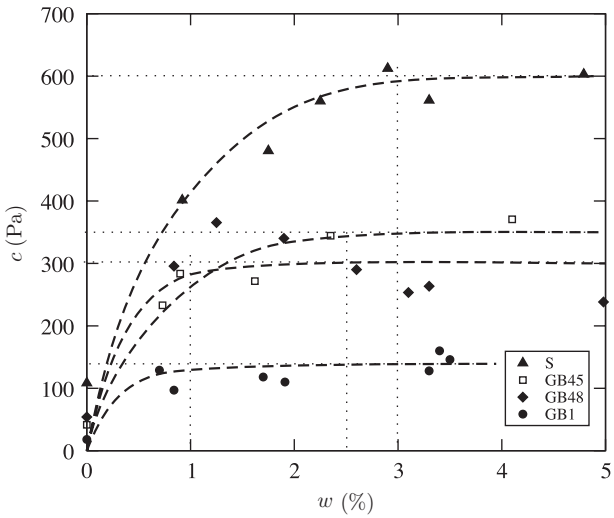

Figure 4. Macroscopic cohesion c as a function of water content w for four tested granular materials. The trends are represented by dashed lines as a guide to the eyes.

Table I. Characteristic data from experimental measurements.

	$\langle D \rangle$ (mm)	φ (deg.)	c_{m} (Pa)	w_{m} (%)
S	0.16	33	600	3
GB45	0.45	30	350	2.5
GB48	0.6	30	300	1
GB1	1	25	150	<1

form of the particles might also affect the value of c_{m}. The value of w_{m} is less clearly defined and is likely to depend on the surface state of the particles [36]. The sand grains have a rough surface requiring more water to form a meniscus than the more smooth GB. On the other hand, partial clustering of water may occur and this might require a larger amount of water for the formation of liquid bridges [21, 22].

3.2. Numerical simulations

3.2.1. Sample preparation. The numerical samples are composed of 7307 spherical particles of diameters 2, 1.5 and 1 mm in proportions of 50, 30 and 20%, respectively. The dimensions and the total volume of the numerical sample are similar to those of the experimental samples. This numerical sample can be compared with the sample GB1 (Table I) although the size distribution of the particles is slightly different. In fact, using exactly the same particle sizes as in experiments with the same total volume would require many more particles in simulations and thus much more computation time. The particles are placed randomly in a cylindrical cell. The initial configuration is prepared under gravity without introducing capillary bonds. Then, we attribute a capillary bond to eligible pairs of particles (within the debonding distance). Finally, the sample is consolidated under

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the action of a vertical confining pressure with a zero coefficient of friction. The consolidation is stopped and the coefficient of friction set to 0.4 as soon as the solid fraction $\phi = 0.6$ is reached. The subsequent compaction is negligibly small.

As in experiments, the cylindrical cell is composed of two disjoint parts. The lower part is fixed whereas the upper part moves horizontally, giving rise to a shear plane along the common section of the two parts. We apply a constant vertical load σ, the same as in experiments, on the top of the sample. However, in contrast to experiments, shearing is controlled by imposing a constant horizontal velocity on the upper part. The numerical sample has exactly the same dimensions as in experiments.

During shearing, the number of liquid bonds evolves and the available liquid must be redistributed in the system. We used two different methods for redistribution: (1) we simply apply the above procedure every time the contact list is updated (Protocol 1); (2) the volume of a broken liquid bond is split between the corresponding particles (proportional to their diameters) and conserved for the formation of new liquid bonds when a contact occurs with the same particles (Protocol 2). In this method, the volume of free liquid left after debonding is kept with the two particles (and not distributed to the other bonds of the same particles) and used only if a new contact is formed. This implies that if the initial liquid distribution is homogeneous, then it will remain so during deformation as in the first method. In other words, the liquid will not migrate considerably and one should expect quite similar results from both methods. Indeed, in different tests, we found that both methods lead to nearly identical results (see Figure 12 in Section 4.2.2).

