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Computer simulation of random loose packings of micro-particles in presence of adhesion and friction

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ABSTRACT

With a 3D discrete-element method specially developed with adhesive contact mechanics, random loose packings of uniform spherical micron-sized particles are fully investigated. Characterized by a dimensionless adhesion parameter *Ad* proposed in the previous work, four packing regimes are identified: random close packing (RCP) regime with $Ad < 0.01$; random loose packing (RLP) regime with $0.01 < Ad < 1$; adhesion regime with $1 < Ad < 20$ and an asymptotic limit regime with $Ad > 20$. The evolution of the radial distribution function with respect to *Ad* is analyzed and divided into three stages. Force distribution of these adhesive loose packings follows $P(f) \sim f^{\theta}$ for small forces and $P(f) \sim e^{-\beta f}$ for big forces, respectively, which shares a similar form with that in packings without adhesion but results in distinct exponents of $\theta = 0.879$, $\beta = 0.839$ for normal forces. A local mechanical equilibrium analysis demonstrates that adhesion enhances both sliding and rolling resistance so that the fairly loose packing structures of adhesive particles can still be mechanically stable.

1. Introduction

Jammed particle packings have been studied to understand the microstructure and bulk properties of liquids, glasses and crystals [1,2] and frictional granular materials [3,4]. Two packing limits have been identified for disordered uniform spheres: the random close packing (RCP) and random loose packing (RLP) limits [1,5–11]. The upper RCP limit is reproduced for frictionless spheres at packing fraction $\phi_{RCP} \approx 0.64$ and has been associated with a freezing point of a 1st order phase transition [2,4,10,12,13], among other interpretations [2,13]. Only in the presence of friction, packings reach lower packing fraction up to the RLP limit $\phi_{RLP} \approx 0.55$ for mechanically stable packings [6,8,11]. However, most packings of dry small micrometer-sized particles in nature are not only subject to friction, but also *adhesion* forces as well. For instance, van der Waals forces generally dominate interactions between particles with diameters of around 10 μm or smaller. In this case, the adhesive forces begin to overcome the gravitational and elastic contact forces acting on the particles and change macroscopic structural properties [14,15].

Despite the ubiquity of adhesive particle packings in almost all areas of engineering, biology, agriculture and physical sciences [15–18], there have been few systematical investigations of these kinds of packings [19–25]. The multi-coupling of adhesion, elastic contact forces and frictional forces in the short-range particle-particle interaction zone and their further couplings with fluid forces (e.g. buoyancy, drag and lubrication) across long-range scales make it highly difficult to single out the effect of the adhesion forces, let alone to investigate the packing properties experimentally. With the progress of computer simulation techniques, discrete element simulation has become an efficient and accurate method to study the packing problems of micron-sized particles [14,19,23], which are rather difficult to achieve in the experiment condition. In a dynamic packing process, particles will be arrested and eventually form a packing when all the kinetic energy is dissipated after a series of collision. To better understand the dynamic behavior during the packing process, various dynamic models were proposed to describe the impact process with a combination of quasi-static contact theories and dissipation mechanisms [14,15,26–28]. While the dissipation mechanisms account for the dynamic effects such as viscoelasticity, the quasi-static contact theories fundamentally describe the contact between particles, of which Hertz contact theory is the most successful to characterize the relation of applied forces and contact area of non-adhesive particles. However, as particle sizes go down to micron scales, van der Waals force becomes the most predominant interaction among other forces like gravity, drag or electrostatic forces. Several mesoscale models are put forward to describe the effects of van der Waals adhesion on the elastic forces between static contacts of particles, among which the JKR (Johnson, Kendall and Roberts), DMT (Derjaguin, Muller and Toporov) and M-D (Maugis-Dugdale) models are widely accepted ones [29–31]. Recently, Li and Marshall [32], and Marshall [33] developed a three-dimensional, mesoscopic discrete-element method (DEM) for adhesive micron-sized particles based on the JKR model, which has been successfully applied to dynamic simulations of micron-particle deposition on both flat and cylindrical surfaces with

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experimental validations [14,34]. With this approach of adhesive DEM, both macroscopic and microscopic parameters during the dynamic process can be predicted.

