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CFD-DEM simulation of fluidization of multisphere- modelled cylindrical particles

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A hybrid Open-MP (Shared memory) – MPI (Distributed memory) parallel Computational Fluid Dynamics (CFD)-Discrete Element Method (DEM) model has been developed for simulating fluidization of cylindrical particles in a fluidized bed. In the DEM model, five, seven, nineteen and sixty overlapping spherical particles in different formation methods including single-row, multi-row and hybrid formations have been used to represent one cylindrical particle. The simulation results of the hybrid representation for mimicking a cylindrical particle are more accurate than other representations; particularly in terms of, particle number density along the bed height and particle orientation distribution in the bed, in comparison with previously reported experimental data. The simulation results show that the preferential orientation of the particles is horizontal in the fluidize bed, but the number of particles with vertical orientation increases when they approach to walls. Only multi-row and hybrid formations could capture this increase near the walls.

1. Introduction

Gas-fluidized beds are widely applied in various industries such as chemical, energy, pharmaceutical and environmental industries [1]. Understanding the hydrodynamics and particle movement in the bed is of paramount importance for designing, optimizing and scaling-up in fluidization process. Numerical simulation has played a significant role in revealing the fundamentals in fluidized beds [2,3]. Multi-scale modelling approaches, such as a combination of Discrete Element Method (DEM) and Computational Fluid Dynamics (CFD), has been developed to describe the hydrodynamics of both gas and solid phases in fluidized beds [4,5]. Spherical particles are often adopted for CFD-DEM modelling of fluidized beds for simplicity. However, as most particles in industrial processes are actually non-spherical, recently modelling of non-spherical particles has been receiving an increasing amount of attention [6–8]. Cylindrical particles are common in several industrial processes including polymer suspension, biomass combustion and fluidized beds [9–12]. In pharmaceutical industry, extrusion is a common process in the manufacture of various drug delivery systems such as granules, pellets and tablets which results in cylindrical shape products [13]. Therefore, understanding the aerodynamic behaviour of cylindrical particles is of great importance. Representation of non-spherical particles and detection of particle-particle contact are the main challenges of using DEM for non-spherical particles [14]. There are three main approaches for representing a non-spherical particle in DEM, namely multi-sphere, polyhedral and super quadratic representations [14]. Super quadratic and polyhedral shape representation methods have been used for simulation of various non-spherical particles in fluidized beds [8,15,16]. However, these approaches demand complicated and computationally expensive contact detection algorithms [14]. On the other hand, in the multi-sphere method, a non-spherical body is represented by a certain number of overlapping spheres. This method is easy to be implemented and can be readily extended from the DEM code for spherical particles [17]. Since the multi-sphere approach employs a fast and well-validated sphere-sphere contact detection algorithm, it is the most efficient and versatile in DEM simulation of non-spherical particles [14]. In this representation method, an increase in the number of spheres may lead to more accurate representation of non-spherical surfaces, while this also increases the computational costs [17]. Therefore, one challenge for this multi-sphere approach is to determine the optimal number of spheres [14,17], especially the topology assembled from spheres to capture particle behaviour in the multi-phase system. There are many studies that emphasise the significant effect of the particle shape on fluidized bed dynamics [6,15,16,18,19], but very few on the effect of particle representation [20].

Zhong et al. [21] pioneered in using a multi-sphere approach to investigate particle behaviour of cylindrical particles in fluidized beds.

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In their study, 5 overlapping spheres with a diameter of 2.6 mm are used to represent a cylindrical particle with the same diameter and a length of 6 mm. Reasonable accuracy of predictions from this approach has been achieved when comparing their simulation results with experimental data. Ren et al. [22,23] continued to examine the dynamic behaviour of corn-shaped and cylindroid particles in a spouted bed using this multi-sphere representation approach. They used 4 overlapping spheres to represent a 10 mm long cylinder with a diameter of 4 mm. Their simulation results captured the spouting action of non-spherical particles with great accuracy. Recently, Oschmann et al. [20] studied various elongated non-spherical particles in a fluidized bed with a focus on orientation and mixing of cylindrical and cuboidal particle. They compared the results from polyhedral and multi-spherical shape representation and concluded that the accuracy of the particle shape representation has a significant influence on the simulation results [20]. In their study 36 overlapping spheres is used to represent a cylinder of 6 mm length and 6 mm diameter.

Despite the popularity of multi-sphere approach for simulation of non-spherical particles in fluidized beds [14,20,22], the effect of number and formation of spheres on the accuracy of simulation results is so far not fully understood.

In this study, a detailed investigation on the effect of cylindrical particle representation by the multi-sphere method on particle orientation and bed hydrodynamics in a fluidized bed is presented. The soft-sphere DEM method is used for simulation of particles movement and the MFIX CFD solver for fluid flow. The simulation results, including pressure drop, particle distribution, and particle orientation distribution, are compared to experimental data of Vollmari et al. [16].