3.2.2. Numerical results and comparison with experiments. We performed a series of direct shear simulations with different values of the water content from 0 to 2%.

Figure 5 shows the shear strain τ for a dry and a wet sample with $w = 1\%$ as a function of horizontal displacement $\delta\ell$. The initial configuration is the same in both simulations. The residual state is reached without passing by a stress peak and for a displacement of the order of one particle diameter for all tested values of the water content. The steady-state deformation involves numerous instabilities that occur throughout the system and appear in the form of rapid stress drops on the stress–strain plots. We see that in transition from dry to wet materials, the frequency of such instabilities declines.

The evolution of the Coulomb cohesion can be analyzed as a function of water content w as in experiments. Figure 6(a) shows fitted yield loci from 15 simulations with three different values of the confining pressure σ and five different values of w. The Coulomb cohesion c is drawn as a function of w in Figure 6(b). The latter is very similar to the corresponding experimental plot (Figure 4(c)) for monodisperse GB. We observe a saturation of c at still lower levels of water content ($w_{\mathrm{m}} \simeq 0.1\%$).

The limit value c_{m} of the Coulomb cohesion as a function of water content, as observed here both in the simulations and experiments, is not intuitive. Although the liquid bond volume appears in Equations (6) and (11), it is important to remark that failure is initiated at contacts where the maximum capillary force f_0 is reached and this force is independent of the local liquid volume. For this reason, the Coulomb cohesion is mainly controlled by the density of liquid bonds or equivalently by the bond coordination number z. In order to illustrate the effect of z, in Figure 7 we show the stress–strain plots for two samples differing in the number of liquid bonds for the *same* water content. The initial particle configuration is the same in both samples but there are two times less bonds in one sample (obtained by removing half of the bonds in the first sample). We see that in the initial stages of deformation, the cohesion is close to half that of the sample

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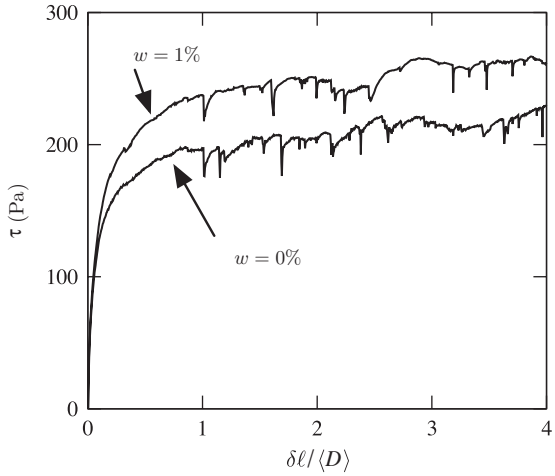

Figure 5. Stress–strain plot for $w=0$ and 1%, $\sigma=300\,\mathrm{Pa}$. The displacements are normalized by the average particle diameter $\langle D\rangle$.

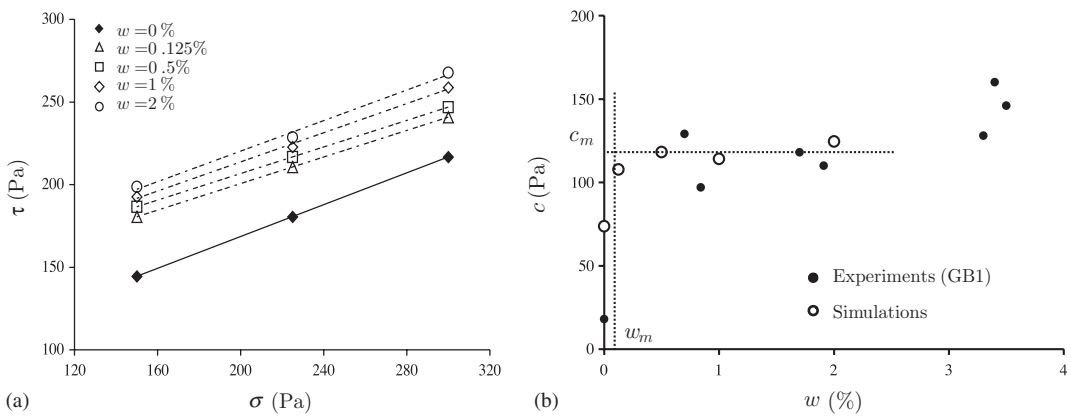

Figure 6. Simulation results: (a) estimated yield loci and (b) Coulomb cohesion as a function of water content (experiments were carried out with 1 mm glass beads).

