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# LES–DEM investigation of the solid transportation mechanism in a 3-D bubbling fluidized bed. Part II: Solid dispersion and circulation properties

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ABSTRACT

The gas–solid flow in a 3-D bubbling fluidized bed is numerically simulated with the coupling of computational fluid dynamics (CFD) and discrete element method (DEM). The gas phase is described by the Navier–Stokes equations while the solid phase is tracked individually. The distribution properties of the local and global dispersion coefficients of solid phase are initially investigated. The granular temperature of solid phase is studied to capture its turbulent behavior. Then, solid circulating pattern is explored. Besides, the influences of superficial velocity, the particle diameter and the scale-up of the bed width on these aspects are discussed. The results show that the vigorous lateral dispersion of solid phase appears in the central region near the inlet, while intensively vertical ones exists in the region of bubble eruption. Furthermore, the vertical dispersion intensity of solid phase is larger than the lateral ones in nearly an order of magnitude. Vigorously turbulent behavior of the solid phase is observed to be in the upper central region of the bed. The larger the superficial velocity or the smaller the particle diameter, the enhanced dispersion and more chaotic motion of solid phase appear. The scale-up of the bed width not only enlarges the lateral dispersion intensity but also leads to more chaotic and turbulent motion of solid phase. Besides, three patterns of solid circulation can be observed, namely the gross circulation, the local circulation and the local exchange. The numbers and intensities of both gross and local circulations increase with enlarging the superficial velocity.

## 1. Introduction

The dense gas–solid flows are frequently encountered in many fluidizing processes, such as the coating of tablet, drying of granulation, mixing of binary mixture, and coal combustion [1–5]. In order to achieve an optimized design and operation of the fluidizing apparatus, deep understanding on the latent dynamic properties of the system is required. Important aspects related to the solid transportation in the fluidized bed are the dispersion, the turbulent property and the circulating pattern of solid phase [6,7].

Extensive experiments focusing on these important properties of the solid phase in the fluidized bed have been conducted in the past years. Niklasson et al. [8] proposed a method to estimate the lateral dispersion coefficient of solid phase in a fluidized-bed combustor based on a combination of a model for drying and devolution of the fuel and cross-sectional measurement of water concentration in the steady operation condition. The effective dispersion coefficient was found to be on the order of 0.1 $m^2/s$. Pallarès and Johnsson [9] experimentally investigated the fuel dispersion of a tracer particle by means of video recording in a 2-dimensional fluidized bed operated under ambient condition. The result showed that the local dispersion coefficient reaches the maximum around the locations of bubble eruptions, and the increase of the fluidization velocity or particle number leads to a higher dispersion system. Olsson et al. [10] qualified the fuel mixing through the lateral dispersion coefficients by tracking a batch of tracer particles in a large-scale fluidized bed operated under ambient conditions. They found that the dispersion coefficient of the solid phase in the bed is in a scale of $1 \times 10^{-3}$ $m^2/s$, and the diffusion-type models are not suitable for the calculation of the dispersion in the system with only a few mixing cells or large solid concentration gradient. Laverman et al. [11] conducted experiments using the PEPT measuring 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.

Besides the experimental research, numerically exploring the dynamic behaviors of the gas–solid phases in the fluidized bed has been frequently adopted due to the development of high performance computation in the last two decades [12–15]. The widely used numerical approaches modeling the gas–solid motion can be categorized into the Eulerian–Eulerian method and the Eulerian–Lagrandian method, between which the distinct difference mainly lies in method adopted to track the solid motion. The solid phase is considered as a continuous medium in the Eulerian method, while it is tracked individually at the particle scale in the Lagrangian approach [16,17]. Due to the ability to

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obtain the trajectory of each particle, the discrete element method in the Lagrangian framework is more and more popular to investigate the dispersion, turbulent property and the particle circulating pattern in the fluidized bed. Zhou et al. [18] modeled the gas–solid motion in the bubbling fluidized bed with discrete element method–large eddy simulation (DEM–LES) coupling to study the gas/particle flow structure and their turbulent intensities. The result showed that the presence of the reactively large particles in the fluidized bed significantly affects the gas and particle turbulent intensities. Norouzi et al. [19] 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. At the same time, increasing the gas velocity enhances both internal and gross circulations of solid phase, leading to an improved solid mixing and decreased deviation from the well-mixed state. Liu and Chen [20] numerically studied the lateral dispersion coefficient of solid phase at different levels of the bed width under different superficial velocities. They found that the lateral dispersion coefficient first increases sharply, and then its increase rate declines. Finally, a constant value is reached with increasing the bed width. Again, the solid motion was found to become more intense with increasing the gas velocity.

