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CFD–DEM study of mixing and dispersion behaviors of solid phase in a bubbling fluidized bed

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ABSTRACT

Three-dimensionally coupled computational fluid dynamics (CFD) and discrete element method (DEM) are used to investigate the gas–solid hydrodynamics and mixing characteristics of a three-dimensional rectangular bubbling fluidized bed. The numerical study is conducted referring to the quasi-3D experimental apparatus investigated by Goldschmidt et al. [1]. The simulation results turn out that time-averaged solid volume fraction and instantaneous particle height agree well with the experimental data. To investigate the solid behavior, the solid velocity and flux distribution are extracted and the influence of the gas velocity on the solid velocity is discussed. It is found that higher gas velocity induces the formation of double-recirculation pattern in which solid phase mainly moves from the near wall region to the central region in the lower bed and oppositely in the upper bed. At the same time, the solid mixing is faster under higher inlet velocity, and that particles in vertical directions tend to mix better than those in lateral directions. At last, we find the particle dispersion coefficient is very anisotropic in three normal directions. In accordance with the results of most experiments, the geometry structure strongly influenced the coefficient value. We also find when inlet gas velocity is higher, the dispersion coefficient increases, for the particle velocities are higher due to greater momentum exchange.

1. Introduction

Fluidized bed has its unique characteristics, including good particle circulation, effective fluid-particle contact, high rates of heat and mass transfer and is widely used in industries as a major flow mode in chemical processes [2–4]. Many studies have been made in the past in order to gain a thorough understanding of the fundamentals of gas–solid fluidized beds, and there are abundant literature relating experimental studies on 2D or pseudo-2D fluidized beds, of which the primary aim has been to investigate the fundamentals of fluidization, such as bubble properties [5], flow behavior [6], and solid mixing [7], using non-invasive visual or imaging techniques. Pallarès and Johnsson [8] experimentally investigated the fuel dispersion of a tracer particle by means of video recording in a 2-dimensional fluidized bed operated under ambient condition. Laverman et al. [9] conducted experiments using the PEPT technique to study the influence of the superficial velocity, the packed bed aspect ratio and the bed material on the macroscopic circulation patterns of the solid phase in a 3-D bubbling fluidized bed.

However, experimental study of particle mixing behavior in fluidized bed is restricted by the practical conditions, and a series of defects may occur during the experimental work. Examples are defects caused by the sampling method, the locations of the sampling, the lack of the information of the size and number of the samples, and the absence of the information of the particle trajectories in bed. Moreover, the requirement of particle properties such as the particle diameter and density can also be a demanding restriction on experimental tests.

In recent years, numerical simulation, considered to be a useful tool to obtain more detailed information on dense gas–solid flow than experimental research without disturbing the flow field, has become a popular method in the field of gas–solid two-phase flow [10–12]. As widely known, there are mainly two models for modeling the gas–solid interactions in fluidized beds. One is the two-fluid model (TFM), in which the solid phase is treated as continuous phase like the gas; the other is Eulerian–Lagrangian model in which the motion of the particle is calculated at the particle level using a trajectory model, one of which is the Discrete Element Model (DEM) [13,14]. The model coupled with CFD (CFD–DEM) is more fundamental, which employs a continuum description for gas phase and can provide dynamic information, such as the trajectories of and transient forces acting on individual particles, which is extremely difficult to obtain by physical methods [15,16]. The CFD–DEM approach is especially suitable to provide an insight into the solid mixing in dense gas–solid flows, for the DEM algorithm allows the dynamic simulation of the solid phase motion by tracking individual particles along the system. With this advantage, the CFD–DEM model is more suitable for investigating solid mixing behaviors [17]. Li and Kuipers [18] observed that an elevated pressure reduces

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the incipient fluidization velocity, widens the uniform fluidization regime, shortens the bubbling regime and leads to a quick transition to the turbulent regime. Liu and Chen [19] carried out a simulation to investigate the influences of superficial velocity and bed width on the lateral solid dispersion coefficient in the bubbling fluidized bed. They found that with increasing the superficial velocity and the bed width, the lateral solid dispersion coefficient increases. Norouzi et al. [20] conducted a 2-D numerical simulation on the information of solid mixing and circulation properties in a fluidized bed with the CFD–DEM approach. The results illustrated that the flow patterns of solid phase change obviously by changing the aspect ratio.