involving a double the number of water bonds, and it increases as the wet coordination number grows. The Coulomb cohesion saturates when the bond coordination number saturates as the total liquid volume is increased. This means that the main effect of the liquid volume (factor $V_{\mathrm{b}}^{1/3}$ in Equation (6)) is to increase the debonding distance $\delta_{\max}$ and thus the bond coordination number as liquid volume is increased in the sample. The bond coordination number saturates when each particle has already a bond with all of its first neighbors.

We observe that the maximum cohesion $c_{\mathrm{m}}=120\,\mathrm{Pa}$ in the simulations is below that ($c_{\mathrm{m}}=150\,\mathrm{Pa}$) for 1 mm GB. The lower value of c_{m} in simulations can be attributed to the larger average diameter of the particles compared with experimental samples. Indeed, it can be shown that the

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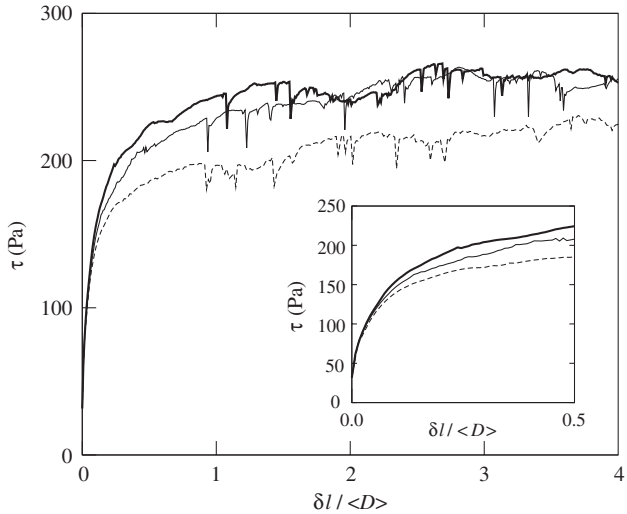

Figure 7. The shear stress τ as a function of shearing distance $\delta\ell$ normalized by the average particle diameter $\langle D \rangle$ for a dry (dashed line) and two wet samples (solid lines) with a high bond coordination number (thick line) and with two times less bonds (thin line). The inset shows a zoom for small deformations.

Coulomb cohesion varies in inverse proportion to the average particle size [33]. This effect of the particle size can also be observed for other experimental samples in Figure 4 where c_{m} and w_{m} are lower for larger values of $\langle D \rangle$.

4. SIMPLE COMPRESSION

In this section we consider the influence of water content on the strength of our granular samples under simple compression loading. The strains are known to be more homogeneous in compression than in direct shear. On the other hand, the strengths are weaker and thus the capillary effects are straightforward to measure. The experimental data are borrowed from Soulié [41], who compared also his results with numerical simulations and found qualitative agreement between them. He explained the quantitative differences of numerical data with experimental data by invoking the distribution of water. We will revisit below the same data in the light of our new numerical developments.

4.1. Review of experimental results

The experimental tests were carried out with samples of GB of diameters ranging from 0.8 to 1.3 mm. The samples were of cylindrical shape with a diameter of 25 mm and a height of 17 mm. The water content was varied from 0.5 to 12%. The beads were wetted in a hermetic seal by mixing a mass of 0.1 kg of dry beads with the amount of water required to reach the targeted water content. The wetted particles were then molded in a cylindrical vessel. Figure 8(a) shows a photograph of a typical sample prepared according to this protocol.

