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Modelling of the flow of ellipsoidal particles in a horizontal rotating drum based on DEM simulation

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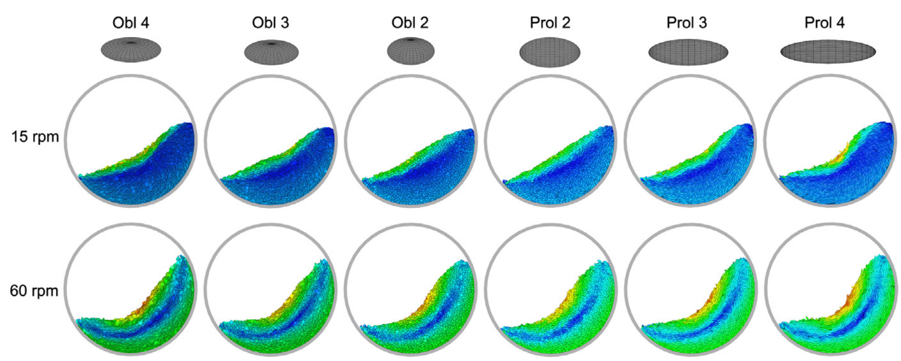
HIGHLIGHTS

- The flow of ellipsoidal particles in a rotating drum is investigated by DEM.
- The ellipsoidal particles are modeled by super-ellipsoids.
- The effects of the aspect ratio and the rotation speed on the mixing are concerned.
- Ellipsoids with lower sphericity have higher consistency of the particle orientation.
- Better coating could be achieved at lower rotation speed in rolling/cascading regime.

GRAPHICAL ABSTRACT



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ABSTRACT

The granular flow involving ellipsoidal particles in a horizontal rotating drum is investigated by DEM, in which ellipsoidal particle is modeled by super-ellipsoids and periodic boundary condition is adopted. Recurring to the abundant information obtained from the DEM simulation, a comparably synthetical investigation is performed for the better understanding of the fundamental of the granular flow involving ellipsoidal particles in a horizontal rotating drum. All cases utilized in this work are characterized by the continuous flow, namely in rolling/cascading regime. How the aspect ratio and the rotation speed of the drum influence the transverse mixing is surveyed. And some attempt has been made to elucidate the above influence on the particle mixing from the perspective of particle diffusion and particle convection. A brief description about the influence of the aspect ratio and rotation speed of the drum on the axis dispersion is also provided. The Euler angles, including the precession angle, nutation angle and spin angle, are utilized to study the distribution profiles of the orientation for ellipsoidal particles. Simultaneously, some simple methods have been devised for different investigation purposes involving particle orientation.

1. Introduction

Rotating drum is a common device in industry while coating, drying, mixing or milling particles. Therefore, some experimental methods, including MRI (Magnetic Resonance Imaging) (Kawaguchi et al., 1998; Nakagawa et al., 1993), RPT (Radioactive Particle Tracking) (Dubé et al., 2013; Sherritt et al., 2003) and PEPT (Positron Emission Particle Tracking) (Ingram et al., 2005; Parker et al., 1997), and numerical simulation methods, including MC (Monte Carlo) and DEM (Discrete Element Method) (Cundall and Strack, 1979) have been developed for a comprehensive understanding of the granular flow in a rotating drum. Comparing with the numerical simulation, experiment requires great effort to gain

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the necessary information, particularly the information in particle level. The high prices of the related laboratory equipment also restrain the utilization of the experimental method. Nevertheless, DEM can offer a cost-efficient alternative and rich information with less effort compared with experiments. Therefore, DEM has been predominated in studying granular flow in a rotating drum. After years of research, the investigation of the granular flow in a horizontal drum by DEM has progressed significantly (Lu et al., 2015; Zhong et al., 2016; Zhu et al., 2008). Considering the main purpose of this paper is to lay the foundation for our future work about the coating of the non-spherical particles with the help of DEM, the corresponding previous investigations involving particle mixing and particle orientation in a rotating drum will be briefly reviewed in the following.

Past research focus is primarily put on granular flow involving spherical particles because of the easiness in modelling a sphere and the limitation of the computation power. While investigating the mixing and flow of particles in a drum, Wightman et al. (1998) demonstrated the difference in mixing patterns between the particles close to walls and the slices in the center. And they found that the introduction of the rocking motion can enhance the particle mixing in comparison with the purely rotational motion. Schutyser et al. (2001) found that the particle mixing is a function of filling degree and dimension of the drum while studying the mixing behavior of the solid substrate particles. They also suggested the implementation of the large, straight baffles can improve mixing performance. The research focus of Finnie et al. (2005) was put on the influences of the operating conditions on the longitudinal and transverse mixing. They found that the filling degree and the increscent rotation speed of the drum go against the acceleration of the transverse mixing at identical number of revolutions. For longitudinal mixing, there is an increasing linear relationship between the longitudinal mixing and the rotation speed, whereas the effect of the filling degree is comparably small. Subsequently, the comparison between the research of Finnie et al. (2005) and the relevant experiments made by Van Puyvelde (2006) implies the obtained results of Finnie et al. (2005) qualitatively concur with the experimental observations. While investigating the particle diffusion in a rotating drum, Taberlet and Richard (2006) suggested the diffusivity is independent of the particle size and is not impacted by the radial segregation. Using a two-dimensional DEM, Cleary et al. (1998) had ever used the circular particles to predict the mixing rate of salt cubes. However, the predicted results indicated that the mixing rate is three to ten times lower than corresponding experiments. Subsequently, super-quadric particles were utilized to model the salt cubes, in which the blockiness, size and aspect ratio for super-quadric particle are chosen to agree the experimental material as close as possible, and the corresponding DEM model established by Cleary (2000) can predict the mixing reasonably. The work of Cleary (2000) and Cleary et al. (1998) indicated that the particle shape has a significant influence on the flow of the particles in a horizontal drum.

