ARTICLE IN PRESS

PTEC-11821; No of Pages 10

Powder Technology xxx (2016) xxx–xxx

Contents lists available at ScienceDirect

Powder Technology

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

Maximally dense random packings of intersecting spherocylinders with central symmetry

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ARTICLE INFO

Article history:
Received 12 May 2016
Received in revised form 27 June 2016
Accepted 24 July 2016
Available online xxxx

Keywords:
Maximally dense random packing (MDRP)
Intersecting spherocylinder
Non-convex particle
Empirical formula

ABSTRACT

The packing of rod-like particles has arisen in a variety of scientific and industrial applications. For the factors that attribute to the packing properties of such particles, elongation effect is one of the most important. However, rod-like particles can be easily assembled into non-convex shapes, in which the effects of non-convex deformations should be concerned. In this paper, the dense random packings of identical intersecting spherocylinders with central symmetry are numerically simulated through an analytical model and the relaxation algorithm. The maximally dense random packing (MDRP) states of 2D and 3D intersecting spherocylinders with various aspect ratios are determined from the order maps. In the MDRP states, the specific volume V, defined as the reciprocal of the packing density ϕ, shows a highly linear correlation with the aspect ratio ($w \geq 1.0$), which is similar to the monophasic packing of spherocylinders. This indicates that the elongation effect is the main shape factor that attributes to the packing density. Consequently, the explicit formulas to predict the packing densities of 2D and 3D intersecting spherocylinders are built as single-variable functions of the aspect ratio. The dense random packing density of 2D intersecting spherocylinders equals to that of identical spherocylinders when $w = 1.25$. This suggests that a balance exists between the relative excluded volume effect and the multi-point contact effect to the packing density of non-convex particles.

1. Introduction

The packing of rod-like particles, which is common in physical and mathematical studies, has arisen in a variety of industrial applications, such as fibers, ceramic and aggregate particles [1–4]. Studies on the packing problem will help to better understand many natural phenomena, including the liquid, glassy, and crystalline states of condense matter, such as liquid crystals [5,6] and silica rods [7]. Different from spherical particles, a rod-like particle usually has an anisotropic shape with uniaxial orientation. Elongation effect is one of the most important factors that attribute to the packing properties. During the densification of the packing configurations, rod-like particles can be easily self-assembled into clusters, in which particles align in parallel with cylinder-cylinder contacts to the neighbors [8–11]. Order in clusters has been identified as the main form of local order in packings of rod-like particles, resulting in a significant increase in the degrees of orientational order [12]. The existence of local order will further affect the packing properties, e.g., the packing density will increase sensitively with the growth of local order. Consequently, in the studies of disordered packings composed of different particle shapes, degrees of local order should be quantified to ensure the same packing state for comparison. How to choose proper order metrics and define the critical packing states add to the difficulties of disordered packing studies.

Rod-like particles can be easily bent or assembled into non-convex shapes, in which the effects of non-convex deformations should be concerned. Deformation into a non-convex shape effectively prevents the self-assembling of particles, which largely reduces the degree of local order in the configurations [13,14]. With multi-point contacts in the configuration of non-convex particles, interactions among neighboring particles are possible in completely different ways such as by interlocking or entanglement [15–18]. During the compaction dynamics, rotational motions are limited and strongly reduced for non-convex particles. Configurations packed by non-convex particles possess more stability due to the strong interlocking of particles. Ludewig and Vandewalle [19] used a sphere assembly model to numerically simulate the random packings of non-convex grains and proposed that the force network of the configuration is deeply affected by the grain shape and the occurrence of multi-point contacts, resulting in the less dense but more stable configurations than spherical particles. If carefully designed, particles with non-convex shapes can even be employed in applications of architectural materials, such as tumbling units [20] and

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http://dx.doi.org/10.1016/j.powtec.2016.07.059
0032-5910/

Please cite this article as: L. Meng, et al., Maximally dense random packings of intersecting spherocylinders with central symmetry, Powder Technol. (2016), http://dx.doi.org/10.1016/j.powtec.2016.07.059

Nomenclature

V	specific volume
V^p	particle volume
V^{ex}	excluded volume
V_{cd}	volume of a circumscribed disk
V_{cs}	volume of a circumscribed sphere
w	aspect ratio
L	length of the cylinder part
D	diameter of the cylinder part
R	radius of the cylinder part
N	number of particles assembled in a configuration
N^{SC}	number of spherocylinders assembled in a particle
N^{Nb}	number of particles located in the neighborhood of a specific particle
S_{Local}	local order metric
$\overline{P_4}$	cubatic order parameter
Q_6	bond-orientational order metric
$\mathbf{u}$	unit vector along a relevant particle axis
$\mathbf{n}$	director unit vector
$\langle c \rangle$	a constant which is usually related to the contacts between particles
Z	coordination number
Z_C	contact number

Greek symbols

ϕ	packing density
γ	convex ratio
δ	distance between two sphero-polyhedra
θ	angle between the normal directions of two particles
μ	expectation of the order metric obtained from the MC statistical results
σ	standard deviation of the order metric obtained from the MC statistical results

Subscripts

i	type of the particle, $i=1,2,3$
j	intersecting spherocylinder j in each particle, $j=1,2\ldots N_i^{SC}$
k	type of the order metric, $k=1,2,3,4$
m	particle m
n	particle n

aggregate architectures [21–23]. To achieve this, how the shape factors affect the packing properties should be well understood, which is what we concern in this work.