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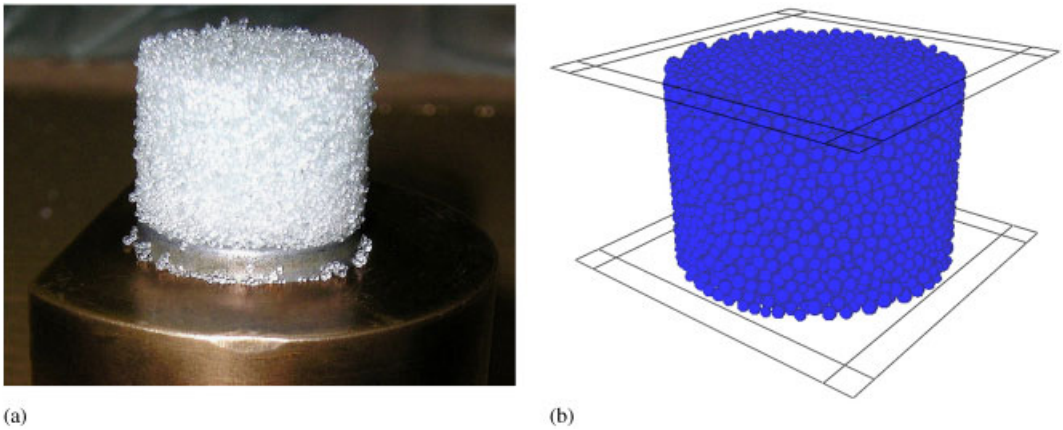

Figure 8. Typical sample used in simple compression tests: (a) glass beads for $w = 3\%$ and (b) spherical particles in simulations.

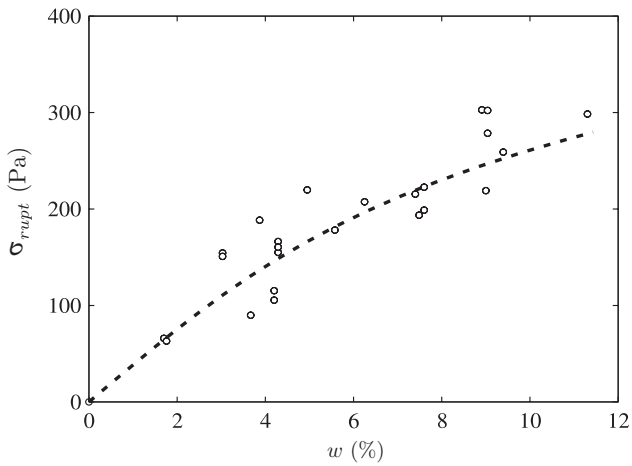

Figure 9. Compressive strength as a function of water content. Experimental data obtained by Soulié [41].

Each cylindrical sample is subjected to axial compression up to failure. Figure 9 shows the compressive strength σ_{rupt}, corresponding to the axial stress at failure, as a function of water content.

4.2. Numerical study

4.2.1. Sample preparation. The numerical samples are of cylindrical shape and composed of 8000 spherical particles with diameters ranging from 0.8 to 1.3 mm, as in experiments. The particle size grading is given in Table II.

The samples are prepared by initially letting the particles fall into a cylindrical box of diameter 25 mm. Then, the sample is 'sealed' by adding an upper wall loaded vertically. At this point, the

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Table II. Particle size grading in numerical samples.

Diameter (mm)	0.8	0.9	1	1.1	1.2	1.3
Proportion (%)	10	20	20	20	20	10

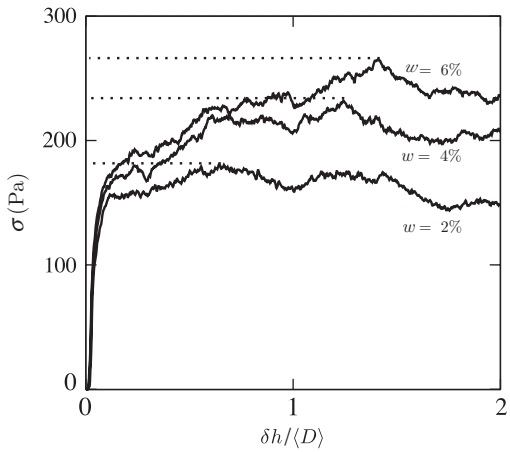

Figure 10. Axial stress as a function of axial strain for three different values of the water content.

