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Original Research Paper

Numerical analysis on the fluidization dynamics of rodlike particles

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ABSTRACT

Fluidization of non-spherical particles widely exists in various engineering applications, such as biomass utilization and catalytic reaction. In this work, a mathematical analysis of particle fluidization has been carried out by employing a combined approach of discrete element method (DEM) and computational fluid dynamics (CFD). The emphasis is focused on the influence of the aspect ratio on the fluidization behavior of rodlike particles. The predictions of the minimum fluidization velocity are comparable to the available empirical correlations. The bed permeability and coordination number are determined by both the bed porosity and the particle shape. Meanwhile, the particle shape has a significant effect on the contact force and particle velocity. The results suggest that the shape parameters such as the sphericity or aspect ratio should be taken into account when establishing a phase diagram in terms of the coordination number and porosity. The evolution of particle orientation is strongly related to the dynamics of bubbles, and the degree of horizontal alignment of particles could be greatly reduced as the bed is well fluidized. These findings would be of interest from applied standpoints as well as showing fundamental effects of the particle shape on the fluidization dynamics.

1. Introduction

Fluidization is extensively used in many physical and chemical applications, such as material preparation, coal combustion and catalytic reactor. It is a typical fluid-solid multiphase flow system, and has been explored in numerous studies. The particles used in those studies are mainly spherical, which are not representative of the reality. In practice, most particles are non-spherical (i.g. ellipsoids, rods and polygons). For example, the straws in the energy utilization and conversion of biomass fuel are of rodlike shape. As one of the most important properties of particles, particle shape has a significant influence on the fluidization behavior such as flow permeability, chemical reaction and segregation [1]. Therefore, to optimize the realistic design and have a reliable operation of the fluidized bed, it is necessary to gain a comprehensive understanding of the effect of particle shape on the fluidization system.

In the past, some work has been done experimentally to investigate the effect of particle shape on the fluidization behavior. Liu and Litster [2] investigated the minimum spouting velocity and fountain height in a spouted bed with non-spherical particles. It was found that the predicted fountain heights were much lower than the experimental values if the influence of particle shape was ignored. Escudié et al. [3] showed that segregation could occur due to the shape difference between the particles in liquid-fluidized beds. Liu et al. [4] observed that non-spherical particles gave poor fluidization quality as compared to spherical particles in terms of the pressure drop and fluidization velocities. The results also showed that non-spherical particles had lower fluidization velocities than that of spheres with the same volume equivalent diameter. Shao et al. [5] explored the minimum spouting velocity of non-spherical particles in a conical-cylindrical spouted bed. The study revealed that the minimum spouting velocity increased as the particle sphericity decreased. Several researchers [6–11] presented some useful correlations to estimate the pressure drop of the fluid flow through the packed beds comprised of non-spherical particles such as cylinders and cubes. Those experimental studies highlight the importance of particle shape on the macroscopic behavior of the fluidization system. However, those results mainly focus on the pressure drop and minimum fluidization velocity, without detailed information about the dynamic behavior. To date, experimental studies of the fluidization behavior of non-spherical particles at a microscopic scale are limited.

On the other hand, mathematical modeling has become an important alternative approach in the study of fluidization dynamics. Among various numerical methods, the combined approach of computational fluid dynamics (CFD) and discrete element method (DEM) has been increasingly used in the simulation of the complex

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fluid-solid flow in fluidized bed [12–14]. In this method, particles are modeled as discrete phases and their motions are tracked individually by solving Newton's laws of motion, while the fluid phase is still considered as a continuum. Clearly, this approach could provide plentiful information about the flow behavior at a microscopic scale, such as the number of contacts between particles and instantaneous forces on particles, which may be extremely difficult to obtain experimentally. Since it has been successfully employed in the simulation of the plug flow of spherical particles in a horizontal pipe by Tsuji et al. [15], significant advances have been accomplished in the DEM-CFD simulation of fluidization behavior [16,17], as reviewed by Zhu et al. [18]. One of the major developments recently is its application in the research of the fluidization of non-spherical particles. Zhong et al. [19] studied the fluidization of cylinder-shaped particles with the aspect ratio of 2.3, including the bed expansion ratio and particle volume fraction. Hilton et al. [20] studied the gas fluidization of cuboid, ellipsoid and spheres, and claimed that particle shape had a significant effect on the dynamics of fluidized bed, including increased pressure gradient within the bed and lower fluidization velocities when compared to beds comprising of spherical particles. Zhou et al. [21] showed that particle shape significantly affected the bed permeability and the minimum fluidization velocity of coarse ellipsoidal particles with the aspect ratio from 0.25 to 3.5. Ren et al. [22,23] studied the fluidization of corned-shape particles in the spouted bed, and the results confirmed the validity of the multi-sphere method in the simulation of fluidization of non-spherical particles. Oschmann et al. [24] claimed that slender particles tended to mix slower with increasing elongation if the same gas velocity was applied. Vollmari et al. [25,26] compared the DEM-CFD simulation results with their experimental work, and shown that the particle orientation had a great influence on the pressure drop. These results provide some useful and interesting information to reveal the fluidization dynamics of non-spherical particles. However, compared to numerous studies on the spherical particles, the available work on the fluidization dynamics of non-spherical particles is not sufficient. There is still much work to be done to fully understand the influence of particle shape on the flow behavior of fluidization system, especially for the slender particles (such as rods) with much large aspect ratio. The feature of slenderness of rodlike particles makes the effect of excluded volume become more significant and promotes the interlocking between particles. According to authors' knowledge, Only Zhong et al. [19] and Vollmari et al. [25,26] did some related work on this kind of particles with aspect ratio less than 4. However, the effect of aspect ratio on the particle dynamics for much slender particles is not clear and has not been addressed adequately, such as the influence of particle orientation on the fluidization behavior. It is therefore worth exploring the fundamental roles of the rod shape and aspect ratio on the fluidization dynamics.