Previous studies using a discrete element method (DEM) found that the packing fraction decreases for adhesive micron-sized particles in a range of $\phi = 0.165 \sim 0.622$ with smaller sizes [19]. A similar result of $\phi \approx 0.2 \sim 0.55$ was found for 4–52 μm particles both in simulation and experiment [23]. As for other experimental investigations, a random ballistic deposition and fluidized bed technique was used respectively to produce the packing fractions of $\phi = 0.15 \sim 0.33$ for both uncompressed and compressed samples [21] and of $\phi = 0.23 \sim 0.41$ with particle diameter of 7.8–19.1 μm [20]. From these studies, we can conclude that for particles smaller than 100 μm, packing density has a positive correlation with particle size. Nevertheless, the effects of other physical parameters, such as velocities, strength of adhesion, frictions etc., on the packing process have little been discussed or analyzed.

In this paper, a prototypical packing system is introduced for the simulation of random loose packings of *soft-sphere*, *non-Brownian*, uniform adhesive particles with a discrete element method. We explore the very low density regime of small particles with van der Waals adhesion interaction by changing physical parameters. The paper is organized as follows: the adhesive DEM simulation approach based on the JKR theory is briefly described in Section 2.1; the simulation conditions and parameters used in this work are given Section 2.2; and the results and discussions on the packing properties involving packing fraction, coordination number, radial distribution function, etc., are included in Section 3. Section 4 gives the conclusions.

2. Models and method

2.1. Computational method: adhesive DEM

In a DEM framework specifically developed for adhesive grains [14,15], both the translational and rotational motions of each particle in the system are considered on the basis of Newton's second law,

$$m\frac{d\boldsymbol{v}}{dt} = \boldsymbol{F}_F + \boldsymbol{F}_A + \boldsymbol{F}_g, \quad I\frac{d\boldsymbol{\Omega}}{dt} = \boldsymbol{M}_F + \boldsymbol{M}_A \tag{1}$$

where $\mathbf{v}$ and $\mathbf{\Omega}$ are, respectively, velocity and rotation rate of an individual particle, m is the particle mass, and I is the moment of inertia. $\mathbf{F}_g$ is gravity. $\mathbf{F}_F$ and $\mathbf{M}_F$ stand for the fluid forces and torques acting on the particle, which are ignored here as we assume a vacuum environment. $\mathbf{F}_A$ and $\mathbf{M}_A$ denote the adhesive contact forces and torques on the particle. They include

$$\begin{aligned}\boldsymbol{F}_A &= F_n\mathbf{n} + F_s\mathbf{t}_s \\ \boldsymbol{M}_A &= r_p F_s(\mathbf{n}\times\mathbf{t}_s) + M_r(\mathbf{t}_s\times\mathbf{n}) + M_t\mathbf{n}'\end{aligned} \tag{2}$$

where F_n is the normal force including adhesive elastic contact force F_{ne} and damping force F_{nd}, F_s is the tangential force due to the sliding friction, M_r is the rolling resistance and M_t is the twisting resistance. r_p is the particle radius. $\mathbf{n}$, $\mathbf{t}_s$ and $\mathbf{t}_r$ are the normal, tangential and rolling direction unit vectors, respectively.

