Simulation of the packing of cohesive particles

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Abstract

The packing behaviour of cohesive particles differs from that of coarse, cohesionless particles. To understand the underlying fundamentals, we have conducted a series of studies by means of discrete particle simulation.The forces involved vary with packing conditions. The packing structures are characterised in terms of porosity, coordination number and radial distribution function, and the particle-particle or pore-pore connectivity is analysed with the Voronoi or Delaunay tessellation. The force structures and their link with jamming states are also discussed. Structural properties are shown to be correlated with porosity which links directly to the cohesive force acting on a particle.

Key words: Packing; Cohesive particles; Computer simulation

1. Introduction

Packing of particles has been widely used to model structures of liquids and amorphous materials [1], and to study phase transition [2] and, more recently, "jamming" [3-5]. Proper description of particle packing is also of prime importance to many industrial processes ranging from raw material preparation to advanced material manufacturing [6]. In the past, many studies have been made to understand and model particle packing at either macroscopic or microscopic level. Macroscopic study often focuses on porosity or packing density (=1-porosity) in relation to, e.g., particle characteristics such as particle size distribution and shape [7]. Microscopic study focuses on packing structure, mainly supported by numerical simulation [8]. To date, the work is mainly for dry and coarse particles where gravity is the dominant force.

Cohesive forces are involved in many situations, and they affect the packing behaviour significantly [6]. For example, the van der Waals force plays a very important role for micro-sized particles. The capillary force gives a similar effect for wet particles. When particles settle in liquid, the effect of the cohesive force can be enhanced as a result of the reduced gravity effect. The different packing behavior of cohesive particles from cohesionless particles can be highlighted by the variation of porosity with particle size, moisture content and liquid density [9-11].

To understand the fundamentals governing the packing of cohesive particles, we have conducted a series of studies by means of discrete particle simulation [12-19]. This paper briefly reviews these studies for further development in this area.

2. Numerical Method

Discrete element method (DEM) uses an explicit numerical scheme in which the motion of individual particles and their interaction with each other are traced [12]. Each particle can possess translational and rotation motion which can be described by Newton's second law of motion. The forces vary with packing conditions, but normally include grav-

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ity, and the normal and tangential forces between two contacting particles [12,13]. Other forces considered include the van der Waals force, the capillary force, and the particle-fluid interactions when particles are settled in liquid. The detailed description of these forces can be found in [13,16,18,19].

Three types of packing were simulated in our work: packing and compaction of fine particles [13,19], packing of wet particles [16] and settling of particles in liquid [18]. The properties of particles largely correspond to those of glass beads but they can also vary [14]. A packing is formed with monosized particles whose size ranges from 1 to 1000 μm. It is formed in a rectangular container with periodic boundary conditions applied in the horizontal directions. The packing process is similar for all the types of packing considered. A simulation begins with particles randomly generated in the container with no overlap among them. The particles are then allowed to settle down under gravity. After a certain time, a stable packing is formed when all particles have velocities essentially equal to zero. Compaction is simulated by applying a pressure to the so formed packing in the axial direction [19].

3. Model validation

To validate the proposed DEM models, the simulated results have been compared with the measured macroscopic properties such as porosity. Fig. 1 shows the dependence of porosity on particle size for the packings of fine particles [13]. The results confirm that porosity increases significantly with decreasing particle size as particle size is less than 100μm. This is because of the increased van der Waals force relative to gravity. The capillary force functions similarly [9,10,20]. The relationship between porosity and moisture content can be well reproduced by the DEM approach [16].

Fig. 2 shows porosity as a function of the effective gravitational acceleration for the settling of different sized particles in liquid mixtures of diiodomethane and toluene [18]. The change of liquid compositions changes liquid density and viscosity, and the Hamaker constant as well. Smaller particles give a larger porosity because of the increase of the van der Waals force relative to the gravity. As liquid density increases, the effective gravitational acceleration decreases, and the effect of the van der Waals force is enhanced, leading to increased porosity.

