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## **Original Research Paper**

## Numerical study of the motion behaviour of three-dimensional cubic particle in a thin drum

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### ABSTRACT

The motion of three-dimensional cubic particles in a thin rotating drum is simulated by the SIPHPM method. The drums with frictional or smooth front and rear walls, and the particles of cubic and spherical shapes, and different particle numbers are considered to study the effect of cubic particle shape, end-wall frictions and filling levels. Different flow patterns of cubic particles are observed, which are significantly dominated by the friction from the end-walls. The probability density function of velocity components, the flatness factors are used to analyze the motion behaviour of cubic particle. The Froude number, ensemble mean and time averaged particle velocities are also analyzed. A primary and secondary mode of driving from the end-wall frictions are indicated and the mechanisms on the influences of wall friction, particle shape and filling levels are fully explained.

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#### 42 1. Introduction 43

As a widely applied mixer for mixing, drying, heating and coat-44 ing of granular particles, the rotating drum or cylinder mixer has 45 46 been extensively studied in the past decades on the rich phenomena (e.g. mixing [26], segregations and stratification [2], sur-47 face flow [27], granulation [4], axial dispersion [25], cohesion 48 [6]), statistical features (e.g. velocity analysis [7], the Markov pro-49 50 cess [9] and poly-dispersion [1]). Meanwhile, various influencing effects on the aforementioned phenomena and features have also 51 52 been explored extensively, including the operating conditions [24], noncircular drum effect [3], non-spherical particle effect 53 [22], internal baffle effect [21], particle density effect [29]), and 54 55 heat transfer [12]. But, the majority of these studies are based on spherical particles. Compared to the drum filled with spherical par-56 ticle, the dynamical behaviours of non-spherical particles in the 57 drum have not been well explored, although it is well accepted that 58 particle shape has a significant impact on flow behaviour [10]. 59

60 Recently, as the particle shape has a strong influence on the dynamics of particulate systems, some studies have been con-61 tributed to the non-spherical particles, from theoretical, experi-62 mental and modeling, to application aspects [20,19]. In 63 experimental study, Williams et al. [28] analyzed separated and 64

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lumped particle images to assess particle shape descriptors through a digital image segmentation technique and implement particle shape parameters into generation of irregular shaped particles. Various particle shape descriptors were obtained using the combinations of image segmentation algorithms, and nonspherical particles were subsequently created in DEM modeling using the particle shape results. Rasouli et al. [22] compared the flow behaviour of cylindrical and spherical particles using the multiple radioactive particle tracking technique to capture the positions and orientations of cylindrical particles simultaneously. The boundary between the active and passive layers and the velocity profile on the free surface were analyzed. Dubé et al. [10] also used the radioactive particle tracking technique (RPT) to follow large non-spherical particles inside a rotating drum, and three crucial aspects of particle: residence time, mixing/segregation, and axial dispersion were studied. It was found that particles of high aspect ratio have significant deviations in velocity profile and residence time. Unexpected core segregation patterns and lower axial dispersion coefficient were also found for non-spherical particles. In simulation [20], using the super-quadric equation, discrete element method simulation was performed to study the cross-sectional flow of non-spherical particles in horizontal rotating cylinders. The effects of the degree of squareness and wall rougheners on flow behaviors were studied. In their work, the typical challenging strategies for non-spherical particle modeling include the orientation representation by using quaternions and the contact

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detection by super-quadric equation [19]. Thus, the compositesphere method is still an alternative approach frequently applied in non-spherical particle simulation [18,5,8].

94 Moreover, the effect of drum wall on particle is also an impor-95 tant issue. For example, besides the work by Lu et al. [20], Santomaso et al. [23] also studied the effect of wall roughness on 96 97 the axial segregation in horizontal rotating drums. They showed 98 that modification of the geometry and roughness of internal surface of mixer could modify the segregation patterns. With regard 99 to the friction effect of walls, Guo et al. [17] studied the angle of 100 internal friction and concerned the particle shape on the angle of 101 102 internal friction experimentally by powder rheometer. Three regions can be divided for various binary granular systems based 103 on the magnitudes of aspect ratio, and a power function exists 104 105 between  $\Delta \tan \Phi$  and granular shape factors. In addition, although 106 my recent work has indicated the important influence of end-107 wall on mixing of spherical particles [30], the wall effect on the 108 mixing of non-spherical particle is still unclear.

109 In particular, we have proposed three kinds of numerical models to simulate the interaction between non-spherical particles. It 110 111 includes an analytical solution model of non-spherical particle col-112 lision of rigid materials (the GHPM model [15,16]), a soft-sphere imbedded pseudo-hard particle model (the SIPHPM model [13]), 113 and a coupled approach of the hard and soft models (the EHPM-114 115 DEM [14]). We think the SIPHPM model is particularly suitable 116 for simulating very dense granular flows of non-spherical particles 117 for its robustness, good validation and numerical reliability.

118 In conclusion, the motion behaviours and characteristics of nonspherical particles (especially under three-dimensional case) in 119 120 rotating drums are significant to practical applications. The effects 121 of non-spherical shape, filling level and wall friction are also important issues, which are still poorly understood. As a funda-122 mental research, this work is aimed at exploring the mechanisms 123 of cubic particle motion in a thin layer and the effects of cubic 124 125 shape, filling level and wall friction. To accomplish that purpose, 126 the rotating drums filled with about 400–989 cubic particles with 127 or without frictions on the front and rear walls are simulated by 128 the SIPHPM model, and the results are analyzed in details.

