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DEM simulation on the packing of fine ellipsoids

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HIGHLIGHTS

- The packing of fine ellipsoids is studied by DEM simulation.
- Particle size and shape markedly affect the porosity and CN.
- The porosity is correlated with particle size or force ratio and aspect ratio.
- The RDF peaks become obscure and even disappeared when particle size reduces.

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ABSTRACT

In this work, discrete element method (DEM) is used to study the effect of particle size and aspect ratio on packing structure of fine ellipsoids. It shows that porosity and coordination number significantly change with particle size and shape. The porosity-aspect ratio curve has minima at around 0.5 for oblate spheroids and 1.5 for prolate spheroids, but the cusp at 1.0 varies from convex to concave when particle size reduces as a result of the increasing role of the cohesive forces between particles. The coordination number-aspect ratio curves change from a strong to weak "M" shape when particle size reduces. Based on the results, equations are formulated to describe the correlation between bed porosity, aspect ratio, and particle size or force ratio. Microscopically, the radial distribution function is also affected by both particle size and shape. Fine particles have more disordered structure than coarse particles, and the packing of fine spheres is more ordered than fine ellipsoids. For coarse ellipsoids, majority of particles tend to orient horizontally, but the preferred orientation become worse when reducing particle size.

1. Introduction

Particle packing is one of the simplest particulate systems, and has been an important research topic in engineering and physics fields. For example, the densification of a powder mass is important in the shaping of solids in ceramics, powder metallurgy, and composite synthesis. Proper description of particle packing at either microscopic or macroscopic level is fundamental to many industrial processes such as solid-liquid separation, raw material handling and primary extractive processes. Thus, particle packing has been extensively studied for decades (Gray, 1968; German, 1989; Yang et al., 2000; Farrell et al., 2010; Silbert, 2010; Baranau and Tallarek, 2014).

There are many variables affecting the packing of particles. Among these variables, particle size and shape are of most importance. Many studies have been done to study the effect of particle size on the packing of spheres (Yen and Chaki, 1992; Watson et al., 1997; Yang et al., 2000; Jia et al., 2012). Generally, the packing structure becomes looser and the mean coordination number decreases as particle size decreases. For mono-sized spheres, the correlation between porosity and particle size or interparticle forces have been established by macroscopic (Yu et al., 2003) and microscopic (Feng and Yu, 2000; Yang et al., 2000) approaches. Besides particle size, particle shape also affects packing structures profoundly. For example, a small deviation of particle shape from spherical decreases the porosity of random packing significantly, but further deviation of shape may increase porosity (Zou and Yu, 1996; Sherwood, 1997; Williams and Philipse, 2003; Donev et al., 2004; Man et al., 2005; Chaikin et al., 2006; Zhao et al., 2012; Wegner et al., 2014; Dong et al., 2015). The highest packing densities obtained are 0.70 for spherocylinders with aspect ratio at 0.4 (Williams and Philipse, 2003) and 0.74 for ellipsoids with aspect ratio around 1.25 (Donev et al., 2004; Man et al., 2005; Chaikin et al., 2006). Moreover, nonspherical particles experience a tendency of orientation, and prefer laying horizontally due to the influence of gravity. Local alignment was found for the fibre-shaped particles (Evans and Ferrar, 1989), ellipsoids (Buchalter and Bradley, 1994; Zhou et al., 2011b), and bean, nail

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and cylinder shaped particles (Nolan and Kavanagh, 1995). Recently, it was reported that particle shape also shows a significant effect on the properties of the so called Voronoi cells, such as the volume, surface area and sphericity, in packings of ellipsoidal and cylindrical particles (Dong et al., 2016). So far, although the dependence of porosity on particle size for spherical particles and particle shape for coarse nonspherical particles are well established, it is still not clear how the porosity changes with both particle size and shape. Also, when the van der Waals force involves, how the orientation preference changes with both particle size and shape is unclear.