A JKR (Johnson-Kendall-Roberts) model is employed to account for F_{ne} between the relatively compliant micro-particles, implying the length scale of elastic deformation is larger than that of the adhesive force (with the particles' Tabor parameter larger than unity) [15,29]. The solid-phase dissipation force F_{nd} caused by viscoelasticity of materials is assumed to be proportional to the rate of change of the material deformation. Thus, the normal force F_n is given by

$$F_n = F_{ne} + F_{nd} = 4F_C\left[(a/a_0)^3 - (a/a_0)^{3/2}\right] + \eta_N\mathbf{v}_R\cdot\mathbf{n}, \tag{3}$$

where F_C is the critical pull-off force derived from the JKR theory, $F_C = 1.5\pi wR$ [29], a is the radius of the contact area with a_0 at equilibrium in the JKR model, η_N is the normal dissipation coefficient defined in [35], $\mathbf{v}_R$ is the relative velocity at the contact point on particle surfaces. Here R is defined as the effective radius between two contacting particles, $1/R = 1/r_{p,i} + 1/r_{p,j}$, and w is the work of adhesion with typical values about 10–30 mJ/m^2, from either measurements [36,37] or Lifshitz theory's predictions.

The dissipative friction terms, including the sliding, twisting and rolling frictions in the presence of adhesion, are all approximated by a linear spring–dashpot–slider model with model parameters given in [34]. The slider considerations mean that the sliding, twisting and rolling resistances all reach critical values, $F_{s,crit}$, $M_{t,crit}$ and $M_{r,crit}$, as three related displacements exceed the certain limits. For displacements larger than those limits, the resistances stay constant and the particles start to slide or spin. The critical limits in presence of adhesion are given in the following equations [15,16,38,39],

$$\begin{aligned}F_{s,crit} &= \mu_f|F_{ne} + 2F_C|, \\ M_{t,crit} &= 3\pi a F_{s,crit}/16, \\ M_{r,crit} &= -4F_C(a/a_0)^{3/2}\theta_{crit}R.\end{aligned} \tag{4}$$

Here μ_f is the friction coefficient that is fixed at 0.3, θ_{crit} is the critical angle for the relative rolling of two particles, which is around (0.6–1.0)% according to the measurement by atomic force spectroscopy [40].

2.2. Simulation conditions

The generation of the packing starts with the successively random free falling of 1000 uniform spheres with an initial velocity U_0 at a height H under gravity. The horizontal deposition plane has two equal edges of length L along with periodic boundary conditions on both directions. A stable packing structure is achieved when all the particles are settled after a time long enough. Here, the fluid effect is filtered out by assuming packing under a vacuum condition and friction coefficient is fixed at $\mu_f = 0.3$. More importantly, the gravitational effect with respect to particle inertia (namely the kinetic energy) can be neglected when the system satisfies $Fr = U_0/\sqrt{gH} > 1$, where Fr is the *Froude* number (ratio of inertia to gravity). To precisely characterize the gravitational effect, we define the relative velocity increment as $\Delta U = (U - U_0)/U_0$, where $U = \sqrt{U_0^2 + 2gH}$ is the final velocity. For all runs in the numerical simulations, we ensure that ΔU is <4%. Thus the acceleration caused by gravity during the dynamic deposition process can be ignored, indicating that the deposition velocity can be treated as the same with the initial inlet velocity. It should be noted that the gravitational force is kept from beginning to end (as seen in Eq. (1)), though it is much smaller with respect to particle inertia before deposition and then lower than adhesion force between contacting micro-particles after deposition. As a primary concern of our work, interstellar dust particles always transport with a relatively large velocity before they form large aggregates. Therefore, the adhesive packings simply arise due to the competition between the particle inertia and particle-particle interactions (e.g., adhesion, elasticity and frictions). Most importantly, the negligible gravitational effect distinguishes our system from that of [19,22], which generate particles randomly in a box without touching each other and wait them to deposit due to gravity. The geometrical and physical parameters used in the DEM simulations are listed in Table 1.

3. Results and discussions

3.1. Packing fraction

Typical packing structures and connecting networks of loose and dense packings are shown in Fig. 1. The packing fraction is calculated from the vertically middle part of the packing ($0.3h \le X \le 0.8h$, with h as packing height), avoiding the so-called wall effect from both bottom and top of the packing structure. It has been well accepted that packing