Particuology 23 (2015) 109–117

Contents lists available at ScienceDirect

Particuology

journal homepage: www.elsevier.com/locate/partic

Random packing of tetrahedral particles using the polyhedral discrete element method

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ARTICLE INFO

Article history:
Received 8 December 2014
Received in revised form 28 January 2015
Accepted 2 February 2015
Available online 14 July 2015

Keywords:
Discrete element method
Random packing
Tetrahedral particle
Coordination number
Packing density

ABSTRACT

The random packing of tetrahedral particles is studied by applying the discrete element method (DEM), which simulates the effects of friction, height ratio, and eccentricity. The model predictions are analyzed in terms of packing density and coordination number (CN). It is demonstrated that friction has the maximal effect on packing density and mean CN among the three parameters. The packing density of the regular tetrahedron is 0.71 when extrapolated to a zero friction effect. The shape effects of height ratio and eccentricity show that the regular tetrahedron has the highest packing density in the family of tetrahedra, which is consistent with what has been reported in the literature. Compared with geometry-based packing algorithms, the DEM packing density is much lower. This demonstrates that the inter-particle mechanical forces have a considerable effect on packing. The DEM results agree with the published experimental results, indicating that the polyhedral DEM model is suitable for simulating the random packing of tetrahedral particles.

1. Introduction

The random packing of granular materials is ubiquitous in nature and industry. Their interesting structural properties have been the focus of a considerable body of research (Stillinger & Weber, 1984; Pouliquen, Nicolas, & Weidman, 1997; Glotzer & Solomon, 2007; Jaoshvili, Esakia, Porrati, & Chaikin, 2010). Earlier studies investigated the packing of spherical particles in the laboratory (Bernal, 1959; Scott, 1962; Finney, 1970). However, such experiments are labor intensive and often involve large uncertainties at the microscopic scale of interest. To overcome these difficulties, numerical methods have been developed to generate random packing of spheres (Jodrey & Tory, 1981; Nolan & Kavanagh, 1992). However, given that these methods are geometry based, i.e. they do not account for the mechanical particulate forces, some investigators have incorporated the discrete element method (DEM) (Cundall & Strack, 1979) to investigate the random packing of spherical particles. DEM has gradually become a most effective tool in the numerical simulation of particle packing.

Particle shape has a significant effect on packing structure (Wouterse, Williams, & Philipse, 2007; Baker & Kudrolli, 2010; Kyrylyuk & Philipse, 2011; Athanassiadis et al., 2014). The packing of non-spherical particles is considerably different from that of spherical particles (Li, Zhao, Lu, & Xie, 2010). Lu, Li, Zhao, and Meng (2010) investigated the random packing of binary mixtures of spheres and spherocylinders using a sphere assembly model and relaxation algorithm, yielding relationships between packing density and aspect ratio. Kyrylyuk and Philipse (2011) carried out a similar investigation using mechanical contraction methods. Li et al. (2010) reported the maximum random packing densities of basic 3D objects using sphere assembly models. Jiao and Torquato (2011) specialized their approach to random packings of Platonic solids using the adaptive-shrinking-cell method (Torquato & Jiao, 2009) and determined the influence of the shape and symmetry of a polyhedral particle on its packing density. The aforementioned studies were geometry based. The random packing of non-spherical particles has also been investigated using DEM. For example, Zhou, Zou, Pinson, and Yu (2011) simulated the random packing of ellipsoidal particles and reported that the maximum packing density occurs at an aspect ratio of 0.6 for oblate spheroids and 1.8 for prolate spheroids. Deng and Davé (2013) used the multi-sphere

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http://dx.doi.org/10.1016/j.partic.2015.02.007
1674-2001/

method to investigate the effects of particle size and aspect ratio on the packing of spherocylinders. Using a similar technique, Nan, Wang, Ge, and Wang (2014) studied the random packing of rigid fibers with variable aspect ratios and curvatures.

To date, few investigations into the packing of polyhedral particles using DEM have been reported, even though polyhedra are common geometric shapes. One reason for this is that modeling polyhedra in DEM is much more complex than modeling the types of non-spherical particles mentioned above. In principle, the DEM element can be any shape (Cundall & Strack, 1979). However, the simplest spherical element is most commonly used because it is computationally efficient, especially in terms of particle-particle contact detection (Theuerkauf, Witt, & Schwesig, 2006; Siiriä & Yliruusi, 2007; Suikkanen, Ritvanen, Jalali, & Kyrki-Rajamäki, 2014). In view of this, the clump technique can be employed to produce non-spherical particles from multiple spheres. However, Höhner, Wirtz, and Scherer (2012) found considerable differences between the packing properties of polyhedral and multi-sphere particles in a simulation of hopper discharge. Therefore, we used accurate particle shape in this work.