It is clear that the proposed DEM models are able

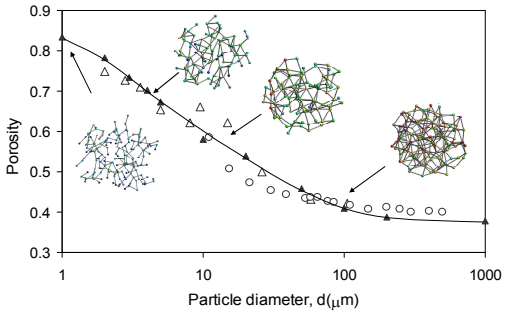

Fig. 1. Porosity as a function of particle size. Δ and o are measured data [9]); ▲ are the simulated results. Insets show the contact networks.

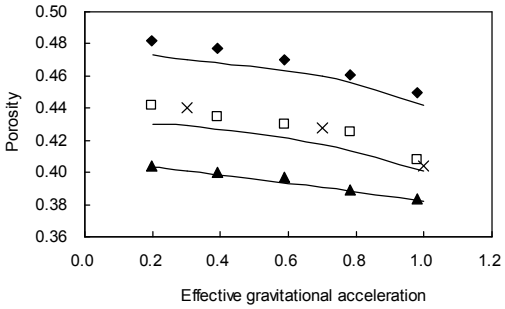

Fig. 2. Porosity of different sized glass beads as a function of the effective gravitational acceleration (Δg = (1-ρ_f/ρ_p)g). Points are the measured data [18]: ♦, d=500μm; □, d=250μm; ▲, d=110μm; ×, Onoda and Liniger [11]. Lines are the simulated results.

to generate results comparable with the measured data under different conditions. The discrepancy between the simulated and measured results is mainly attributed to the assumptions to simplify the consideration and effect the simulations. Some equations used to determine the forces are not so well developed. Nevertheless, the good agreement between the simulated and measured results in Figs. 1 and 2 confirms the validity of the present DEM models, at least qualitatively. The resultant microscopic information is useful for understanding the packing fundamentals of cohesive particles.

4. Structural analysis

Structural analysis is key to elucidating the packing mechanisms and the underlying physics. Various techniques have been adopted in this work. These include those commonly used in the literature, such as the radial distribution function (RDF) and coordination number (CN) distribution, and the so-called Voronoi or Delaunay tessellation to quantify the particle-particle or pore-pore connection in a

packing. Figs. 3 and 4 show some typical results for the packing of fine particles, taken from [13, 15, 17].

Fig. 3 shows the RDFs for different particle sizes. For 1000 μm particles which are largely cohesionless, RDF exhibits a split second peak, a well-known short-range feature observed in the random close packing [1,8]. When particle size decreases (or porosity increases), the first peak becomes narrower with a sharp decrease to the first minimum and the component of the second peak disappears while the peaks beyond the second one gradually vanish. Fig. 4 shows the area distribution of the Voronoi polyhedron face, where the areas are relative to the particles surface area. There are two peaks in the distribution. The first one is very strong and realized when the area tends to zero. The second one is obtained at a higher value of face area and shifts slightly towards higher face areas and gradually flattens out as porosity increases.

For the packing of wet particles and the settling of particles in liquids, the variation of packing structure with porosity is similar to that for the packing of fine particles [16,18,20]. The combined results also show that microscopic variables can be correlated with a single macroscopic variable, i.e. porosity. So the so-called "quasi-universality" [21] reasonably holds, although careful studies are needed to identify its possible limitation [14].

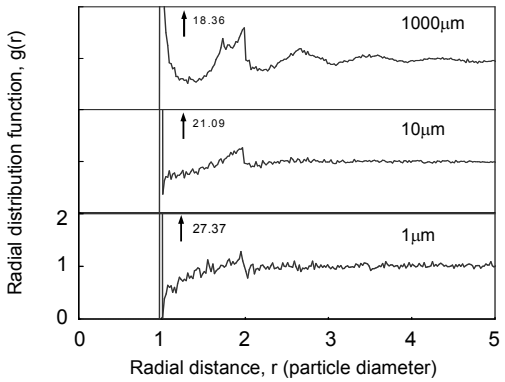

Fig. 3. Radial distribution functions for different sized particles.