sample is 17 mm high and has a solid fraction of 0.62. Finally, the capillary cohesion is introduced between eligible pairs of particles and the surrounding cylindrical wall is removed. The sample relaxes to equilibrium due to capillary cohesion with only a slight settlement of about 0.1 mm due to gravity, see Figure 8(b).

4.2.2. Numerical results and comparison with experiments. Numerical simulations were carried out for 2, 4 and 6% of water content. In each simulation, the upper wall moves at 1 mm/s for 2 s. The axial stress σ is simply estimated from the axial resultant of the forces acting on the upper wall divided by its area, as in experiments. The axial stress σ is shown in Figure 10 as a function of axial shorting δh normalized by the average particle diameter $\langle D \rangle$. The compressive strength σ_{rupt} corresponds to the axial stress at the peak. Remark that the axial stress declines beyond the stress peak.

In Figure 11, a snapshot of the sample of $w = 2\%$ is displayed at the end of the simulation. We observe the barrel shape of the sample, as observed in experiments with granular soils. Figure 11 shows a vertical section of the sample with color-coded particle displacements. We observe an immobile cone at the lower central part of the sample, which can be attributed either to the motion of the upper wall or to the effect of gravity.

The compressive strengths are plotted as a function of water content in Figure 12 together with the numerical data of Soulié and the experimental data of Figure 9. We see that the numerical data of our simulations are closer to the experimental data than the initial numerical data of Soulié. It should be noted that the capillary law used by Soulié is different from the one employed in the present work. However, the fits to the data obtained from direct integration of Young–Laplace equations are quite similar.

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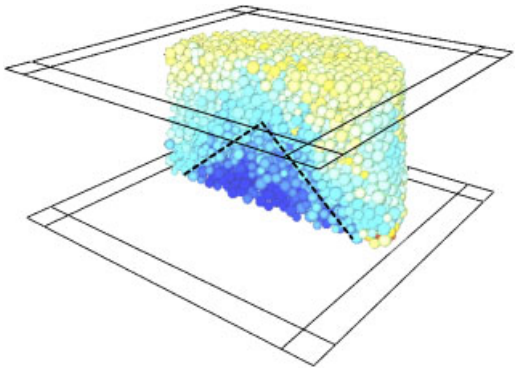

Figure 11. Numerical sample at the end of the simulation with $w = 2\%$. We observe a nearly immobile region indicated by dashed lines.

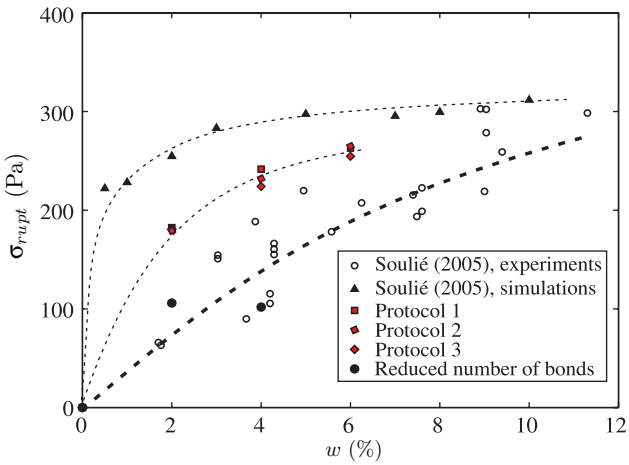

Figure 12. Compressive strengths as a function of liquid content in simple compression tests from experiments and simulations for three different redistribution protocols (see text).

