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Structure analysis on the packing of ellipsoids under one-dimensional vibration and periodic boundary conditions

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ABSTRACT

This paper presents a numerical study on the packing structure of ellipsoidal particles under one-dimensional vibration and periodic boundary conditions by discrete element method. It is shown that after vibration, packings of ellipsoids become denser, and the coordination number increases slightly for oblate ellipsoids (aspect ratio between 0.25 and 0.75), but decreases for most of the prolate ellipsoids due to the conspicuous excluded volume effects. It is found that packings of ellipsoids are more random after vibration, showing opposite trend to spheres. The analysis of Voronoi tessellation for ellipsoids packing indicates that after vibration, some bridges or arches collapse, and particles reorganize to fill voids, leading to denser packings. The Voronoi cell volume becomes smaller for both oblate and prolate particles, and more uniform for oblate particles. Therefore, the bed becomes densely packed by obtaining smaller and more uniform Voronoi cell (or void structure) at the sacrifice of particle orientational order.

1. Introduction

Particle packing is important and widely found in nature and industry. Proper description of particle packing is fundamental to many industrial processes ranging from raw material preparation to advanced material manufacturing in many industries. Vibration or tapping has the potential to densify the packing if conditions are right [1–4]. It is known that if uniform hard spheres are poured in a container, a random loose packing (RLP) can be formed with the packing density $\rho \approx 0.60$. Properly controlling vibrational and charging conditions, the transition from disordered to ordered, densest packing of particles can be obtained consistently [5]. For example, the initial RLP structure can be densified to a random close packing (RCP) with $\rho \approx 0.64$ by utilizing tapping or vibrations. Many studies have been carried out on randomness and its transition from loose packing to close packing, particularly for spheres [4–6]. In the meantime of the change of packing density, microstructural properties also change. A looser packing often corresponds to smaller coordination number (CN), less peaked radial distribution function (RDF) and larger but more widely distributed pores [4].

As one of the key parameters affecting packing structure, particle shape plays equally important role as particle size. It was found that particle shape affects the packing structure significantly [7–9]. 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 [7,10–15]. The highest packing densities obtained are 0.70 for spherocylinders with aspect ratio at 0.4 [12] and 0.74 for ellipsoids with aspect ratio around 1.25 [7,16,17]. However, the definitions of RLP and RCP widely used for spheres are not applicable to uniform non-spherical particles, especially spheroids, since the packing is no longer random. Ordered packing structures have been observed in packings of ellipsoidal particles [7–9]. For example, oblate spheroids were found to face upward/downward, and the prolate spheroids with the symmetry axes pointing to the horizontal direction [8,9]. However, when ellipsoidal particles are subjected to vibration conditions, some basic questions are still unclear, including: will the packing become denser? If yes, what causes this change? Will the packing become more ordered after vibration? Is there any relationship between packing density and particle orderness? The answers to these questions have been less reported in the literature, and will be addressed in this work.

Hence, a three-dimensional DEM model is used in the present work to study the packing of ellipsoids under both poured packing and one-dimensional vibrated conditions. The variation of packing density with vibration is captured, and the transition of packing structures in terms of microstructural properties such as coordination number (CN), particle orientation and Voronoi cells are analyzed. Such information is useful for structural understanding and further development in this area.

2. DEM model and simulation conditions

The present work follows our previous work on DEM packing of coarse [9] and fine ellipsoids [8], and focuses on packings under vibration conditions. Note that due to the high computational time cost for contact detection as a result of the numerical solution of a sixth-order

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Table 1
Particle parameters used in the DEM simulation.

Parameters	Values
Bed size (width × thick × height)	200 mm × 200 mm × 900 mm
Particle number	15,000
Volume equivalent particle size (2a, 2b = 2c, d_v)	$d_v = 2(abc)^{1/3} = 10$ mm
Particle aspect ratio ($\eta = a/b$)	0.15–4.0
Particle density	2500 kg/m^3
Sliding friction coefficient, μ_s	0.4
Rolling friction coefficient, μ_r	0.002 d_v
Normal damping coefficient, c_n	0.3
Tangential damping coefficient, c_t	0.3
Young's modulus, E	1×10^7 g/(m·s^2)
Poisson ratio, ν	0.3
Time step, Δt	1×10^{-4} s

NB: i) *a* is the principal radius in the polar direction, *b* and *c* are principal radii in the equatorial plane. ii) For a prolate spheroid, aspect ratio $\eta > 1$; for a sphere, $\eta = 1$; and for an oblate spheroid, $\eta < 1$. And iii) wall is assumed to have the same physical properties as particles.

polynomial equation [18,19], our recently developed GPU parallelization technology [20] is applied in this work.

The size, aspect ratio and other physical properties of particles and parameters used in DEM simulation are given in Table 1. Particles used are spheroids with aspect ratios varying from 0.15 to 4.0. All the particles with different aspect ratios have the same volume hence the same equivalent diameter d_v. Here, aspect ratio α is defined as $\eta = a/c$, where a is the principal radius in the polar direction, and b and c are two principal radii in the equatorial plane, where $b = c$ for spheroids. For prolate spheroids ($a > b = c$), aspect ratio $\eta > 1$; for a sphere ($a = b = c$), $\eta = 1$; and for oblate spheroids ($a < b = c$), $\eta < 1$.