5. Force analysis

Formation of a packing is a dynamics process in which the motion of a particle is controlled by various forces and torques. Such force information is quite difficult – if not impossible – to obtain in experiment. It is readily available in the DEM simulation. As shown by Dong et al. [18], the forces can be classified into two categories: process dependent and process independent. For example, for the settling of particles in liquids, the first category includes the contact and van der Waals forces, and drag and lift forces. The second category includes the gravity and buoyancy force. The process dependent forces vanish or become constant once a packing reaches its stable state. The force structure of cohesive particles in a static state has been examined [13,16,18,19]

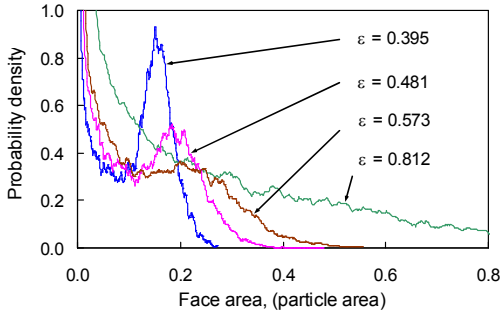

Fig. 4. Distributions of the face area of Voronoi polyhedron as a function of porosity.

Fig. 5 illustrates the evolution of force structures for the compaction of 10μm particles [19]. The force structure is characterised in terms of the non-dimensional normal contact force, which is defined as the ratio of the normal force and the mean value. The red lines represent the large forces of magnitude larger than 1.618 times the averaged value. Three jamming regions can be identified from the structure of large forces. When ε>0.44, the pressure causes some large but isolated force clusters being formed in the packing due to the local plastic deformation. When 0.36<ε<0.44, the large forces have formed a continuous network and the applied pressure can be transmitted through this network. However, at this stage the particles still have flexibility to re-arrange themselves in response to the pressure. Therefore, with increasing pressure, more large forces are generated and the orientation of some force connections changes. When ε<0.36, all particles are jammed, so the force network becomes rigid. Further increase in pressure can not increase the connections between particles but larger deformation of particles.

The cohesive force plays a key role in controlling the packing behavior of cohesive particles. The force may have different forms, e.g. the van der Waals force or capillary force, which however function similarly. It is therefore very helpful to formulate a general equation to describe the relationship between

porosity and cohesive forces in a packing. Fig. 6 plots porosity as a function of χ ($= |\sum \mathbf{F}_{ij}^c|/m\Delta g$) for all the three packing types considered. Although scattered, the data show one trend. A general equation has been proposed to describe the relationship between microscopic inter-particle forces and macroscopic porosity [9,13,16,18].

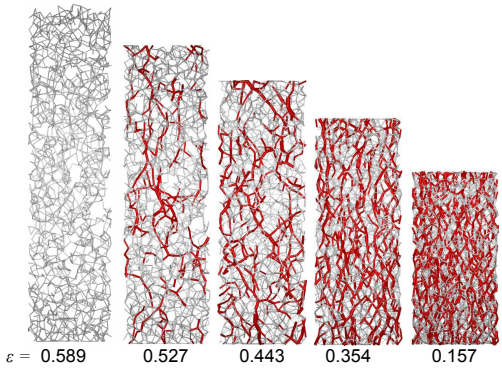

Fig. 5. Force structures of 10μm particles subjected to compaction giving different porosity. The red bonds are the large forces.

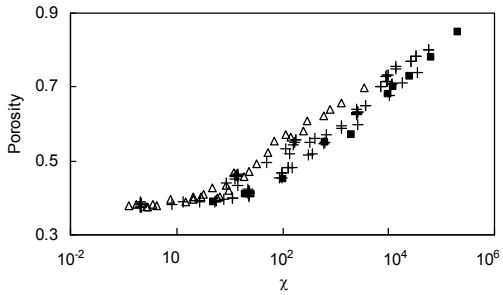

Fig. 6. Porosity as a function of the force ratio χ. Points are data from simulations of ■, packing of fine particles; +, packing of wet particles; and Δ, settling of particles in liquids.

6. Conclusions

Cohesion between particles due to the van der Waals and capillary forces plays an important role in the packing of cohesive particles. This effect can be effectively studied by DEM-based simulation. By use of this method, we have studied the packing of fine or wet particles under different conditions. The resultant information is useful to understand the packing and force structures of cohesive particles and the underlying mechanisms, as highlighted by the results presented in this paper. Future work will be conducted for more complicated systems, e.g. multi-sized particles, in order to generate results which may have direct application in practice.

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