In order to find hints to explain the observed discrepancies, we carried out more simulations using different protocols for water redistribution. In addition to the two protocols introduced in Sections 2.4 and 3.2, we used another protocol in which the effect of gravity is accounted for by transferring the liquid from broken bond between two particles to the lowest contact located on the lower hemisphere of each of the two particles (Protocol 3). In this protocol, the volume of the liquid bond is shared by the two particles proportional to their sizes. During shearing the liquid is gradually transported downward according to the bonding–debonding dynamics of the material. This dynamics being generally slow, the transport of liquid by this mechanism is not effective for small deformations.

Two points were checked in more detail: (1) the rule for the redistribution of water when a capillary bond fails according to the three protocols introduced in Sections 2.4, 3.2 and 4.2 and

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(2) the bond coordination number z which simply depends on the initial selection of eligible pairs of particles. In fact, as in the case of direct shearing, our data from simple compression show that the main influence comes from z. In order to illustrate this point, in Figure 12 two data points are shown for two simulations, $w=2$ and 4%, with reduced number of liquid bonds by a factor 2. We see that the shear strength for these two samples is significantly reduced compared with the other simulations with different protocols.

On the other hand, we see that, as long as z is the same, the protocols for water redistribution have nearly no effect. The difference between our simulations and those of Soulié is thus only related to the initial values of z. Indeed, in contrast to our simulations, Soulié did not allow the sample relax after the removal of the cylinder used to mold the sample. The relaxation of the sample before compression leads to lower liquid bond coordination. In this respect, it should be noted that also in experiments water is not distributed to all present or eligible particle pairs. Shaking might be never efficient enough to allow all pairs to receive liquid bonds. Experimental investigation of water distribution seems thus to be crucial for a better modeling of wet granular media [21, 22].

5. CONCLUSION

In summary, we developed a DEM-type approach for the simulation of 3D wet granular materials with spherical particles. The capillary law implemented in this framework is an analytical expression of the capillary force as a function of geometrical and materials parameters of a liquid bridge, and it was shown to provide excellent fit for the data from direct integration of Young–Laplace equations. This code (tapio-K, see [42]) was applied to simulate the quasi-static behavior of wet granular media for direct shear and simple compression boundary conditions and compared with simulations carried out with nearly the same parameters and boundary conditions. The experimental setup was specially designed to allow for the measurement of weak stresses, a necessary condition for the evaluation of the effects of capillary cohesion with millimeter-size particles.

Experimental direct shear tests were performed with GB and sand, and the shear strengths were analyzed in the Mohr–Coulomb space for weak confining stresses (below 1 kPa). We found that the internal angle of friction was not sensitive to water content w, and the Coulomb cohesion increased in a nonlinear fashion with w to saturate to a well-defined level c_{m} of cohesion independent of water content for $w>w_{\mathrm{m}}$. A similar behavior was observed in numerical simulations. The cohesion c_{m} was found to be quite close between the experiments and numerics for the samples of the same particle size distribution ($c_{\mathrm{m}}=120\,\mathrm{Pa}$ in numerics *vs* $c_{\mathrm{m}}=150\,\mathrm{Pa}$ in experiments). The numerical values of w_{m} were found to be systematically below those in experiments.

For simple compression tests, we compared the experimental results of Soulié [41] with numerical simulations performed with cylindrical samples of wet particles. Comparing the influence of water content between experiments and simulations, we found discrepancies that were analyzed by further simulations where the bond coordination number was varied. We found that, in contrast to water content, the bond coordination number plays a major role in compressive strength. Numerically, it was also shown that the details of the redistribution of water at failed capillary bonds has a minor effect on the behavior.

Our findings and the comparisons made with experiments carried out with similar boundary conditions credit the numerical method, and more particularly the implemented capillary law. On the other hand, the observed discrepancies open new queries concerning the distribution of water

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in real samples of wet grains. It seems thus that, in order to progress in understanding the strength properties of wet granular materials, more detailed observations are required. New experiments are presently under way to evaluate the local distribution of capillary bridges and the influence of the mixing protocol.

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