The simulation begins with the poured packing [21] of mono-sized and mono-shaped ellipsoidal particles with random position and orientation in a rectangular box with the width of 20 particle diameter. Periodic boundary conditions are applied to the side walls to eliminate the wall effect and maintain a continuous internal granular flow [22–24]. The bottom wall is assumed to have the same physical properties as particles. After packing, one-dimensional vibration in the vertical direction is introduced for a period of 20 s, then stops. The bed is then allowed to settle for 10 s to reach its static state, as used for spheres done by An et al. [25]. To be consistent, in the DEM simulation, the bottom of the container is vibrated according to $Z(t) = A\sin[\omega(t - t_0)]$ where $Z(t)$ is the vertical displacement at time t, and t_0 is the starting time of vibration. The effect of vibration amplitude A and frequency ω are tested, and shown in Fig. 1. With the increase of A and ω, the bed becomes denser, and the packing density keeps high when A and ω are in a certain range, e.g., A between 0.1 and 0.4 d_v and ω between 100 and 400 *rad/s*. However, when A or ω are too high, the bed becomes looser again, but the value is still higher than that of poured packing. The general tendency agrees well with that of An et al. [4]. In the following sections, unless otherwise specified, the vibration amplitude A and frequency ω are respectively set to 0.2 d_v and 200 rad/s, as used by An et al. [25].

Fig. 2 shows the variation of packing density and bulk-averaged coordination number ‹CN› with time and packings of oblate and prolate spheroids. With the introduction of vibration from 10s to 30s, the packing density fluctuates significantly. The vibration stops at 30 s, then the packings quickly reach the steady state. For oblate spheroids with aspect ratio of 0.15, the packing density is at 0.564 for poured packing, and increases to 0.614 after vibration. For prolate spheroids with aspect ratio of 4.0, the packing density is at 0.603 for poured packing, but reduces to 0.613 after vibration. Although small vibration amplitude is used, the ‹CN› fluctuates dramatically. During the whole vibrating process, the ‹CN› is smaller than the ‹CN› under stable states before and after vibration. From the inset figures, it can be observed that ordered orientation structure can be found in packings of oblate ($\eta = 0.15$, and particles tend to face upward or downward) and prolate ($\eta = 4.0$, and the symmetry axis of particles tend to point to the horizontal direction) particles, consistent with previous studies [8,9]. After vibration, the packing height and particle orientation slightly change, but the difference cannot be visualized clearly from the packings in Fig. 2.

3. Results and discussion

3.1. Packing density and coordination number

The relationship between packing density and aspect ratio has been established in the literature, e.g. by Donev et al. [7] and Zhou et al. [9], generally showing an M-shape curve. Ellipsoidal particles can pack more densely than spheres in a certain range of aspect ratios, e.g. from 0.5 to 2.0. If particles are too flat or too elongated, the packing becomes looser than spheres. The relationship under both poured packing and dense packing is shown in Fig. 3. It can be seen that from Fig. 3(a), the packing densities for different aspect ratios increase to some extent after vibration, and the curve still demonstrates an M shape. It should be noted that the increase of packing density for oblate spheroids with aspect ratio smaller than 0.3 is quite significant. For example, packing density increases by 0.05 for aspect ratio of 0.15, which indicates that the packing structure changes after vibration.

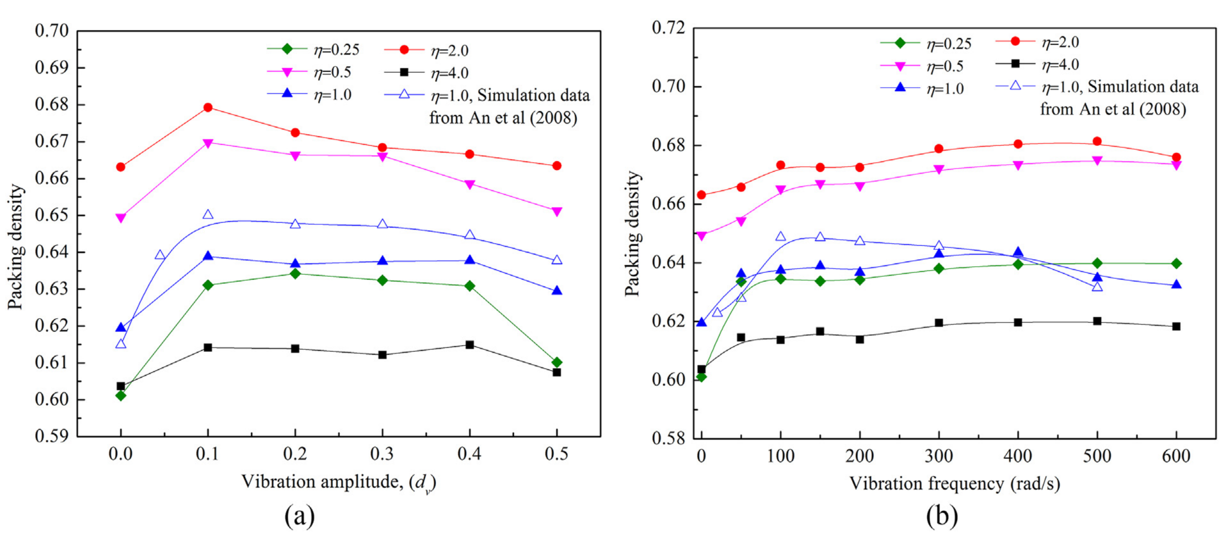

Fig. 1. Effect of (a) vibration amplitude A at $\omega = 200$ rad/s and (b) frequency ω at $A = 0.2\ d_v$ on packing density.