In the bubbling fluidized bed, distinct flow behaviors of solid phase exist in the different regions of the bed, such as the bottom region where the particles are entrained into the bubble wake, the near wall region where the downward flow of solid phase is vigorous, and the central region where particles rise energetically with the bubbles. Although there have existed many studies on the dispersion and circulation behaviors of the solid phase in the fluidized bed, few reports focus on the local distribution of these important aspects of solid phase. Thus, investigating the local distribution characteristics of the dispersion and turbulent behaviors of solid phase is critical for understanding the latent solid transportation mechanism in a 3-D fluidized bed. Furthermore, the responses of these important aspects of solid phase to the variation of particle diameter and the scale-up of the bed width are interesting and estimable for the optimization of design and scale-up of the system.

Thus, the current work presents a numerical modeling of the gas–solid motion in a 3-D bubbling fluidized bed to explore the local distribution properties of the dispersion intensity, the turbulent characteristic and the circulation behavior of solid phase under the framework of CFD–DEM coupling approach, in which the gas motion is solved at the computational grid level while the solid motion is modeled with the discrete element method at the particle level. The local and global distribution properties of solid dispersion and the turbulent property are investigated initially. Subsequently, the circulation behavior of solid phase is discussed. Moreover, the effects of the superficial velocity, the particle diameter and the scale-up of the bed width on these important aspects of solid phase are discussed.

## 2. Mathematical model

### 2.1. Gas–particle hydrodynamics

The computational model adopted in the current work for solving the gas–solid motion is the CFD–DEM coupling approach, which has been well-documented in literature [21]. The gas motion is solved based on the local-averaged Navier–Stokes equations in the framework of computational fluid dynamics. The solid phase is solved at the particle scale level using discrete element method with soft-sphere contacting model to deal with the collision between particles. The governing equations of fluid phase are solved with the PISO algorithm [22] to decoupling the pressure and velocity. The coupling between the gas and solid phases is achieved through the voidage and drag force. When estimating the drag force exerted on each particle, the correlation proposed by Koch and Hill [23] has been adopted. Detailed description of the governing equations is given in Part I of this paper. Particularly, for the front and back walls, the periodic boundary condition is implemented for all the involved variables of both gas and solid phases.

### 2.2. Solid dispersion coefficient

Two methods are available to estimate the solid dispersion coefficient, namely the macro approach and the micro approach [9,20,24]. In the macro approach, the calculation domain of the whole system is divided into many of the sampling cells. Subsequently, the concentration of a specific particle group is calculated in each individual cell, followed by solving a Fickian-type diffusion concentration equation [8]. In the micro method, the solid dispersion coefficient is determined from the trajectory of the tracer by the Einstein's expression [25]. As the DEM approach can provide the position of each individual particle at any time instant, the micro calculation approach is chosen in the current work. The local dispersion coefficient of a specific particle labeled with number $i$ is formulated as

$$D_i = \frac{(\Delta r_i)^2}{2\Delta t} \tag{1}$$

where $\Delta r$ is the local displacement in the time interval $\Delta t$. Thus, the solid dispersion coefficient in the lateral or vertical direction can be obtained from the displacement of the particle in each individual direction. In the simulation procedure, the calculation domain is divided into lots of small computational grids. Then, the instantaneous dispersion property of the solid phase is represented by the quantity of solid dispersion coefficient in the current computational cell. Its value is estimated by averaging all the dispersion coefficients of the particles locating in the current cell as

$$D_{k,\tau} = \frac{\sum_{i=1}^{N} D_{i,\tau}}{N} = \frac{1}{N}\sum\nolimits_{i=1}^{N}\left(\frac{\left(\Delta r_{i,\tau}\right)^2}{2\Delta t}\right) = \frac{1}{2\times\Delta t\times N}\sum\nolimits_{i=1}^{N}\left(\left(\Delta r_{i,\tau}\right)^2\right) \tag{2}$$

where $N$ is the total number of particles in the current cell. $k$ is the current cell label. $\tau$ is the current time instant. $D_{i,\tau}$ is the dispersion coefficient of particle $i$ at time instant $\tau$.

For the dispersion property of the solid phase in the whole system at any time instant, the systematic dispersion coefficient of solid phase is estimated by averaging all the dispersion coefficients of particles in the system as

$$D = \frac{1}{NP}\sum_{i=1}^{NP}\frac{(\Delta r_i)^2}{2\Delta t} = \frac{1}{NP}\sum_{i=1}^{NP}\frac{(r_i - r_{i0})^2}{2\Delta t}(i = 1, 2, \ldots, NP) \tag{3}$$

where $NP$ is the total number of particles in the system. $r_i$ is the new position of particle $i$ while $r_{i0}$ is its initial position.

Due to the chaotic motion of solid phase at each time instant, the time-statistical value of systematic dispersion coefficient is needed to investigate the general distribution property of the solid dispersion. It is formulated as

$$\overline{D} = \frac{1}{N_t}\sum_{i=1}^{N_t} D_i\,(i = 1, 2, \ldots, N_t) \tag{4}$$

where $N_t$ is the total number of the time instants. $D_i$ is the instantaneous systematic dispersion coefficient of the whole system.

### 2.3. Granular temperature

Due to the complex interaction between the fluid phase and the particles in the dense gas–solid flow, both fluid and solid phases show a turbulent movement behavior. For the solid phase, its turbulent