2. Mathematical equations

2.1. Solid phase equations

In this work a three dimensional DEM code is developed to model the motion of each particle in the system, based on the Newton's second law [24]:

$$m_i \frac{d\vec{u}_i}{dt} = \vec{F}_i^c + \vec{F}_i^{pf} + \vec{F}_i^g \tag{1}$$

$$\frac{d\left(\vec{I}_i.\vec{\omega}_i\right)}{dt} = \vec{T}_i \tag{2}$$

where m_i, $\vec{u}_i$ and $\vec{\omega}_i$ are mass, translational and angular velocities of particle i, respectively. $\vec{F}_i^c$ is the summation of all contact forces acting on particle i. $\vec{F}_i^{pf}$ and $\vec{F}_i^g$ are particle-fluid interaction and gravity forces, respectively. $\vec{I}_i$ is the particle's moment of inertia, and $\vec{T}_i$ is the summation of all torques acting on particle i.

Since the moment of inertia changes with the orientation of non-spherical particles, the equations of rotational motion (Eq. (2)) are solved in a body-fixed coordinate system. The axes in this system are the principal axes of inertia, therefore, Eq. (2) in the body-fixed frame can be expressed as [17]:

$$I_i' \frac{d\vec{\omega}_i^b}{dt} + \vec{\omega}_i^b \times I_i'\vec{\omega}_i^b = \vec{T}_i^b \tag{3}$$

where I_i', $\vec{\omega}_i^b$ and $\vec{T}_i^b$ are principal moment of inertia, angular velocity in the body-fixed frame and the summation of all torques acting on the particle i in the body- fixed frame, respectively. The rotation matrix A is used to transfer a vector from body-fixed to space fixed frame and vice versa ($\vec{M}^b = A\vec{M}^s$) [25]:

$$A = \begin{bmatrix} q_0^2+q_1^2-q_2^2-q_3^2 & 2(q_1q_2+q_0q_3) & 2(q_1q_3-q_0q_2) \\ 2(q_1q_2-q_0q_3) & q_0^2-q_1^2+q_2^2-q_3^2 & 2(q_2q_3+q_0q_1) \\ 2(q_1q_3+q_0q_2) & 2(q_2q_3-q_0q_1) & q_0^2-q_1^2-q_2^2+q_3^2 \end{bmatrix} \tag{4}$$

where q_0, q_1, q_2, q_3 are components of a unit quaternion which can be represented in terms of Euler angles as [25]:

$$q_0 = \cos\frac{\theta}{2} + \cos\frac{\phi+\psi}{2} \tag{5}$$

$$q_1 = \sin\frac{\theta}{2} + \cos\frac{\phi-\psi}{2} \tag{6}$$

$$q_2 = \sin\frac{\theta}{2} + \sin\frac{\phi-\psi}{2} \tag{7}$$

$$q_3 = \cos\frac{\theta}{2} + \sin\frac{\phi+\psi}{2} \tag{8}$$

2.1.1. Contact force

To calculate particle-particle and particle-wall contact forces, the linear spring-dashpot model proposed by Cundall and Strack [26] is used. In this model, the normal component of the contact force from the linear spring- dashpot model is calculated as:

$$\vec{F}_{ij,n} = -k_n \delta_n \vec{n}_{ij} - \eta_n \vec{u}_{ij,n} \tag{9}$$

where k_n and η_n are the normal spring stiffness and the normal damping coefficient respectively. $\vec{n}_{ij}$ is the unit vector from the centre of particle i to the centre of particle j, and $\vec{u}_{ij,n}$ is the normal relative velocity of the contacting particles. The normal overlap δ_n of spherical particles can be calculated as:

$$\delta_n = R_i + R_i - \mid \vec{r_i} - \vec{r_j} \mid \tag{10}$$

where $\vec{r_i}$, $\vec{r_j}$ are position vectors and R_i, R_j are radii of particle i and j, respectively.

Normal spring stiffness and the damping coefficient are contact parameters. For a contact between particle i and particle j, these parameters are given as [27]:

$$k_n = \frac{4}{3}E^*\sqrt{\frac{R_iR_j}{(R_i+R_j)}} \tag{11}$$

$$E^* = \frac{1-\nu_i^2}{E_i} + \frac{1-\nu_j^2}{E_j} \tag{12}$$

$$\eta_n = \frac{2\ \ln e_n}{\sqrt{\pi^2 + \ln^2 e_n}}\sqrt{k_n \frac{m_im_j}{m_i+m_j}} \tag{13}$$

where E, ν and e_n are Young's module, the Poisson ratio and coefficient of normal restitution, respectively.

Similar to the normal contact force, the tangential force is calculated as [28]:

$$\vec{F}_{ij,t} = \begin{cases} -\mu\left|\vec{F}_{ij,n}\right|\vec{t}_{ij}\ if: \left|\vec{F}_{ij,t}\right| > \mu\left|\vec{F}_{ij,n}\right| \\ -k_t\delta_t\vec{t}_{ij} - \eta_t\vec{u}_{ij,t}\ else \end{cases} \tag{14}$$

In this equation, when $|\vec{F}_{ij,t}| > \mu|\vec{F}_{ij,n}|$, sliding occurs and the tangential force is obtained from the Coulomb friction law [28]. In Eq. (14), k_t,

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