In the bubbling fluidized bed, there exist different flow behaviors of solid phase in different regions. There is a broad existence of the reports focusing on the gas–solid hydrodynamics of the fluidized bed carried out with experimental and numerical methods. For example, Gui and Fan [21] proposed a criterion for identification of the boundary of bubbles which is used to investigate the effect of bubble on particle mixing characteristics; Yuu et al. [22] found that there are many small vortices in bubbles, and the vorticity of the vortices, which exist in relatively small bubbles, is very high. These vortices with high vorticities would play an important role in various operations in fluidized beds.

However, there is little study on the solid velocity and flux distribution, mixing behavior of solid phase, in the bubbling bed. The current work is conducted to provide insights into these two aspects of the bubbling fluidized bed with the CFD–DEM method. The fluid motion is computed at the computational cell level and the solid motion is tracked at the particle scale level. In Section 2, the mathematical model of the fluid phase and the solid phase is described. Then the simulation setting is presented in Section 3. Subsequently the results are presented and discussed in Section 4.

2. Mathematical model

2.1. Governing equations for gas motion

The fluid phase, air to be specific for this study, is treated as a continuum phase. For the gas motion in the bubbling fluidized bed, the governing equations are the Navier–Stokes equations for the incompressible viscous Newton fluid, but taking into account the volume fraction of gas, given by

$$\frac{\partial\left(\varepsilon_g\rho_g\right)}{\partial t}+\frac{\partial\left(\varepsilon_g\rho_g\mathbf{u}_i\right)}{\partial x_i}=0 \tag{1}$$

$$\begin{aligned}&\frac{\partial}{\partial t}\left(\varepsilon_g\rho_g\mathbf{u}_i\right)+\frac{\partial\left(\varepsilon_g\rho_g\mathbf{u}_i\mathbf{u}_j\right)}{\partial x_j}\\&=-\varepsilon_g\frac{\partial p}{\partial x_i}-\sum_{m=1}^{n}\frac{\mathbf{f}_{d,m}}{\Delta V}+\rho_g\varepsilon_g\mathbf{g}+\frac{\partial}{\partial x_j}\left[\varepsilon_g(\mu+\mu_t)\left(\frac{\partial\mathbf{u}_j}{\partial x_i}+\frac{\partial\mathbf{u}_i}{\partial x_j}\right)\right]\end{aligned} \tag{2}$$

where ρ_g, p, $\mathbf{u}$, μ and μ_t are the density, the pressure, the velocity of fluid phase, the dynamic viscosity and the turbulent viscosity, respectively. ΔV is the volume of the computational cell. $\mathbf{f}_{d,m}$ is the drag force exerted on particle m locating in current cell. n is the total number of particles locating in the current cell. ε_g is the gas voidage and can be estimated as

$$\varepsilon_g=1-\frac{\sum_{i=1}^{n}V_{pi}}{\Delta V} \tag{3}$$

where V_{pi} is the volume of particle i occupied by the current cell.

