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DEM simulation of cubical particle packing under mechanical vibration

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ABSTRACT

Packing densification of cubical particles under mechanical vibrations was dynamically simulated by using discrete element method (DEM). Effects of operating parameters such as vibration amplitude, frequency, vibration intensity, and container size (container wall) on packing densification were comprehensively investigated. The macro property such as packing density and micro properties such as coordination number (CN), radial distribution function (RDF), and particle orientation of the packings were analyzed and compared. It is found that mechanical vibration with proper vibration amplitude and frequency is effective for the densification of cubical particle packing. Packing structures of different packing densities display different properties, based on which random loose packing (RLP) and random close packing (RCP) of cubical particles are identified with the packing density of 0.591 and 0.683, respectively. Two densification mechanisms are discussed as the particle rearrangement is dominant for the transition from RLP to RCP and the crystallization along the container wall is dominant for the transition beyond RCP to ordering. The obtained results are useful for optimizing vibration conditions to generate dense packings and understanding the structural information of some fixed beds with cubical particles.

1. Introduction

Particle packing, known as the static assembly of particles, is probably the simplest state of granular matter which are extensively existed both in nature and industries [1,2]. In scientific research, packings of particles can be used to model the structures of liquids [3–5], amorphous metals and alloys [6], solids and crystals [7–9] and their transitions [10–13]. Proper understanding of particle packing is also of primary importance in industrial applications with the following two problems particularly being concerned: i) the packing densification of particles, which is fundamental in powder metallurgy or composite synthesis [14,15]; ii) the quantitative characterization of packing structures, as the permeability and thermal conductivity of granular materials can be quantitatively related to the pore connectivity [16] and particle connectivity [17] of a packing, respectively.

Generally, mechanical vibrations or tapping methods are used to densify the packing of particles [12,13,18–20]. Since the work of Scott [21], it is known if uniform hard spheres are poured in a container, a random loose packing (RLP) can be formed with the packing density $\rho \approx 0.60$; and this initial RLP structure can be densified to a random close packing (RCP) with $\rho \approx 0.64$ by utilizing tapping or vibrations. The obtained RLP and especially RCP of uniform hard spheres exhibit critical features for modelling phase transitions [22–24], thus the mechanism in terms of the transition or densification from RLP to RCP is fascinating for researchers. By using mechanical vibrations, packing densification can be realized due to the rearrangement of particles with the elimination of large pores and arching structures initially formed in the loose packings. As a dynamic process, the densification under sinusoidal vibration is affected by vibration time, amplitude A and frequency ω etc. Particularly, A and ω have direct influence on the vibration energy which affects the vibration efficiency greatly. The dimensionless vibration intensity Γ [25,26], defined as $A\omega^2/g$ (g represents the gravitational acceleration), is thus used to evaluate vibration energy with both A and ω being considered. An et al. [12] reported the densification of spheres from RLP to RCP should be related to Γ with two pore filling mechanisms identified as "pushing filling" when Γ is low and "jumping filling" when Γ is high.

It is noting that previous studies were mainly conducted on the packing of spheres, whereas most of the particles that we encounter in reality are of non-spherical shapes. Actually, some non-spherical particles can be beneficial alternatives of spherical particles in many applications. For example, cubical particles are advantageous in forming denser products in powder metallurgy [27] and acting as the drug-delivery media [28] in certain medical field. In addition, it was shown that packing of cubical particles could also be used to study the phase behavior of colloidal particles [29]. But the understanding of cubical particle packing is presently limited. The crystallized packing of cubical particles is easy to be figured out as particles aligned with the neighbors without voids. However, little is known about the RLP and RCP of cubical particles. The studies of cubical particle packing began with physical experiments. Zou and Yu [30] proposed empirical equations to describe

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the relationship between packing density and particle shape for various non-spherical particles. For mono-sized cubical particles, packing densities of RLP and RCP are predicted as about 0.586 and 0.656, respectively. Recently, Barker and Kudrolli [31] reported the RLP and RCP of five Platonic solids by fluidized or mechanically vibrated methods. The packing density of RLP and RCP of cubical particles are 0.54 and 0.67, respectively. They also examined the randomness of packing structures by calculating the variance among the projected areas of images obtained from the top of the packings. Actually, due to the complexity of particle systems, it is difficult and laborious for physical experiments to understand the underlying densification mechanism and the detailed structural information of packing structures.

