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The effect of air on the packing structure of fine particles

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ABSTRACT

A numerical study of the effect of air on the packing structure of fine particles has been performed by a combined continuum and discrete numerical model. The forces considered are gravity, contact force, drag force, and van der Waals forces. The results are analyzed in terms of particle rearrangement, local porosity, coordination number, radial distribution function, and the distribution of contact forces. The results indicate the degree to which drag and van der Waals forces promote mean porosity increases and mean coordination number decreases. Drag forces allow contacts of particles reaching a state of rest in a packing to be closer to the Coulomb failure criterion for shear displacement when van der Waals forces are small. Increasing van der Waals forces imposes contact conditions that are far away from the Coulomb failure criterion. Increased drag and van der Waals forces tends to lead to more heterogeneous structure. It is demonstrated that average normal contact force is related to the ratio of van der Waals forces to particle weight.

1. Introduction

Particle packing has been studied for many years as it is of fundamental importance to many industries, e.g. the random packing of hard spheres has been used to model the structure of liquids and glassy materials; to study mechanical properties in granular materials such as electrical conductivity, fluid flow, and stress distributions, etc [1]. In previous years, most published papers have been on packing of coarse spherical and/or non-spherical particles [2–9].

Recently, the packing of fine particles has been attracting more and more interest motivated by their wide application in industry [10]. The packing of fine particles differs from that of coarse particles. For fine particles, the interparticle forces, such as van der Waals and electrostatic forces, become more important than gravity. This results in variation of porosity with particle size [11] and open-tree packing [12] or scaffold structures [13]. Yu et al. [14] summarized the literature on experimental studies and generalized the relationship between porosity and interparticle forces, and particle size. A few papers [14,15] reported that porosity for the packing of fine particles is higher than that of coarse particles and the proposed mechanism suggested is that increasing the interparticle forces increases porosity.

It is extremely difficult and expensive to obtain the microstructural information for packing geometries arising from different controlling variables. Recently, the discrete element method (DEM) or molecular dynamics method (MD) has been used to simulate the packing of fine particle [10,11,16–21]. Landry et al. [18] found that the majority of the tangential forces for particle–wall contacts are close to the Coulomb failure criterion while particle–particle contacts in the bulk are far from the Coulomb failure criterion. Although they used 100 μm, 2000 kg/m^3 glass particles, the effect of attractive forces, such as van der Waals forces, were not taken into consideration. Yen and Chaki [21] considered the van der Waals forces and also ignored the rotational motion of particles. They reported that as friction and van der Waals forces reduced rearrangement of the particles, the packing porosity increased, as would be intuitively expected. Yang et al. [7,10,11,16] extended the DEM to the packing of fine particles by considering the effect of van der Waals forces, particle rotation, and rolling friction. They revealed that the material properties and size of particles have a strong effect on the packing structure of fine particles under the conditions of random generation of 1024 monosized fine spherical particles in a rectangular box. In order to avoid the wall effect, a periodic boundary condition along the two horizontal directions was employed.

So far, the effect of air on particles is neglected in all the above work. It is well known that drag force plays quite an important role for fine particles. For example, the discharge rate of coarse powders without aeration under gravity from hoppers can be described by both empirical relations and theoretical models, but for fine particles these correlations largely overestimated discharge rate. This is due to a negative pressure gradient developing near the hopper outlet during flow, resulting in an air flow into the hopper. This causes extra drag force and decreases the discharge rate for fine particles [22–25]. Even for coarse media e.g. in studies of the brazil-nut effect, it has been shown that air drag strongly influences the density dependent behaviour of the intruder in vibrated beds [26]. Using high-speed video and magnetic resonance imaging Mobius studied the motion of a large sphere in a vertically vibrated bed of smaller grains and pointed out air drag caused relative motion between the intruder and the bed during the shaking cycle and played an important role in the observed density dependence of the rise time.

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Table 1
The physical properties of fine particles and dimension of container

Physical properties	
Particle diameter, d	60 μm
Particle density, ρ	2000 kg/m^3
Number of particle, N	100,000
Spring stiffness, k_n, k_t	10 N/m
Friction coefficient, μ	0.3
Restitution, e	0.95
R_{vdw}	0–10,000
Fluid viscosity, μ_f	1.8×10^{-5} pa s
Dimension of container	
Width	0.0276 m
Height	0.0411 m

Note: restitution coefficient is set to 0.95 assuming no cohesive effect.

Forming a packing is a complex dynamic process. Air drag force may influence the structure of packing individually or cooperatively with other forces, such as contact forces, van der Waals and/or electrostatic forces associated with fine particles, and the capillary force with wet particles. It would be a great challenge to study the effect of air on packing structure of fine particles.

