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Disordered packing density of binary and polydisperse mixtures of curved spherocylinders

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ABSTRACT

Particle elongation is an important factor affecting the packing properties of rod-like particles. However, rod-like particles can be easily bent into non-convex shapes, in which the effect of bending should also be of concerned. To explore the shape effects of elongation and bending, together with the size and volume fraction effects on the disordered packing density of mixtures of non-convex particles, binary and polydisperse mixtures of curved spherocylinders are simulated employing sphere assembly models and the relaxation algorithm in the present work. For binary packings with the same volume, curves of the packing density versus volume fraction have good linearity, while densities are plotted as a series of equidistant curves under the condition of the same shape. The independence of size and shape effects on the packing density is verified for mixtures of curved spherocylinders. The explicit formula used to predict the density of binary mixtures, by superposing the two independent functions of the size and shape parameters, is extended to include a non-convex shape factor. A polydisperse packing with the shape factor following a uniform distribution under the condition of the same volume is equivalent to a binary mixture with certain components. The packing density is thus predicted as the mean of maximum and minimum densities employing a weighing method.

Introduction

Hard particles and their mixtures jammed into random packings are ubiquitous in nature and industry. Scientific studies have used the random packing of hard spheres to model the structures of glassy, liquid states of matter (Bernal, 1965), colloids (Chaikin & Lubensky, 2000), granular media (Edwards, 1994), and heterogeneous materials (Torquato, 2002). Among factors affecting the packing density, the particle size distribution is one of the most important. Researchers have long carried out experiments and simulations to explore the optimum particle size distribution that maximizes the packing density of particles (Cumberland & Crawford, 1987; Dodds, 1980; Fuller & Thompson, 1907; German, 1989; Gray, 1968; Kolonko, Raschdorf, & Wasch, 2010; Ouchiyama & Tanaka, 1981, 1986; Rodriguez, Allibert, & Chaix, 1986; Suzuki & Oshima, 1985; Yang, Miller, & Turcoliver, 1996;). On the basis of their results, models have been built to explain the mechanism why a size disparity in a mixture increases the packing density. Subsequently, a series of empirical formulas to predict the packing density of mixtures has been developed, including the simple packing model (Ouchiyama & Tanaka, 1981), the mixture packing model (Yu & Standish, 1988), the linear packing model (Yu, Zou, & Standish, 1996), and the linear-mixture packing model (Yu & Standish, 1991). These predictive models have been successfully used in a variety of industrial applications, such as those in metallurgy, transportation, agricultural, and chemical industries.

As the simplest case in polydisperse packings, following the pioneering works of Furnas (1931), Westman and Hugill (1930), and Westman (1936) in the1930s, researchers began to explore the packing properties of mixtures composed of binary spherical particles. A series of experiments with various components was carried out to build the relation describing how the size ratio and volume fraction affect the packing density. Furnas focused on binary mixtures in which particles have a large disparity of sizes. The model he proposed to predict the packing density has been gradually developed into the upper bound of a binary packing (Farr & Groot, 2009; Kyrylyuk, Wouterse, & Philipse, 2010). In contrast, the Westman equation was developed from the results of experiments on mixtures composed of particles of similar size, which are closer to real packings. Because predictions made with the Westman equation

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Nomenclature

d_v	Diameter of the sphere with the same volume as the non-spherical particle
d_p	Equivalent packing diameter
G	Parameter related to r in the Westman equation
L	Length of the tube
N	Particle number
$[\bar{P}_4]$	Cubatic order metric
R	Radius of the tube
R_u	Curvature distance
r	Size ratio
S_p	Surface area
V_p	Particle volume
V	Specific volume
X	Volume fraction
w	Aspect ratio
θ	Central angle
ϕ	Packing density
ψ	Wadell sphericity

correspond well to the results of experiments, the Westman equation is more widely used in industrial applications. The Westman equation (Westman, 1936) uses a quadratic function of the volume fraction to predict the packing density ϕ, which is:

$$\left(\frac{V-V_LX_L}{V_S}\right)^2+2G\left(\frac{V-V_LX_L}{V_S}\right)\left(\frac{V-X_L-V_SX_S}{V_S}\right)+\left(\frac{V-X_L-V_SX_S}{V_S}\right)^2=1, \quad (1)$$

where V is the specific volume defined as $1/\phi$. V_L, X_L and V_S, X_S are the specific volumes and volume fractions of large and small particles, respectively. For a specific packing, G is a unique parameter that relates to the size ratio r, which is defined as the ratio of the diameter of the smaller sphere to that of the larger sphere.