The deficiencies of studies in physical experiments can be readily overcome by numerical simulations. Generally, two kinds of simulation methods are prevalent in modelling particle packings: 1) methods of or related to Monte Carlo (MC) [32]; 2) the Discrete Element Method (DEM) [33]. MC methods are widely used to obtain the maximum packing densities of particles. Zhao and Li [34] reported the packing density of their obtained RCP of cubes using a MC based method is 0.7755. However, they just focused on the relationship between packing density and sphericity without describing further structural information. And it is worth noting that these MC methods actually cannot realize the truly dynamic packing of particles since they are geometrically based without force considerations, which may fail to reproduce the structural information fully comparable to those measured [35]. Based on Newton's second law of motion, DEM [33] can obtain the dynamic information of every particle at each time step, thus can well realize the dynamic packing of particles with inter-particle forces and dynamics being considered. In addition, the experimental vibration conditions performed on particle packing can also be well achieved by DEM [12,20], thus the investigation of densification mechanism is possible.

In present work, the dynamic packing of mono-sized cubical particles under mechanical vibration is simulated by DEM with the focuses of reproducing the transition from RLP to RCP and identifying the obtained RCP structure and corresponding densification mechanism. The paper is structured as follows: Section 2 describes the DEM approach used for vibrated packing of cubical particles and the simulation conditions; in Section 3, the effects of vibration condition on packing density, microstructural characterization, and densification mechanisms are systematically discussed and analyzed; final conclusions are summarized in Section 4.

2. Simulation method and conditions

2.1. DEM model

In DEM model [33], each particle possesses both translational and rotational motions, which are governed by Newton's second law of motion, given by

$$m_p \frac{dv_p}{dt} = F_p + m_p g \tag{1}$$

$$I_p \frac{d\omega_p}{dt} = T_p \tag{2}$$

where m_p, v_p, ω_p and I_p are respectively the mass, translational velocity, angular velocity, and moment of inertia of particle p; F_p and T_p are the total force and torque acted on the particle p. Due to the geometrical non-uniform characteristics of non-spherical particles, their contact detection is problematic. A number of techniques have been developed in the last decade for solving this problem [36,37]. Especially, the multi-sphere model is widely adopted in DEM simulation. This method is flexible in shape description as a particle of any shape can be constructed by a number of element-spheres; and the contact detection between non-spherical particles can be simplified to the contact calculation of their element-spheres. Therefore, in this paper the multi-sphere model is adopted to describe cubical particles.

By using the multi-sphere model [38], the total force F_p of the particle p is the sum of the forces on its element-spheres.

$$F_p = \sum_{s=1}^{ns} F_{p,s} \tag{3}$$

where ns is the total number of spheres in the particle p; $F_{p,s}$ is the force of sphere s in particle p, and it is the sum of normal forces $F^n_{p,s}$ and tangential forces $F^t_{p,s}$ acting on its contact points:

$$F_{p,s} = F^n_{p,s} + F^t_{p,s} = \sum_{C=1}^{contacts} \left(F^n_{ps,c} + F^t_{ps,c} \right) \tag{4}$$

The normal and tangential contact forces $F^n_{ps,c}$ and $F^t_{ps,c}$ on the contact point c are calculated based on Hertz model [39] and the work of Mindlin and Deresiewicz [40], respectively. The details about the force models can be found in the literature [41,42]. The torque T_p is the sum of three components [43]:

$$T_p = \sum_{s=1}^{ns} \left(T_{tp,s} + T_{np,s} + T_{rp,s} \right) \tag{5}$$

where $T_{tp,s}$ is created by tangential forces, $T_{np,s}$ is created by normal forces when the normal force of the element-sphere does not pass through the center of the particle; $T_{rp,s}$ is the rolling friction torque. $T_{tp,s}$ and $T_{np,s}$ are respectively given as

$$T_{tp,s} = \sum_{C=1}^{contacts} \left(r_{ps,c} \times F^t_{ps,c} \right) \tag{6}$$

$$T_{np,s} = d_{p,s} \times F^n_{p,s} \tag{7}$$

where $r_{ps,c}$ is the vector between the contact point c and the center of element sphere s, belonging to particle p; and $d_{p,s}$ represents the relative position vector between the centroid of particle p and the centre of the element sphere s.

2.2. The orientation representation and rotational solution

The orientation representation and rotational movement of non-spherical particles are much more complicated than that of spherical particles. This is because the inertia tensor of a non-spherical particle in a global coordinate system will be changed at each time step according to its new orientation [37]. To overcome this problem, two coordinate systems as indicated in Fig. 1 are generally adopted: one is the global coordinate system, which is fixed; and the other is a local coordinate system, which moves with the non-spherical particle together. Therefore, the rotational equation can be solved with the inertial tensor obtained in the local coordinate system.

In a local coordinate system, the inertial tensor I of a non-spherical particle can be expressed as:

$$I = \begin{pmatrix} I_{xx} & I_{xy} & I_{xz} \\ I_{yx} & I_{yy} & I_{yz} \\ I_{zx} & I_{zy} & I_{zz} \end{pmatrix} \tag{8}$$

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