The turbulent viscosity is modeled with the k-ε turbulence model as

$$\mu_t=c_\mu\rho_g k^2/\varepsilon_t \tag{4}$$

where c_μ is a constant, $c_\mu=0.09$. k and ε_t are, the turbulent kinetic energy and its dissipation rate, respectively, for which the governing equations are given as

$$\begin{aligned}&\frac{\partial}{\partial t}\left(\varepsilon_g\rho_g k\right)+\frac{\partial\left(\varepsilon_g\rho_g k\mathbf{u}_j\right)}{\partial x_j}\\&=\frac{\partial}{\partial x_j}\left[\varepsilon_g\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right]+\varepsilon_g\mu_t\frac{\partial\mathbf{u}_i}{\partial x_j}\left(\frac{\partial\mathbf{u}_j}{\partial x_i}+\frac{\partial\mathbf{u}_i}{\partial x_j}\right)-\varepsilon_g\rho_g\varepsilon_t\end{aligned} \tag{5}$$

$$\begin{aligned}&\frac{\partial}{\partial t}\left(\varepsilon_g\rho_g\varepsilon_t\right)+\frac{\partial\left(\varepsilon_g\rho_g\varepsilon_t\mathbf{u}_j\right)}{\partial x_j}\\&=\frac{\partial}{\partial x_j}\left[\varepsilon_g\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial\varepsilon_t}{\partial x_j}\right]+\frac{\varepsilon_g c_1\varepsilon_t}{k}\mu_t\frac{\partial\mathbf{u}_i}{\partial x_j}\left(\frac{\partial\mathbf{u}_j}{\partial x_i}+\frac{\partial\mathbf{u}_i}{\partial x_j}\right)-\varepsilon_g c_2\rho_g\frac{\varepsilon_t^2}{k}\end{aligned} \tag{6}$$

where c_1 and c_2 are the model constants, which equal to 1.44 and 1.92, respectively. $\sigma_\varepsilon=1.3$ and $\sigma_k=1.0$ are turbulent Prandtl numbers for ε_t and k, respectively.

2.2. Governing equations for solid motion

The solid phase is treated as a discrete phase and described by the so-called discrete element method [13]. The DEM is particularly suitable to study the characteristics of particle mixing, because of its capability of precise description of both particle–particle and particle–wall interactions. According to the model, the translational and rotational motions of a particle at any time, t, can be described by Newton's law of motion. The equations governing the translational and rotational movements of the particle i with mass m_p can be given as

$$m_p\frac{d\mathbf{v}_p}{dt}=m_p\mathbf{g}+\mathbf{f}_p+\mathbf{f}_d+\sum_{j=1}^{k}\mathbf{f}_{c,j} \tag{7}$$

$$I_p\frac{d\boldsymbol{\omega}_p}{dt}=\mathbf{T}_p \tag{8}$$

where I_p, $\mathbf{v}_p$ and $\boldsymbol{\omega}_p$ are, respectively, the moment of inertia, translational and rotational velocities of particle. The forces exerted on a single particle consist of the gravitational force, the drag force $\mathbf{f}_d$, the pressure gradient force $\mathbf{f}_p$ and the colliding force. T_p is the torque exerted by other particles or wall in the contacting procedure. k is the total elements of the particles and walls colliding with the current one.

The pressure gradient force is calculated as

$$\mathbf{f}_p=-\frac{1}{6}\pi d_p^3\nabla p_g \tag{9}$$

where d_p is the particle diameter.

The particle drag force is calculated on the base of the local solid concentration and the relative velocity between the gas and the particle, which can be formulated as

$$\mathbf{f}_d=\frac{V_p\beta}{\varepsilon_p}\left(\mathbf{u}-\mathbf{v}_p\right) \tag{10}$$

where β is the drag force coefficient and estimated from the correlation proposed by Koch and Hill [23] as

$$\beta_{\mathrm{Koch\&Hill}}=\frac{18\mu\varepsilon_g\varepsilon_p}{d_p^2}\left(F_0\left(\varepsilon_p\right)+\frac{1}{2}F_3\left(\varepsilon_p\right)\mathrm{Re}_p\right) \tag{11}$$

$$\mathrm{Re}_p=\frac{\varepsilon_g\rho_g\left|\mathbf{u}-\mathbf{v}_p\right|d_p}{\mu} \tag{12}$$