The tetrahedron is the basic shape in the family of polyhedra and has some interesting applications and properties. The study of tetrahedral packing is of importance in geotechnical, mining, and transportation engineering; e.g., the study and deployment of tetrahedra is important in river damming. All polyhedra can be discretized into tetrahedra by Delaunay triangulation. Regular tetrahedra exhibit the lower bound (Conway & Torquato, 2006) and upper bound (Jaoshvili et al., 2010) of packing density among convex polyhedra. Latham, Lu, and Munjiza (2001) simulated the random loose packing of angular particles using tetrahedra and obtained a packing density of 0.416. Chen (2008) reported a packing density of 0.779 for regular tetrahedra. Jiao and Torquato (2011) generated random packing of tetrahedra using the adaptive-shrinking-cell method (Torquato & Jiao, 2009) and obtained a lower packing density of 0.763. These investigations were mainly focused on achieving a denser packing of regular tetrahedra. With respect to irregular tetrahedra, Zhao, Li, Jin, and Zhou (2012) investigated the effect of particle shape on packing using the relaxation algorithm. Their study reported that the regular tetrahedron represents the upper bound of packing density in the family of tetrahedra. Nevertheless, almost all these investigations ignore the mechanical forces (e.g., gravity and contact forces) that exist in a physical packing process. Moreover, the packing characteristics of tetrahedral particles when subjected to various physical mechanisms are not well understood.

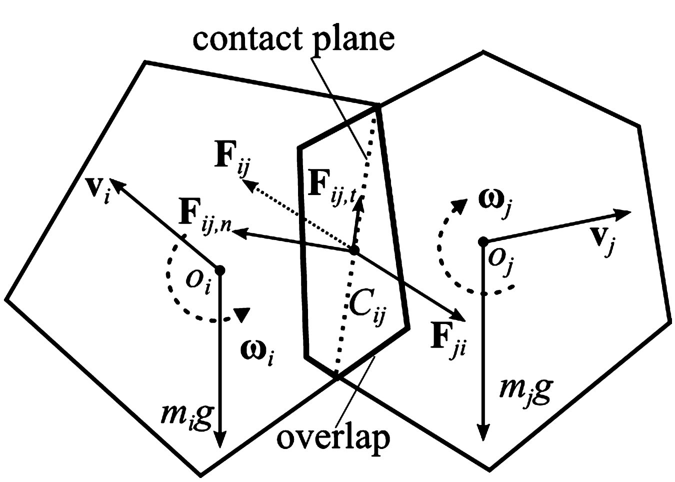

Fig. 1. Two-dimensional illustration of interaction between two particles. The overlap region is exaggerated for clarity.

In this paper we investigate the random packing of tetrahedral particles under the conditions of gravity and contact force using DEM. We consider the effects of different physical and geometric parameters, such as particle friction, eccentricity, and height ratio, on packing density and particle coordination number.

2. Polyhedral discrete element model

2.1. Governing equations

DEM can be applied to computing the individual translating and rotating motion of a large number of particles. It uses an explicit time stepping approach to numerically integrate the motion of each particle. The constitutive force-displacement law and Newton's second law of motion are used, respectively, to calculate the contact force and motion of each particle in each time step. The governing equations for the motion of a particle i with mass m_i and moment of inertia I_i are given as follows:

$$m_i \frac{\mathrm{d}v_i}{\mathrm{d}t} = (1 \pm \alpha) \sum_{j=1}^{n_i} F_{ij} + m_i g, \tag{1}$$

$$I_i \frac{\mathrm{d}\omega_i}{\mathrm{d}t} = (1 \pm \alpha) \sum_{j=1}^{n_i} M_{ij}, \tag{2}$$

where v_i and ω_i are the translational and angular velocities of the particle i, respectively; n_i is the number of neighbors touching the particle i; and α is the damping constant used to dissipate system energy to arrive at a steady state solution in a reasonable number of iterations. As shown in Fig. 1, forces acting on the particle i include the gravitational force, $m_i g$, and the contact forces (including force F_{ij} and moment M_{ij}). When F_{ij} and v_i (or M_{ij} and ω_i) have the same signs, the sign before α in the above equations is a minus, and contrariwise, a plus.

2.2. Contact detection

Detecting particle contacts for polyhedral particles is much more complicated than for spherical particles. For spherical particles, it is easy and efficient to obtain the overlap of two bodies in terms of their positions and radii. However, for polyhedral particles, the overlap region is not regular (see Fig. 1) and has multiple contact points (e.g., at face–face or face–edge contact), making it a resource-intensive computation in most cases. Given that the detection of so many particle collisions must be computed in each time step, a combination of approximate and exact collision detection is performed to reduce the simulation time.

The AABB (axis-aligned bounding box) algorithm is an efficient approach to determine whether a collision between two bodies is likely; this is termed 'approximate detection'. As the name suggests, the AABB is a box consisting of six faces aligned with global coordinate axes that can, in most cases, fit tightly within a contacting body. This makes it straightforward to detect overlap between two AABBs by comparing their lengths along each axis. If there is an axis along which the projections of the AABBs do not overlap, then no overlap exists between the two AABBs, which also means that no overlap exists between the two bodies. On the other hand, if there is overlap between the two AABBs, then overlap may exist between the two bodies. In this case, exact detection should be implemented.

Various methods have been developed for exact detection, such as the common plane (CP) algorithm (Cundall, 1988), the fast common plane (FCP) algorithm (Nezami, Hashash, Zhao, & Ghaboussi, 2004), and the inner potential particle algorithm (Boon, Houlsby, & Utili, 2012). Recently, a dual approach (Muller & Preparata, 1978;