This paper will address these significant issues by numerical simulation. In particular, DEM is used to study the effect of both particle size and shape on packing structure. As demonstrated in the previous studies (Zhou et al., 2011b; Gan et al., 2016a, 2016b), ellipsoids can represent a large range of particle shapes varying from platy to elongated, and therefore are used in the present work. In particular, spheroids are used as they can be described by one single shape parameter – aspect ratio. Thus, various relationships can be established by this parameter. The results are analysed in terms of porosity, coordinate number, and radial distribution function. Particles with size ranging from 2 μm to 1 mm, and aspect ratio ranging from 0.25 to 3.5 are used.

2. Simulation method and conditions

2.1. Governing equations

Many modelling techniques have been used in the literature to study particle packing, for example, Monte Carlo algorithms and those based on either sequential or collective arrangement (Williams and Philipse, 2003). In particular, as a dynamic simulation model, DEM has been widely used to study particle packing under various conditions, as summarized by Zhu et al. (2008). DEM has its unique advantage in providing dynamic information, such as the trajectories of and transient forces acting on individual particles, which is extremely difficult, if not impossible, to obtain by physical experimentation at this stage of development. DEM has been successfully applied to study particle packing of nonspherical particles, e.g. ellipsoids (Džiugys and Peters, 2001; Peters et al., 2009; Hilton et al., 2010; Zhou et al., 2011b; Dong et al., 2015, 2016). The present work follows that of Zhou et al. (2011b). For convenience, a brief description of the method is given below.

According to the DEM, a particle can have two types of motion: translational and rotational, which are determined by Newton's second law of motion. The governing equations for the translational and rotational motion of particle i with radius R_i, mass m_i, and moment of inertia I_i can be written as

$$m_i \frac{d\mathbf{v}_i}{dt} = \sum_{j=1}^{k_c} (\mathbf{f}_{c,ij} + \mathbf{f}_{d,ij} + \mathbf{f}_{v,ij}) + m_i\mathbf{g} \tag{1}$$

and

$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \sum_{j=1}^{k_c} (\mathbf{M}_{t,ij} + \mathbf{M}_{r,ij} + \mathbf{M}_{n,ij}) \tag{2}$$

where $\mathbf{v}_i$ and $\boldsymbol{\omega}_i$ are the translational and angular velocities of the particle, respectively, and k_c is the number of particles in interaction with the particle. The forces involved are: the gravitational force $m_i\mathbf{g}$, and interparticle forces between particles, which include elastic force $\mathbf{f}_{c,ij}$, and viscous damping force $\mathbf{f}_{d,ij}$. For fine particles, the van der Waals force $\mathbf{f}_{v,ij}$ need to be considered (Yu et al., 2003). These interparticle forces can be resolved into the normal and tangential components at a contact point. The torque acting on particle i by particle j includes two components: $\mathbf{M}_{t,ij}$ which is generated by the tangential force and causes particle i to rotate, and $\mathbf{M}_{r,\ ij}$, commonly known as the rolling friction torque (Brilliantov and Pöschel, 1998), is generated by asymmetric normal forces and slows down the relative rotation between particles. For ellipsoids, addition torque $\mathbf{M}_{n,ij}$ should be added because the normal contact force and van der Waals force do not necessarily pass through the particle centre. Moreover, particle may undergo multiple interactions, so the individual interaction forces and torques are summed over the k_c particles interacting with particle i.

Equations used to calculate the interaction forces and torques between two spheres have been well-established in the literature (Zhu et al., 2007). These equations can be extended to ellipsoids (Zhou et al., 2011a, 2011b; Gan et al., 2016a, 2016b). The ellipsoidal particles have smooth/continuous surfaces like a sphere, so the Coulomb condition or sliding/rolling friction models are the same for spheres and ellipsoids. Other important forces, such as the normal and tangential contact forces, are recently also proved to be valid for ellipsoidal particles by using finite element method (Zheng et al., 2013). Therefore, these force models previously formulated for spheres can be reasonably used in this work. The equations to calculate the particle-particle interaction forces and torques are listed in Table 1.

Table 1
Components of forces and torque acting on particle *i*.