In this work, the DEM-CFD approach is extended to study the fluidization of rodlike particles. The minimum fluidization velocity of particles with three different aspect ratios is compared with available literature correlations. And the effect of aspect ratio on the dynamic behavior such as the flow pattern and coordination number as well as the particle orientation is quantitatively investigated in detail. To elucidate the effect of particle shape, the fluidization behavior of spheres has also been analyzed and presented for comparison.

2. Numerical methods

2.1. DEM for rodlike particles

According to the DEM originally proposed by Cundall and Strack [27], the movement of an individual rod could be reduced to the translational and rotational motion, described by:

$$m_i \frac{d\boldsymbol{v}_i}{dt} = \sum \boldsymbol{F}_{c,i} + m_i \boldsymbol{g} + \boldsymbol{f}_{pf,i} \tag{1}$$

$$\frac{d(\boldsymbol{I}_i \cdot \boldsymbol{\omega}_i)}{dt} = \boldsymbol{R}_i \cdot \left(\sum \boldsymbol{M}_{c,i} + \boldsymbol{M}_{pf,i}\right) \tag{2}$$

where m_i, $\boldsymbol{I}_i$, $\boldsymbol{v}_i$ and $\boldsymbol{\omega}_i$ are the mass, moment of inertia, translational velocity and angular velocity, respectively. $\boldsymbol{F}_{c,i}$ is the contact force, originating from its interaction with neighboring rods or wall. $\boldsymbol{f}_{pf,i}$ is the fluid-particle interaction force on the rod. $\boldsymbol{M}_{c,i}$ is the contact torque, arising from the tangential and normal contact force. $\boldsymbol{M}_{pf,i}$ is the torque due to fluid flow, including the pitching torque and rotational resistance torque. $\boldsymbol{R}_i$ is the rotation matrix from the global to the local coordinate system. The calculation of the rotation expressed by Eq. (2) is accomplished in a local coordinate system which is a moving Cartesian coordinate system fixed to the rod and whose axes are superposed by the axes of inertia, as shown in Fig. 1 where the aspect ratio r_f is defined as the ratio of the total length L to the diameter $d = 2R$. And the transformation of the angular velocity and torque between the local and global coordinate systems can be realized by the rotation matrix. If not specified, all torques and angular velocities are with respect to the global coordinate system in following paragraphs.

Though various analytical methods have been developed to detect the contacts and calculate the contact force between non-spherical particles, such as composite particle representation and continuous function representation, as reviewed by Dong et al. [28]. Among these methods, the multi-sphere model introduced by Favier et al. [29] has enough accuracy with a relative simpler algorithm. As a result, this method is employed in the representation of rods in this work, though it may encounter an increased computational effort as a large number of spheres have to be used to construct an individual rod. In this model, the rod is assumed to be a chain of overlapping spheres (as shown in Fig. 1), with their centers consecutive one-by-one on the symmetry. Thus, the possible interactions such as the collision and slip, between any two rods can be simplified as that of spherical particles. As a consequence, the total contact force/torque of the rod can be readily obtained, given that all contact forces on its spherical elements are known. It should be noted that there are no inter-sphere forces between the spheres in the same rod though they can overlap. Detailed expressions to calculate the contact forces of the spherical element are presented in Appendix A, where the cohesiveness among particles is assigned to zero in this study. Obviously, the difference between the real rod and one represented by the multi-spheres can be adjusted by controlling the separation fraction of neighboring spheres ($\delta = x/R$, the ratio of the normal overlap of two adjacent spheres to the radius of the rod). According to our

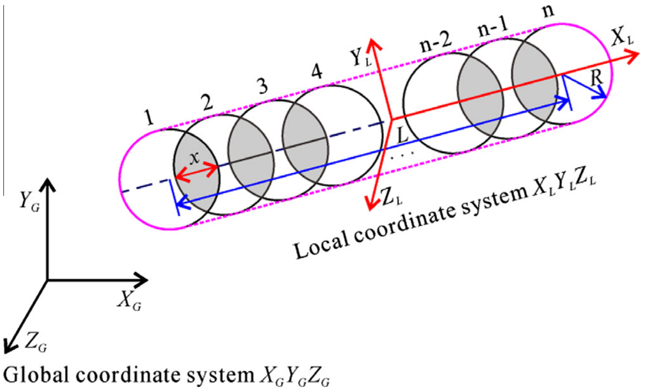

Fig. 1. The representation of the global and local coordinate systems for multi-sphere represented rod.