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Radical tessellation of the packing of ternary mixtures of spheres

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ABSTRACT

The packing of ternary mixtures of spheres with size ratios 24.4/11.6/6.4 is simulated by means of the discrete element method. The packing structure is analyzed by the so called radical tessellation which is an extension of the well-established Voronoi tessellation. The topological and metric properties of radical polyhedra are quantified as a function of the volume fractions of this ternary packing system. These properties include the number of edges, area and perimeter per radical polyhedron face, and the number of faces, surface area and volume per radical polyhedron. The properties of each component of a mixture are shown to be strongly dependent on the volume fractions. Their average values can be quantified by a cubic polynomial equation. The results should be useful for understanding the packing structures of multi-sized particles.

1. Introduction

The packing of multi-sized particles is an important operation related to the mineral, materials, pharmaceutical, chemical and other industries [1]. Packing structure plays a very important role in characterizing properties such as conductivity and permeability, which directly affect product quality or process performance [2,3]. However, it is not easy to estimate structural properties by theoretical models. In fact, to date, it is still difficult to measure experimentally structural properties, in spite of the recent developments in non-invasive techniques [4,5]. Computer simulation provides an effective alternative to study the packing structure of particles. Previous studies were mainly conducted by two types of models: sequential addition (see [6–8] for example) and collective rearrangement (see [9–11] for example). However, these models have to use different assumptions to determine the motion of particles, which may not be able to generate results satisfactorily comparable with experimental observations [12–17]. The discrete element method (DEM) can overcome this deficiency because the dynamics of forming a packing is properly taken into account. The validity and advantage of this simulation technique have been demonstrated by various investigators [16–27]. Recently, we used this simulation method to study the packing of ternary mixtures of particles [28], and found that the simulations are in good agreement with the measured coordination number, one of the most important structural properties [29,30].

It has been well established that the structure of a packing can be quantified in terms of the metric and topological properties based on the so called Voronoi tessellation [31]. Such analysis can provide much more detailed information than the one-dimensional radial distribution function [32] and coordination number as well. The Voronoi method has a rich history in the characterization of particle packing since the work of Bernal [33] and Finney [34]. The original Voronoi method tessellation is mainly used for the packing of uniform or monosized spheres in the early studies [2,32–45]. But it has been extended to handle the packing of multisized particles, giving the so called radical tessellation [46] and Johnson–Mehl tessellation [47]. The studies thus far are mainly focused on binary mixtures of particles [48–52]. These studies are based on the results generated by the sequential addition or collective rearrangement, which, as discussed above, may not be so realistic for granular materials.

In this paper, we perform a radical tessellation analysis on the packing of ternary mixtures, in connection with our previous study of the coordination number [28]. The metric and topological properties of each polyhedron are studied as a function of the volume fractions of constituent components. Such detailed quantitative results are useful for a better understanding of the complicated packing structures of particle mixtures.

2. Numerical method

DEM is used to generate the packing of a ternary mixture of spheres. The translational and rotational motions of each particle are described by Newton's second law of motion, where the gravity and interparticle forces as well as torques are explicitly considered. Normally, the interparticle forces involved include the contact and non-contact forces. As we are only concerned with coarse and dry particles, it is reasonable to ignore the relatively long range inter-particle forces, such as the van der Waals, capillary and electrostatic forces [53,54].

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The detailed descriptions of the forces involved in the present study can be found elsewhere [17,28], and thus will not be repeated here for brevity.

Table 1 lists the parameters and their values used in this work. The particle properties are the same as those used in our previous work [28], which are close to those of glass beads. The present study focuses on the effect of volume fractions X_L, X_M and X_S (where L, M or S represents the large, medium and small components respectively, and $X_L + X_M + X_S = 1$) for a given ternary particle system, with other properties kept constant.

A simulation starts with the random generation of spherical particles of pre-set sizes in a rectangular container of the length of $10d_L$ (diameter of the large component) with no overlaps in particles, and the porosity of the initial state is set to about 0.9 for all mixtures to ensure consistency. Periodic boundary conditions are applied in two horizontal directions to eliminate the wall effect [24,28,55]. To produce a stable packing, the particles are allowed to settle down, under gravity and all other forces considered, until their velocities are essentially zero.

The radical tessellation used here is an extension of the Voronoi tessellation to a multi-sized particle system. Similar to the Voronoi tessellation, the radical tessellation divides the whole packing space into a set of non-overlapping convex polyhedra and each polyhedron contains only one particle. The plane used in the radical tessellation to separate two close particles is the assembly of points with equal tangential distance to the two spheres, other than the bisecting plane. Thus the polyhedron face as part of the plane is guaranteed to be outside the particles and will not intersect with any particles. The radical tessellation retains most of the features of the Voronoi tessellation, and it recovers the Voronoi bisecting plane for monosized particles. The generation of radical tessellation in the present work is facilitated by an open source program developed by Rycroft [56]. A typical illustration of the tessellation of a ternary mixture is given in Fig. 1.