Note that most of these models, built from the results of experiments using a finite number of spherical particles, are applicable only to the packings of spherical particles. However, real particles are usually non-spherical, which means the size distribution is not the only geometric factor that affects the packing density. The particle shape is not only related to the flowing and fractional properties of a particulate system. It also affects the behavior of particles in the storage, transportation, mixing, separation, crystallization, sintering, and fluidization processes of powders. In packing problems, particles with various shapes exhibit richer characteristics. For example, the random-close-packing (RCP) density of identical spheres is around 0.64, which is far below the maximum random packing density of other basic three-dimensional objects, such as spherocylinders (Kyrylyuk, van de Haar, Rossi, Wouterse, & Philipse, 2011; Zhao, Li, Zou, & Yu, 2012), spheroids (Donev et al., 2004; Man et al., 2005), Platonic solids (Simth, Fisher, & Alam, 2011; Torquato & Jiao, 2009), superballs (Jiao, Stillinger, & Torquato, 2009), and superellipsoids (Delaney & Cleary, 2010).

For mixtures composed of non-spherical particles with a polydisperse size distribution, the problem becomes more complex and the shape effect should be evaluated. More generally, the shape parameters are also not identical in a mixture. Analysis can be further extended to explore the maximum packing density if both the shape and size parameters are polydispersely distributed in a mixture. Choosing the proper parameters for the quantification of the shape disparities of various objects and determining the relation between the shape parameter and the packing density of non-spherical particles remain as future work. Researchers have made great efforts toward solving these problems by producing a series of empirical formulas (Liu & Ha, 2002; Yu, Standish, & Mclean, 1993; Zou & Yu, 1996a). According to the experimental packings of spheres, cylinders and disks, Zou and Yu (1996b) proposed the concept of equivalent packing diameter, which is a function of the particle volume and the Wadell sphericity (Li et al., 2012). By introducing the concept of equivalent packing diameter, the mixture density of non-spherical particles can be predicted from that of spherical particles with certain size distributions; i.e., the shape disparity is considered to make a similar contribution to the packing density as the size distribution in spherical systems. The equivalent packing diameter d_p of anon-spherical particle (Zou & Yu, 1996a) is described as

$$d_p=\psi^{-2.785}\exp\left[2.946\left(\psi-1\right)\right]d_v, \quad (2)$$

where d_v is the diameter of the sphere with the same volume as the aspherical particle, and ψ is the Wadell sphericity (Li et al., 2012; Wadell, 1935), defined as the ratio of the surface area of a sphere having the same volume as the original particle to the surface area of the particle. This equivalence method has been verified to be applicable to mixtures of simple and basic three-dimensional objects; e.g., cylinders and disks (Yu et al., 1993). However, the empirical formula used to calculate the equivalent packing diameter was developed from finite experimental results. The sphericity, describing how round a particle is, is the only shape parameter that contributes to the empirical formula. For other complex particle shapes, the application of the equivalent packing diameter to predict the packing density of mixtures should be verified. More importantly, the similarities between spherical and non-spherical particle packings should be guaranteed, at least in terms of the mechanism that decreases the variation of the specific volume during a mixing process. The universality of this similarity is directly related to the question of whether the effect of the particle shape is equivalent to that of the particle size on the density of a mixture. This will help us understand whether a corresponding correlation exists between the macroscopic packing density and the microscopic configuration because the contacts of neighboring non-spherical particles are more complex and should be obviously different from those of spherical particles.

Basis and previous works

Our previous studies on binary mixtures of spherocylinders revealed that for binary spherocylinders having the same volume, there is a linear correlation between the packing density and the volume fraction with both end values determined by the shape effect. However, for mixtures of binary spherocylinders having the same shape, the densities can be plotted as a series of equidistance curves with similar varying trends and peak loci. This suggests that the geometric factors of particle shape and size independently affect the packing density in packings of binary spherocylinders. On the basis of this correlation, we proposed an explicit formula (Meng, Lu, Li, Zhao, & Li, 2012) that predicts the packing density (ϕ) of binary spherocylinders as

$$\phi\left(r,w_1,w_2,X_i\right)=f\left(r,X_i\right)+g\left(w_1,w_2,X_i\right), \quad (3)$$

where r is the size ratio of the two particles. w_1 and w_2 are the aspect ratios of two components. X_i is the volume fraction of component i, which satisfies the relation $\sum_{i=1}^{2}X_i=1$ in a binary packing. In the explicit formula, the packing density of binary spherocylinders is described as a linear superposition of two functions of the size ratio and shape factor without coupling terms, which is considered to reflect the physical essence of mixtures of non-spherical particle.

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