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CFD-DEM simulation of fluidization of rod-like particles in a fluidized bed

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ABSTRACT

In chemical and energy industries, fluidization concerning rod-like particles is often encountered, but little effort has been made in this respect. Understanding fluidization of rod-like particles is crucial for the guidance of relevant industrial process. To investigate the fluidization of the rod-like particles with different aspect ratios, CFD-DEM coupling algorithm is employed in this article to simulate a bubbling fluidized bed, in which the rod-like particles are modeled by super-ellipsoids. The simulations results show that, in the case of same particle volume, the rod-like particles with smaller aspect ratio obtain larger force from the gas and the particles can absorb more energy from fluid flow, and the fluidization phenomenon, like slugging and bubbles, is easier to form. The local voidage fraction and particle's projected face area perpendicular to fluid flow direction are directly related to particle orientations, which have great influence on drag force and fluidization. Due to the significance of particle orientation, a further investigation is made for the factors that influence the distribution of particle orientation. The results show that particle orientation is greatly affected by fluidization time, fluidization velocity, and the structure of the fluidized bed.

1. Introduction

Fluidized beds involving rod-like particles are often used in chemical and energy industries, such as gasification and combustion of biomass, drying and pharmacy [1–3]. Understanding fluidization properties of rod-like particles and knowing how particle shape influence these properties are important for the design, control and optimization of relevant industrial process. However, little effort has been made in studying the fluidization of rod-like particles, only several investigators have put their attention on the research in this respect [1–7].

Currently, experiment method [8–14] and numerical simulation [9, 15–21] can be applied to study fluidization. And the numerical simulation is an important tool to investigate fluidization of particles in the fluidized bed because more information can be easily obtained with the help of numerical simulation. On the basis of different theories, various numerical simulation methods have been proposed, such as TFM (Two fluid method) based on CFD (Computational fluid dynamic) [9], DSMC (Direct simulation Monte Carlo method) [16,22], CFD-DEM (Computational fluid dynamic–discrete element method) [15,23]. Comparing with other numerical simulation methods, CFD-DEM coupling method can provide detailed micro-scale information, which is important for the comprehension of fluidization of rod-like particles in the fluidized bed. So it has attracted many attentions in fluidization research field, and is also applied in this article to investigate the fluidization of rod-like particles.

Owing to the most of the non-spherical particles approximate to spherical particle and the model of non-spherical particles is difficult to establish, CFD-DEM have been broadly used in studying fluidized bed involving spherical particles instead of non-spherical particles. DEM is an approach that can numerically simulate dynamic behaviors of particulate matter and is firstly proposed by Cundall and Strack [23]. Particles are treated as discrete phase in DEM rather than continuum media as used in TFM. DEM, therefore, have become more and more prevalent in the field of granular flow because of its capability to capture the more accurate physics. Tsuji et al. firstly reported the CFD-DEM model by coupling DEM with CFD when they investigated the fluidization properties of spherical particles in the fluidized bed [15]. The simulation results such as the mixing and motion of particles and the generation of slugging and bubbles match well with corresponding experimental results owing to the introduction of micro-scale model. Subsequently, the availability of CFD-DEM model had been verified by many researchers and CFD-DEM has been got widely acceptance [22, 24–26]. With the help of CFD-DEM, the flow behaviors of spherical particles in the fluidized bed have been investigated detailedly. As the development of DEM, the increasing amount of particles can be processed simultaneously in CFD-DEM model, and more importantly, the particle shape can be modeled by more complicated DEM model. As a result, the attention of researchers has put on the simulation of fluidization behaviors of non-spherical particles in fluidized bed by CFD-DEM numerical simulation.

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The DEM modeling approaches for cylindrical particles include multi-sphere model [27–29], real shape model [7,29–31], super-ellipsoid model [32–35], etc. And the merits and faults of these models had been detailedly discussed by Lu et al. [21]. The rod-like particles used in this study is modeled by super-ellipsoids that possess the relatively high accuracy, which was firstly proposed by Williams and Pentland [32], and Cleary established the three-dimensional super-ellipsoid model subsequently [35]. For avoiding the complex calculation algorithm necessary for contact detection, simpler super-ellipsoid formula has been proposed to model non-spherical particle [35–37], but this is unpractical for the description of cylindrical particle. On the other hand, the adoption of standard super-ellipsoid equation [38] will increase calculation time, but this can be applied to model cylindrical particle. To achieve the higher accuracy and lower calculation consumption, various contact detection accelerate algorithms have been proposed for cylindrical particles [7]. Besides the particle model, drag force model, which is treated as the coupling term between gas and solid phase and is the base of description for the fluidization behaviors of particles, is also very important in CFD-DEM simulation. Different formulas of drag coefficient considering the influence of particle shape have been presented [39–43]. On the base of previous research results, Hölzer and Sommerfeld put forward a new formula of drag coefficient specific to non-spherical particles, and they had demonstrated that the error compared with relevant experimental results is very small [43]. So this drag force model has been accepted in fluidization field [44–47] and is also utilized in this paper for investigation of the fluidization for rod-like particle in the fluidized bed.