3. Results and discussion

3.1. Structural properties and their distributions

We considered the following properties of the radical tessellation: (1) the polyhedron face related properties, which are the number of edges e, perimeter L and area A of a polyhedron face; and (2) the polyhedron related properties, which are the number of faces f, surface area S and volume V per polyhedron. Of these parameters, e and f are known as typical topological properties, and the rests as metric properties. They are widely used in the structural analysis [32–52]. All these properties are distributed variables, as a natural consequence of the disordered structure of a packing. For each property x, we consider its mean value for the whole packing, denoted as $<x>$, and that for component i, namely, the individual mean value $<x_i>$, where $i = L$, M or S. We also consider the distributions of these properties and individual component in terms of the probability density functions $p(x)$ and $p(x_i)$, respectively.

Table 1
Input values for simulating the packing of a ternary mixture of spheres.

Parameter[a]	Value
Particle size, d (mm)	24.4, 11.6 and 6.4
Particle density, ρ (kg/m^3)	2.5×10^3
Number of particles, N	1000–55,400
Young's modulus, Y (N/m^2)	1.0×10^7
Poisson ratio, $\bar{\sigma}$	0.29
Sliding friction coefficient, μ_s	0.3
Rolling friction coefficient, μ_r	0.002
Normal damping coefficient, γ_n	2.0×10^{-5}
Time step (s)	1.0×10^{-6}

[a] It is assumed that the container has the same properties as particles.

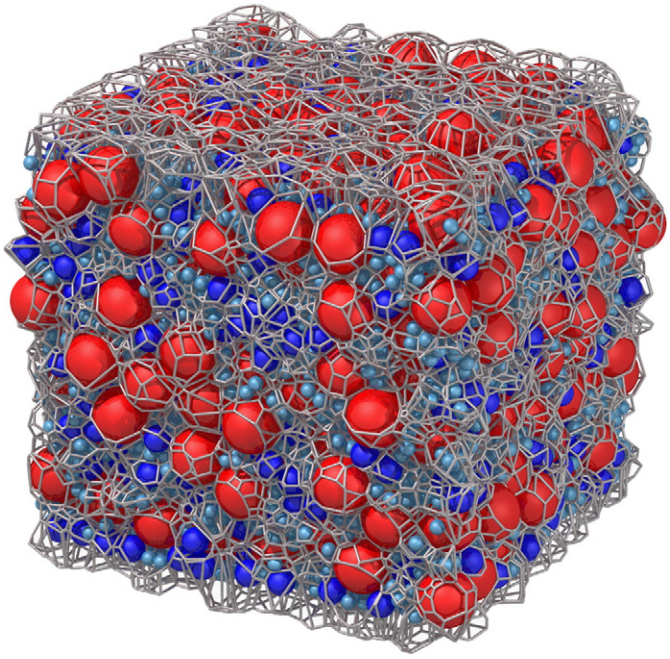

Fig. 1. An isometric view of the radical tessellations for the packing of a ternary mixture of the volume fractions of X_L:X_M:X_S = 66%:17%:17%.

For the polyhedron related properties, the overall and individual mean values and distributions satisfy the following relationships:

$$p(x) = \sum_i n_i p(x_i) \tag{1a}$$

$$\langle x\rangle = \sum_i n_i \langle x_i\rangle. \tag{1b}$$

Similarly, the relationships for the polyhedron face related properties are:

$$p(x) = \left(\sum_i n_i p(x_i)\langle f_i\rangle\right)/\langle f\rangle \tag{2a}$$

$$\langle x\rangle = \left(\sum_i n_i \langle x_i\rangle\langle f_i\rangle\right)/\langle f\rangle \tag{2b}$$

where n_i is the number fraction of component i, which can be related to volume fraction X_i by definition. The overall mean values and packing densities are shown in Table 2 for the 28 mixtures simulated. Note that the 28 mixtures in this work include all the 15 mixtures in our previous work [28], although their numbering may not be the same. The added mixtures can add more information for the ternary system considered.

The simplest topological properties are derived from the knowledge of the number of faces per polyhedron, which provides the information on the number of topological neighbors of the particle enclosed by the polyhedron. For the random packing of monosized spheres, the average face number is about 14 [57]. Interestingly, for the ternary system considered, the average number of faces $<f>$ shows the same value and can be treated as a constant as shown in Table 2, which is consistent with the study of a binary packing system [48]. The number of edges per face can be obtained according to Euler's formula [57,58]

$$\langle e\rangle = 6 - 12/\langle f\rangle. \tag{3}$$

Thus, $<e>$ is insensitive to the changes in volume fractions X_i. By contrast, the average metric properties all depend on X_i.