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Random adhesive loose packings of micron-sized particles under a uniform flow field

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ABSTRACT

The effects of hydrodynamic interactions on random adhesive loose packings of monodisperse spherical microparticles are investigated via a two-way coupled CFD-DEM approach. It is found out that the packing fraction and coordination number do not follow the regression of the adhesion number, which was proposed recently to well characterize the bulk properties of adhesive packings. Based on the balance between particle adhesion and fluid drag force, we propose a modified fluid adhesion number, Ad_f, which successfully normalizes the packing fraction and coordination number. Besides, the pressure drop through the packed bed shows a critical behavior, which validates the jamming threshold of fine powders, but occurs at a fixed packing fraction of $\phi \approx 0.22$ under the present protocol. The normalized permeability of the packed bed for different parameters is analyzed, which is in good agreement with the derivation of Kozeny-Carman equation.

1. Introduction

Understanding the properties of random packings of uniform spherical particles has long been a fundamental challenge in both physical science and industrial applications. Random packings have been widely applied as classical models to investigate glass transition [1], colloidal suspension [2] as well as the mechanical properties of granular materials [3,4]. While in a variety of engineering applications, such as dust removal [5,6], fibrous filtration [7,8], segregation [9] and clogging [10,11], the packing problems have not drawn much scientific attraction and are still not well addressed. Defined as the volume ratio of the particle phase to the occupied space, packing fraction serves as the most fundamental and important bulk property. It has been well validated and accepted that the random packing fraction of large elastic and frictional grains lies between two limits, denoted as random close packing (RCP) and random loose packing (RLP) [12–14]. Specifically, a phase diagram is derived through a statistical mean-field theory based on the Edwards ensemble approach [15,16] to describe the jammed packing states, which theoretically delimits the regions where mechanically stable packings could exist.

However, most real particles in nature and industries are around micron-sized, which are subject to not only elastic and frictional forces, but also adhesive forces, electrostatic forces and hydrodynamic forces [17,18]. In this case, both the structural and mechanical properties of micro-particle packings could be intrinsically different in presence of such interactions. Previous simulations and experiments have shown that both the packing fraction and coordination number of microparticle packings can go far below the RLP limit when van der Waals adhesive forces are incorporated [19–23]. The effect of adhesion is scaled by a dimensionless adhesion number, which uniquely determines the packing properties from a dynamic perspective [24,25]. Furthermore, by varying the adhesion number and friction coefficient, a modified packing phase diagram for small adhesive particles is interpreted based on the improvements of the statistical mechanics theory of granular matter [26], which provides a universal framework to understand the packing problems of fine powders. As for the electrostatic forces, a few attempts have been made to explore their influence on the particle assembly [27–29].

Regarding the hydrodynamic interactions, packings under a flow field are known as filtration or clogging problems, which have been extensively studied in the community of chemical engineering. Previous investigations have provided abundant descriptions on the performance of particle cake, including pressure drop, collection efficiency and permeability [7,8,30–35]. However, most of these studies only focus on the macroscopic operational parameters. Little attention has been paid to uncover the underlying physical relationship between the macro and micro properties. One of the challenges lies in the great difficulty to obtain experimental measurements like packing fraction and coordination number for such small micro-particles, which calls for the development of numerical simulations. In the past decades, discrete element method (DEM) has become a powerful technique, which can be coupled into other numerical method such as computational fluid dynamics (CFD), lattice Boltzmann methods (LBM) and smoothed particle hydrodynamics (SPH), to study all kinds of particle

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problems [36–38]. Various dynamic models have been proposed to describe the inter-particle collision process [17,39–43], which helps to better understand the dynamic behavior of the small adhesive particles.

In this work, we study the effects of hydrodynamic interactions on random packings of micron-sized spherical particles by means of a CFD-DEM coupled approach. The influence of the particle clusters on the fluid flow is well considered, through a two-way coupling of the fluid motion and the particle motion. Our results show that the packing bulk properties do not follow the scaling law that is proposed previously. Instead, a new dimensionless parameter is deduced based on the balance between inter-particle adhesive forces and drag forces, which universally regresses the simulation results. Furthermore, we report a jamming phenomenon for adhesive particles, of which the jamming point is found to be independent of neither particle size nor surface energy. Finally, the pressure drop through the packed bed as well as the permeability are also discussed and compared with theoretical equations.

2. Models and methods

2.1. Two-way coupled CFD-DEM approach

We perform numerical simulations of micro-particle packings via a discrete element method (DEM), which is coupled into a framework of the open-source CFD codes MFIX. The governing equations of the fluid-phase are the mass and momentum conservation, expressed as

$$\begin{aligned}&\frac{\partial \varepsilon_f}{\partial t}+\nabla\cdot(\varepsilon_f\mathbf{u})=0,\\&\frac{D}{Dt}\left(\varepsilon_f\rho_f\mathbf{u}\right)=\nabla\cdot\bar{S}_f-\mathbf{I}_{fs}.\end{aligned}\tag{1}$$

Here, ε_f is the fluid-phase volume fraction, ρ_f is the mass density of the fluid, $\mathbf{u}$ is the volume-averaged fluid velocity, $\bar{S}_f$ is the stress tensor of the fluid and $\mathbf{I}_{fs}$ is the momentum transfer term between the fluid and particle phases, which is extraordinarily important in the two-way coupling algorithm. In every computational time step, $\mathbf{I}_{fs}$ is calculated at every grid node by summing up the fluid forces $\mathbf{F}^j_{drag}$ acting on all the particles in the fluid cell,

$$\mathbf{I}^i_{fs}=\frac{1}{V_i}\sum_{j=1}^{m}H^j_i\mathbf{F}^j_{drag}\tag{2}$$

where m is the total number of particles in the ith grid cell, and V_i is the volume of the cell. H^j_i is the generic kernel with compact support, which represents the impact of the particles inside this grid cell on the grid node. By incorporating $\mathbf{I}_{fs}$, the disturbance of particle motions on the flow field is well considered.