Forces and torques	Symbols	Equations
Normal elastic force	$\mathbf{f}_{\mathrm{cn,ij}}$	$-4/3E^*\sqrt{R^*}\,\delta_n^{3/2}\mathbf{n}$
Normal damping force	$\mathbf{f}_{\mathrm{dn,ij}}$	$-c_n(8m_{ij}E^*\sqrt{R^*\delta_n})^{1/2}\mathbf{v}_{n,ij}$
Tangential elastic force	$\mathbf{f}_{\mathrm{ct,ij}}$	$-\mu_s\lvert\mathbf{f}_{cn,ij}\rvert(1-(1-\delta_t/\delta_{t,\max})^{3/2})\hat{\boldsymbol{\delta}}_t\ \ (\delta_t<\delta_{t,\max})$
Tangential damping force	$\mathbf{f}_{\mathrm{dt,ij}}$	$-c_t(6\mu_s m_{ij}\lvert\mathbf{f}_{cn,ij}\rvert\sqrt{1-\lvert \mathrm{V}_t\rvert/\delta_{t,\max}}/\delta_{t,\max})^{1/2}\mathbf{v}_{t,ij}\ (\delta_t<\delta_{t,\max})$
Coulomb friction force	$\mathbf{f}_{\mathrm{t,ij}}$	$-\mu_s\lvert\mathbf{f}_{cn,ij}\rvert\hat{\boldsymbol{\delta}}_t\ \ (\delta_t\ge\delta_{t,\max})$
Torque by normal force	$\mathbf{M}_{\mathrm{n,ij}}$	$\mathbf{R}_{ij}\times(\mathbf{f}_{cn,ij}+\mathbf{f}_{dn,ij})$
Torque by tangential force	$\mathbf{M}_{\mathrm{t,ij}}$	$\mathbf{R}_{ij}\times(\mathbf{f}_{ct,ij}+\mathbf{f}_{dt,ij})$
Rolling friction torque	$\mathbf{M}_{\mathrm{r,ij}}$	$\mu_{r,ij}\lvert\mathbf{f}_{n,ij}\rvert\hat{\boldsymbol{\omega}}_{t,ij}^{n}$

where, $1/m_{ij} = 1/m_i + 1/m_j$, $1/\mathrm{R}^* = 1/\lvert\mathrm{R}_i\rvert + 1/\lvert\mathrm{R}_j\rvert$, $E^* = E/2(1-\nu^2)$, the angular velocity unit vector $\hat{\boldsymbol{\omega}}_{t,ij}$ is defined as $\hat{\boldsymbol{\omega}}_{t,ij} = \boldsymbol{\omega}_{t,ij}/\lvert\boldsymbol{\omega}_{t,ij}\rvert$, $\delta_n = \lvert\boldsymbol{\delta}_n\rvert, \delta_t = \lvert\boldsymbol{\delta}_t\rvert$, the unit vector $\hat{\boldsymbol{\delta}}_t$ is defined as $\hat{\boldsymbol{\delta}}_t = \boldsymbol{\delta}_t/\lvert\boldsymbol{\delta}_t\rvert$, $\delta_{t,\max} = \mu_s(2-\nu)/2(1-\nu)\cdot\delta_n$, $\mathbf{v}_{ij} = \mathbf{v}_j - \mathbf{v}_i + \boldsymbol{\omega}_j\times\mathbf{R}_j - \boldsymbol{\omega}_i\times\mathbf{R}_i$, $\mathbf{v}_{n,ij} = (\mathbf{v}_{ij}\cdot\mathbf{n})\cdot\mathbf{n}$, $\mathbf{v}_{t,ij} = (\mathbf{v}_{t,ij}\times\mathbf{n})\times\mathbf{n}$.
Note that tangential forces ($\mathbf{f}_{\mathrm{ct,\ ij}} + \mathbf{f}_{\mathrm{dt,\ ij}}$) should be replaced by $\mathbf{f}_{\mathrm{t,\ ij}}$ when $\delta_t > \delta_{t,\max}$.