A spherocylinder is a usually used 3D object in the packing studies, which can be easily modelled through a mathematical way or by a sphere assembly model. The aspect ratio w, defined as the ratio of the length L to the diameter of the cylinder part D, is the most employed shape parameter to quantify the elongation effect. Previous work indicated that for monophasic packings of spherocylinders, the dense random packing density first increases until a peak around $w=0.5$, and decreases with the growth of the aspect ratio [12,24–33]. To explore the shape effects on the packing properties of non-convex particles, we focus on the monophasic packings of cross-shaped and jacks-like particles, which are assembles of spherocylinders. A cross-shaped particle is composed of two spherocylinders with their axes located in a plane, which is similar to the "fat crosses" [34]. Similarly, a jacks-like particle is composed of three spherocylinders with each axis orthogonal to each other. It is a type of hexapods consisting of a central sphere with six radial arms [15,35]. For simplification, the cross-shaped and jacks-like particles studied in this work are respectively named as 2D and 3D intersecting spherocylinders. Similar to spherocylinders, elongation is also a main shape factor that makes shape diversities. The excluded volume, referring to the volume that is inaccessible to other particles as a result of the presence of the first one, will obviously increase with the growth of elongation.

In the present work, we use an analytical model to simulate the monophasic packings of 2D and 3D intersecting spherocylinders. The relaxation algorithm is employed to generate a whole profile of packing configurations with a diversity of densities and degrees of order. By analyzing these configurations, we identify the main forms of local order and use the local order metric S_{Local} to quantify the degrees of local order in the packings of non-convex particles. The cubatic order parameter $\overline{P_4}$ is also employed to measure the degrees of layering order and inplane order. For particles of each aspect ratio, the maximally dense random packing (MDRP) states [15,36] are identified from the order map, which reflects the packing density-order metric relation from comprehensive numerical simulations via a geometrical algorithm. The MDRP state is defined as the maximally dense packing without nontrivial spatial correlations, which corresponds to the transition point in the boarder curve and characterizes the on-set of nontrivial spatial correlations among the particles. With the increase of the packing density, there is a spectrum of packing states with varying densities but similar and very low degrees of order, that are statistically indistinguishable from those associated with a state in which the particle positions and orientations are Poisson distributed. These packing states are considered "fully random". The MDRP is then the one possessing the largest packing density among all those "fully random" packings.

Given the definition of the MDRP state, elongation effects on the packing properties of the MDRP states are then studied, which is also compared with spherocylinder packings. Correlations between the specific volume and the aspect ratio are studied. We then propose empirical formulas to predict the packing densities of identical intersecting spherocylinder packings by using the shape parameter of the aspect ratio w. Excluded volumes and the contacts are also studied to explain the non-convex effects on the variation of the packing density.

2. Geometries

In this work, an intersecting spherocylinder is defined as a central symmetric object composed of several spherocylinders. The centers of each particle coincide with their axes orthogonal to each other. The number of spherocylinders assembled in an intersecting spherocylinder is defined as N^{SC}. N^{SC} equals to 2 and 3 in a 2D and 3D intersecting spherocylinder, respectively. Note that a spherocylinder can be treated as a special intersecting spherocylinder, in which N^{SC} degenerates to 1. In each particle, diameters of the spherical caps are identical while the aspect ratios of each spherocylinder can be different. With a constant diameter of the spherical caps D, the shape of an intersecting spherocylinder is uniquely determined by the parameters of the aspect ratios w_j, where $j=1,2\ldots N_i^{SC}$ for particle type i. For simplification, intersecting spherocylinders studied in this work have an identical aspect ratio, i.e., $w_i=w$. Intersections among the spherocylinders are also limited within the cylinder part. Consequently, the minimum w of the intersecting spherocylinders studied in this work is set to be 1.0. Fig. 1 illustrated instances of 2D and 3D intersecting spherocylinders with various aspect ratios.

The particle volume of an intersecting spherocylinder with an identical aspect ratio can be described as a function of the diameter D and the aspect ratio w, illustrated as

$$V_2^p=\left(\frac{\pi}{3}+\frac{\pi}{2}\cdot w-\frac{2}{3}\right)D^3 \tag{1}$$

$$V_3^p=\left(\frac{\pi}{2}+\frac{3\pi}{4}\cdot w-\sqrt{2}\right)D^3 \tag{2}$$

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