#### 129 2. Numerical method

#### 2.1. SIPHPM model 130

The soft-sphere imbedded pseudo-hard particle model 131 (SIPHPM) [13] is applied in this study to simulate the collision 132 between cubic particles. Herein, the cube model (see the inset of 133 Fig. 2a) is composed of 56 sub-spheres and 6 surfaces. The cube-134 135 cube interaction is then transformed to the interaction between 136 spheres and surfaces. In SIPHPM, the interactions between the subspheres of the same cube are not needed to be computed, as a 137 138 pseudo-hard assumption of the material of the cube is always 139 guaranteed. However, the interaction between the subspheres of 140 different cubes must be solved by the discrete element method, 141 as well as the subsphere-surface interaction between different 142 cubes. In addition, the subspheres can oscillate about their equilibrium position within the cube, where the equilibrium position is 143 144 determined by the position and orientation of the cube. Thus, the governing equations of the cubes and subspheres are coupled 145 and solved respectively as follow: 146

For sub-spheres:

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$$\mathbf{F}_{i,s} = \mathbf{k}_c \delta \mathbf{x}_{i,s} - \eta_c \delta \dot{\mathbf{x}}_{i,s}, \text{if} (\mathbf{F}_{i,s} \cdot \mathbf{t}_{i,s}) > \mu(\mathbf{F}_{i,s} \cdot \mathbf{n}_{i,s}), (\mathbf{F}_{i,s} \cdot \mathbf{t}_{i,s}) = \mu(\mathbf{F}_{i,s} \cdot \mathbf{n}_{i,s})$$
(1)  
$$\mathbf{T}_{i,s} = \mathbf{r}_{i,s} \times \mathbf{F}_{i,s}$$
(2)

$$\boldsymbol{R}_{i,s} = k_r \Delta \boldsymbol{\zeta}_{i,s} - \eta_r \Delta \dot{\boldsymbol{\zeta}}_{i,s} \tag{3}$$

 $\dot{\boldsymbol{v}}_i = (\boldsymbol{F}_{i,s} + \boldsymbol{R}_{i,s})/m_s - \boldsymbol{g}$  $(\mathbf{4})$ 

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where  $\delta \mathbf{x}_{is}, \mathbf{r}_{is}, \Delta \zeta_{im}$  are the deformation displacement, position 151 vector (relative to the cube center), deviation displacement from 152 the equilibrium position of the  $i^{th}$  subsphere, respectively. 153  $F_{is}$ ,  $R_{im}$ ,  $T_{is}$  are the damping elastic collisional force, restoring force, 154 and the torque generated by the  $i^{th}$  subspheres with respect to the 155 cube respectively. **n** and **t** are the normal and tangential directions 156 at the collision point, and **g** is the gravity acceleration.  $k_c$ ,  $\eta_c$ ,  $k_r$ ,  $\eta_r$ , 157 are the stiffness factor and damping coefficient of collision and 158 restoration, respectively.  $\mu$  is the friction coefficient for subspheres. 159  $\boldsymbol{v}_i, m_s$  are the velocity and mass of the sub-spheres, respectively.  $\cdot \cdot$ 160 is the inner operator. Note that the self-rotation of sub-sphere is 161 omitted since it may be regarded as an additional degree of freedom 162 within the large non-spherical particle (apart from the most com-163 monly encountered translational, rotational, vibrational degrees of 164 freedom for a large composite particle), which is not true in 165 practice. 166

For cubes:

$$M_c \dot{\boldsymbol{V}}_{j,c} = \sum_{i}^{N_s} \boldsymbol{F}_{i,s} - \boldsymbol{G}$$
(5)

$$I_{c} \cdot \dot{\Theta}_{j,c} = \sum_{i} T_{i,s} \tag{6}$$

where  $V_{i,c}, \Theta_{i,c}, M_c$  and  $I_c$  are the translational velocity, rational 171 velocity, mass, and moment of inertia of the cubic particle respec-172 tively. **G** is gravity force of the cube.  $N_s = 56$  is the number of subspheres a cube contains.

By solving Eqs. (1)–(6), the collision and motion of both subspheres and cubes can be obtained. In similar manners, the cubewall and cube-surface collisions can also be transformed into subsphere-wall and subsphere-surface collision, and solved by discrete element method as well.

## 2.2. Model validation

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In our recent work [13], the SIPHPM has been validated through 181 comparison with experimental observations on the arching struc-182 tures, both in 2D and 3D cases. In addition, as the GHPM model 183 [15,16]) was validated firstly by theoretical consistency and exper-184 imental comparison, it was used to validate the SIPHPM for cube-185 cube collision process. However, in this section, an additional val-186 idation on cubic particle discharge is performed according to the 187 experimental work by Fraige et al. [11]. 188

200 cubes of size 12.5 mm in side length are initially set inside a silo of 500 (height) \* 200 (width) \* 30 (depth) mm, and discharged through the orifice (width  $B_0 = 60, 80, 116 \text{ mm}$ ) at the bottom center. Notice that the exact positions of all particles cannot be obtained in experiment. Therefore, we just used randomly initial particle velocities in simulation, and let the particles fall freely from some distances from the bottom when the orifice is closed to build similar initial packing states. After that, the orifice is opened, and the discharge starts. The parameters used in current validating simulation are listed in Table 1.

For example, the snapshots of discharge at t = 0.1 s for  $B_0 = 60$ , 80, 116 mm are illustrated in Fig. 1a-c respectively. When the orifice size is different, the numbers of particles moving downward are different. Then, the corresponding number flow rates are computed and shown in Fig. 1d compared to experimental data. It is indicated that: although the initial packing states are different, 204 the number flow rates in simulation are close to the experimental 205 data or within the range of variation of flow rates in experiment. 206 Therefore, it shows once again the validity of current model for 207 simulation of cubic particle motions. 208

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