The DEM framework used in this work is specifically developed for micro-particles, which has been well tested and validated by particle/surface impact experiments [17,18]. The governing equations of the particle phase involve the translational and rotational motions of each particle, which follow the Newton's second law:

$$\begin{aligned}&m\frac{d\mathbf{v}}{dt}=\mathbf{F}_f+\mathbf{F}_p,\\&I\frac{d\mathbf{\Omega}}{dt}=\mathbf{M}_f+\mathbf{M}_p.\end{aligned}\tag{3}$$

Here, $\mathbf{v}$ and $\mathbf{\Omega}$ are the velocity and rotation rate of an individual particle, respectively, m is the particle mass, and I is the moment of inertia. Specifically, gravity is not considered in the present study. $\mathbf{F}$ and $\mathbf{M}$ represent the forces and torques exerting on a particle, while the subscript f or p denotes the source of these forces and torques, from either the fluid or the particle collision.

The dominant hydrodynamic interactions on the particles are the viscous drag, which are expressed as

$$\begin{aligned}&\mathbf{F}_{drag}=-6\pi\mu r_P(\mathbf{v}-\mathbf{u})f,\\&\mathbf{M}_{drag}=-8\pi\mu r_P^3\left(\mathbf{\Omega}-\frac{1}{2}\omega_f\right).\end{aligned}\tag{4}$$

Here, μ is the fluid dynamic viscosity, r_p is the particle radius, and ω_f is the fluid vorticity. f is the friction factor given by the HKL (Hill-Koch-Ladd) drag correlation, which is applicable in a large range of Reynolds number [44,45].

Apart from the fluid forces, the inter-particle collisions produce adhesive contact forces and torques, which include

$$\begin{aligned}&\boldsymbol{F}_a=F_n\mathbf{n}+F_s\mathbf{t}_s,\\&\boldsymbol{M}_a=r_pF_s(\mathbf{n}\times\mathbf{t}_s)+M_r(\mathbf{t}_r\times\mathbf{n})+M_t\mathbf{n}.\end{aligned}\tag{5}$$

In the above equations, F_n is the normal force, F_s is the tangential force due to the sliding friction, M_r is the rolling resistance and M_t is the twisting resistance. $\mathbf{n}$, $\mathbf{t}_s$ and $\mathbf{t}_r$ are the normal, tangential and rolling direction unit vectors, respectively. The normal contact force F_n is described by the JKR (Johnson-Kendall-Roberts) model [17,46] along with a damping part, which is assumed to be proportional to the rate of change of material deformation, shown as

$$F_n=F_{ad}+F_{nd}=4F_C\left[(a/a_0)^3-(a/a_0)^{3/2}\right]+\eta_N\mathbf{v}_R\cdot\mathbf{n}\tag{6}$$

Here, F_C is the critical pull-off force derived from the JKR theory, $F_C = 3\pi\gamma R$ [17,46], a is the radius of the contact area which equals a_0 at equilibrium, η_N is the normal dissipation coefficient, and $\mathbf{v}_R$ is the relative velocity at the contact point on particle surfaces. R is defined as the effective radius between two contacting particles, $1/R = 1/r_{p,i} + 1/r_{p,j}$, and γ is the surface energy.

Besides the normal forces, the sliding, twisting and rolling friction forces and torques are all approximated by a spring–dashpot–slider model in the presence of adhesion, which means that these resistances all stay constant after reaching some critical values, $F_{s,crit}$, $M_{t,crit}$ and $M_{r,crit}$. The critical values are given by

$$\begin{aligned}&F_{s,crit}=\mu_f|F_{ne}+2F_C|,\\&M_{t,crit}=3\pi aF_{s,crit}/16,\\&M_{r,crit}=-4F_C(a/a_0)^{3/2}\theta_{crit}R,\end{aligned}\tag{7}$$

where μ_f is the friction coefficient and θ_{crit} is the critical angle for the relative rolling of two particles. The model parameters used in Eq. (7) can be found in our previous literature [47,48].

2.2. Simulation setup

As shown in Fig. 1, the simulation domain is a cuboid with dimensions of $H\times L\times L$, where $L = 20r_p$ and $H = 10\,L$. The domain width L is selected as the characteristic length scale, so that the dimensionless computational domain is set as $-5 \le X^* \le 5$, $-0.5 \le Y^* \le 0.5$ and $-0.5 \le Z^* \le 0.5$, with x-axis set along the direction of height. Periodic boundary conditions are set along the Y^* and Z^* directions. For the computation of the flow field, the domain is enlarged to $-15 \le X^* \le 15$, also with periodic boundary conditions on both Y^* and Z^*. In this case, the wall at $X^* = 5$ acts as a filter, which is solid for particles but permeable for fluid. Our simulation starts from successive random injection of 2000 uniform spheres at $X^* = -5$ with an initial velocity U_0. Note that the gravitational effect is eliminated, so that all the particles are transported by the fluid flow and deposit onto a plane at $X^* = 5$. The initial flow field is set to be uniform, with $U_x = U_0$, $U_y = U_z = 0$, and updated with the current information of particles during every computational time step. Hence, as the computation proceeds, the flow field will become nonuniform. We performed