So far, some researchers have already put their attention on the fluidization of rod-like particles with the help of CFD-DEM. Zhong et al. investigated the fluidized bed involving monodispersed rod-like particles [5], which the discrete phase and continuous phase are handled by DEM and CFD model, respectively, and the particle shape is modeled by multi-sphere model. The results obtained from this investigation presented that local porosity and particle velocity varies as the variation of radial position in the case of low gas velocity. Cai et al. further demonstrated the axial position of setup is also a function of orientation distribution of rod-like particles when they investigated the fluidization properties of rod-like particles modeled by multi-sphere model in circulating fluidized bed by means of CFD-DEM [2]. By constructing a model of fluidized bed with the help of CFD-DEM coupling method, a further inquiry is made by Oschmann et al. to investigate the factors that affect the mixing and orientation distribution of rod-like particles [6]. Except for CFD-DEM method, other numerical simulation methods, such as Lattice Boltzman method [1], have also been applied to the investigation of fluidized bed concerning rod-like particles. However, the above literatures had made little effort to investigate how aspect ratios of rod-like particles impact the fluidization. And the particle model they used, viz. multi-sphere model, cannot describe cylindrical particle more accurately. In this article, the fluidization properties of rod-like particles with different aspect ratios in fluidized bed are studied by means of CFD-DEM coupling method, in which super-ellipsoids are employed to model rod-like particles, and will be detailedly discussed hereinafter.

2. Mathematical model

2.1. Particle shape model

In the current research, rod-like particle and spherical particle are both employed for the comparisons of fluidization properties between rod-like and spherical particles. Spherical model and super-ellipsoid model are employed to describe spherical and non-spherical particles, respectively. The standard formula of super-ellipsoid is written as [38]:

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

where a, b and c represent semi-major axes of particle, respectively. s_1 and s_2 control the curvature of particle edges, which the bigger shape indices induce the sharper curvature of particle edges. The particle shape is sphere when $s_1 = s_2 = 2$ and the shape of particle tend to be cylinder when $s_1 > 2$ and $s_2 = 2$. In this paper, s_1 is set to be 20, which is large enough to describe cylindrical accurately. Cylindrical particle is rod-like particle only when c is larger than a and b, otherwise is disk-like particle.

2.2. Particle motion equations

According to Newton's laws of motion, particle motion equations are given by

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

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

where m and $\boldsymbol{I}$ respectively stand for particle's mass and inertia moment, $\boldsymbol{v}$ and $\boldsymbol{\omega}$ represent the linear velocity of and angular velocity of particle, respectively. $\boldsymbol{F}_c$ is the contact force, $\boldsymbol{F}_d$ is the drag force, $\boldsymbol{F}_b$ is the buoyancy, $\boldsymbol{g}$ is gravitational acceleration and $\boldsymbol{T}_c$ is the contact torque.

The particle information includes position and velocity can be obtained by the integration of Eqs. (2) and (3) on the basis of force and

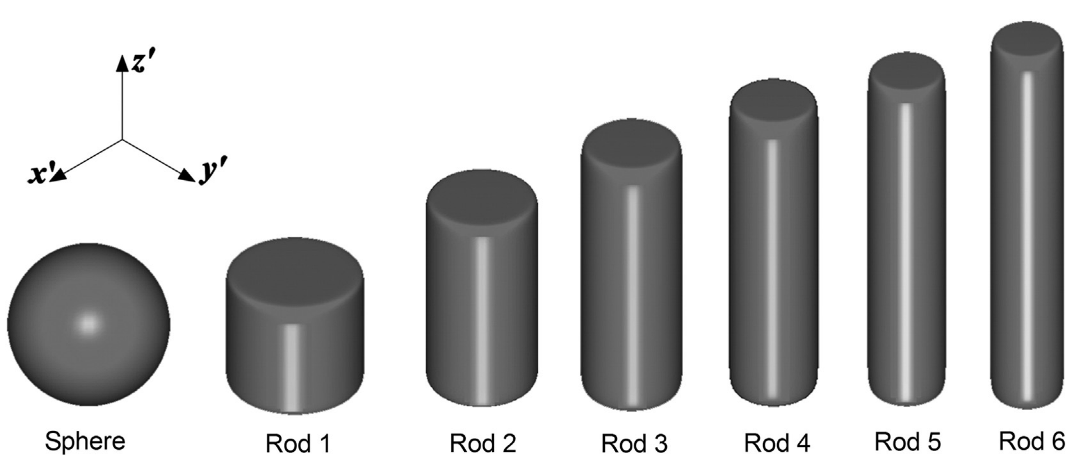

Fig. 1. Spherical particles and super-ellipsoid particles, and body fixed coordinate systems is used here that the center of particle and the origin of coordinate coincide where x'-y' plane lie in the equatorial plane for spherical particles and parallel to end face for rod-like particles.

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