In this paper, a two-dimensional mathematical model has been developed to study the effects of air and van der Waals forces on the packing structure of the poured random packing of fine particles by means of a Combined Continuum and Discrete Model (CCDM) proposed by Xu and Yu [27]. The main advance is a DEM and CFD simulation that combines all the key particulate forces (short of liquid-bridge attractions that affect moist powders) in a coupled simulation that has a sufficiently large system to draw out the statistical emergent properties with confidence. This systematic study focuses on the effect of air on microstructure in terms of particle rearrangement, local porosity, coordination number, radial distribution function, and contact force distribution. The drag force and by implication, air pressure is known from previous work to be important but this study shows more precisely when and how it affects packing structures.

2. Mathematical models

CCDM combines the Discrete Element Method (DEM) and Computational Fluid Dynamics (CFD). In DEM, the translational and rotational motions of particle i at any time t can be calculated according to Newton's second law of motion. A soft sphere model is used for collision of the particles and the spring-dashpot and slider model is employed for calculation contact forces, in normal and tangential directions, $\boldsymbol{f}_{cn,ij}$ and $\boldsymbol{f}_{ct,ij}$. For the fluid phase, the continuum fluid field is governed by the continuity and the Navier-Stokes equations based on the local mean variables over a computational cell. The SIMPLE [28] method is employed to solve the continuity and the Navier-Stokes equations. Details of the original CCDM are given in [27,29].

The effect of this rolling friction on the angle of repose of a sandpile has been demonstrated by Zhou et al. [6,7]. In this work, according to Beer and Johnson's formulae [30], the rolling friction torque, $T_{r,ij}$ is given by

$$|\mathbf{T}_{r,ij}| = \mu_r |\mathbf{f}_{cn,ij}| \tag{1}$$

where μ_r is the dynamic rolling friction coefficient. This coefficient is calculated based on a simplified contact mechanics (for details, see paper [31]).

According to Israelachvili [32], the van der Waals forces, $\boldsymbol{f}_{vdw,ii}$ between two closely spaced spheres i and j, is

$$\mathbf{f}_{vdw,ij} = \frac{Hd}{6z^2}\frac{\mathrm{R}_i}{R_i} \tag{2}$$

$$\text{For particle–wall interaction } d = R_i \tag{3}$$

$$\text{For particle–particle interaction } d = \frac{R_i \times R_j}{R_i + R_j} \tag{4}$$

where H is the so-called Hamaker constant, z is the separation distance between two particles, R_i is the radius of particle i. In order to avoid the singularity in using Eq. (2), a minimum separation distance, z_{min}, is assumed to be 1 nm [33], a cut-off distance is 1% of radius of spheres. In the present work, the Hamaker constant is back-calculated from a set of parameters, R_{vdw} (see Table 1) which is the ratio of van der Waals forces at z_{min} to the weight of particle.

It is worth mentioning here that at the time the investigation was performed, the 3D DEM for spheres was a well tested methodology and van der Waal's forces were implemented in 3D, however, the air flow coupling used a 2D approach. To improve the confidence that the model presented here would capture some of the important physics of a 3D world, the DEM results were in fact generated in a computational domain that is equivalent to a 3D volume that constrains the sphere interactions to be within a cell with frictionless walls just one particle diameter apart. The 2D slice then shown in the results is through all the particle centres. The flow of air is then modeled with no flow in the 3rd dimension. In future, a fully three dimensional mathematical model will be developed but it is suggested that such full 3D models may not reveal major shifts in the regime boundaries and the processes and force interactions presented here. So the porosity is defined as the ratio of the volume of voids to total volume in the 3D closed system considered in order to take into consideration the difference in porosity calculation between 2D and 3D. So in this work, the particles used are spheres not disks or cylinders for calculating the volume of particle i.

3. Simulation conditions

3.1. Packing method

In the present work, the packing method is similar to those in publications [10,11,27]. Uniform spheres with no overlap were randomly generated in the rectangular box with thickness equal to sphere diameter and initial porosity set to 0.75, so that they are effectively suspended in a loosely separated state (see Fig. 1). Then, the particles were allowed to settle down under gravity. In order to avoid wall effects for spheres, periodic boundary conditions were employed

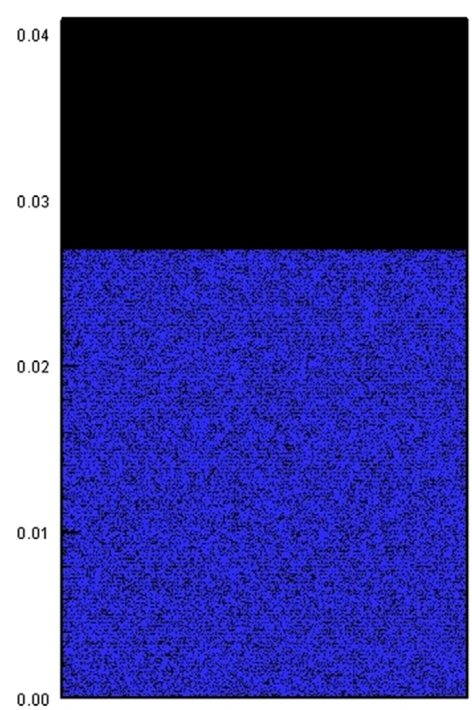

Fig. 1. Initial state of loose pack.