As the development of DEM, different models, including polyhedral model (Hopkins, 2014; Nassauer et al., 2013), multi-sphere model (Kruggel-Emden and Elskamp, 2014; Ning et al., 1997), real shape model for some special shapes (Guo et al., 2012; Kodam et al., 2010) and super-ellipsoid model (Cleary, 2010; Williams and Pentland, 1992), have been put forward to describe non-spherical particle, and the features of these models have been discussed by Lu et al. (2015). Also with the improvement of the computational power, DEM has been popular in investigating the flow of the non-spherical particles in a rotating drum. A 2-dimensional drum filled with the super-quadric particles was modeled by Cleary and Metcalfe (2002). Their simulation results demonstrated that the mixing rate of super-quadric particles was four to seven times higher than that of circular particles. By DEM, Geng et al. (2009) modeled a rotating drum filled with slender particles or spherical particles. They found that the overall mixing rate of spherical particles was lower than that of slender particles. While studying effects of the particle shape on the particle mechanics, Höhner et al. (2014) found that the mixing is impacted considerably while switching from spherical to non-spherical particles, and further reduce the particle sphericity has little influence. Pereira et al. (2011, 2014) made a series of investigations on the formation of the radial streak patterns in a rotating drum filled with binary granular mixtures. In their researches, they evaluated the influence of the particle shape and demonstrated a significant requirement for forming the streak lines.

For the flow of ellipsoid-shaped particles in a rotating drum, some researchers, including Grajales et al. (2012) who surveyed the motion and mixing of rice particles and Gan et al. (2016) who proposed a GPU-based DEM approach, had ever made corresponding investigations. Nevertheless, enough information cannot be obtained from these previous investigations, particularly for the information of particle orientation which is seemingly a little-studied respect. Considering this situation, and also to lay the foundation for our future work involving coating, the fundamental purpose of this paper is to investigate the flow of the ellipsoidal particles in a horizontal drum with the help of DEM. The research focus of this work is to investigate how the aspect ratio and rotation speed of the drum influence the transverse mixing and distribution of the particle orientation while in rolling/cascading regime, and the details will be presented in the following.

2. Mathematical model

2.1. Particle shape model

The mathematical formula of the super-ellipsoid, is written as follows (Barr, 1981):

$$\left(\left|\frac{x}{a}\right|^{s_2}+\left|\frac{y}{b}\right|^{s_2}\right)^{\frac{s_1}{s_2}}+\left|\frac{z}{c}\right|^{s_1}=1, \tag{1}$$

where a, b and c are semi-major axes of an individual particle, respectively. The two shape indices, namely s_1 and s_2 shown in Eq. (1), determine the curvature of particle edges, and a larger shape index indicates a sharper curvature. The DEM code that we developed is general for super-ellipsoidal, and we set $s_1 = s_2 = 2$ to describe an ellipsoidal particle in this paper. Under the above conditions, the cases of $c > a = b$ and $c < a = b$ describe a prolate ellipsoidal particle and an oblate ellipsoidal particle, respectively.

2.2. Particle motion equations

The translational motion and rotational motion of an individual particle obey Newton's laws of motion, and the corresponding kinematic equations are defined as

$$m\frac{d\boldsymbol{v}}{dt}=\sum\boldsymbol{F}_c+m\boldsymbol{g}, \tag{2}$$

$$\boldsymbol{I}\frac{d\boldsymbol{\omega}}{dt}=\sum\boldsymbol{T}_c, \tag{3}$$

where m and $\boldsymbol{I}$ refer to particle's mass and inertia moment, respectively, $d\boldsymbol{v}/t$ and $d\boldsymbol{\omega}/t$ denote the translational and angular acceleration of an individual particle, respectively, $\boldsymbol{g}$ is gravitational acceleration, $\boldsymbol{F}_c$ and $\boldsymbol{T}_c$ are the contact force and contact torque, respectively.

For the calculation of the inertia moment ($\boldsymbol{I}$) and the contact torque ($\boldsymbol{T}_c$), there is minimal effort required for a sphere (Cundall and Strack, 1979; Xu and Yu, 1997; Zhao et al., 2009). Nevertheless,