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Influence of grid resolution, parcel size and drag models on bubbling fluidized bed simulation

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HIGHLIGHTS

- A bubble detection algorithm was developed using connected component labeling.
- Drag models have a large influence on bubble size and voidage distributions.
- EMMS drag model can be used with coarse grid and large parcel size.
- Refining CFD grid and reducing the parcel size can improve the simulation results.

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ABSTRACT

In this paper, a bubbling fluidized bed is simulated with different numerical parameters, such as grid resolution and parcel size. We examined also the effect of using two homogeneous drag correlations and a heterogeneous drag based on the energy minimization method. A fast and reliable bubble detection algorithm was developed based on the connected component labeling. The radial and axial solids volume fraction profiles are compared with experiment data and previous simulation results. These results show a significant influence of drag models on bubble size and voidage distributions and a much less dependence on numerical parameters. With a heterogeneous drag model that accounts for sub-scale structures, the void fraction in the bubbling fluidized bed can be well captured with coarse grid and large computation parcels. Refining the CFD grid and reducing the parcel size can improve the simulation results but with a large increase in computation cost.

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1. Introduction

Gas-solids bubbling fluidized beds are widely used in industry such as methanol to olefins see e.g. [1] and catalyst regenerations see e.g. [2]. In bubbling fluidized bed systems, the heterogeneity introduced by the presence of bubbles significantly reduces the gas-solids contact by creating a way for the gas to easily bypass the bed of solid particles. These heterogeneous structures create circulation of the particles and are the main cause of large-scale turbulence in the fluidized bed. The computer simulation method such as two-fluid model (TFM) [3] and computational fluid dynamic coupled with discrete element method (CFD-DEM) [4–7] have been widely used to understand and predict the dynamics of bubbling fluidized beds. The TFM uses the continuum approach to derive a set of unsteady advection-diffusion equations for both gas and solids phases that are solved on Eulerian computation grid. To capture the small-scale heterogeneous structures, such as small bubbles and clusters of particles, fine grid simulations of about several particle diameters must be carried out with very small time steps to ensure the convergence of the solver [8] [9]. However, this leads to a dramatic increase in computation cost with numerical results that may be questioned as the size of the grid becomes of the scale of particle diameter or smaller. Indeed, previous research [10] questioned the results of fine-grid TFM simulation of gas–solids riser flow using homogeneous drag models. To improve the accuracy of TFM while reducing its computation cost, coarse grid simulation coupled with sub-grid models like energy minimization multi-scale (EMMS) [11–14] and filtered method [15–17] are used by researchers in academy and industry. Benyahia [18] showed that sub-grid models are both useful and needed with continuum models to resolve flow in large-scale industrial systems using coarse computation grids.

The continuum approach requires the formulation of constitutive laws for the solids phase for a wide range of solids

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concentration and energy. However, due to the lack of clear understanding of specific mechanisms, general constitutive relations for granular materials are still literally debatable for the wide span of their flow behaviors, such as the solids-like with the static pile of particles in a stagnant region of the flow and the granular gas dominated by particle-particle collision at intermediate flow regimes, as well as the Knudsen-type flow in very dilute flow conditions. This challenge has been listed as one of the 125 big questions in the 125th-anniversary issue of Science [19] by raising the question: "Can we develop a general theory of the dynamics of turbulent flows and the motion of granular materials?". Discrete particle models (DEM) avoid the challenging derivation of constitutive models by following the trajectory of every particle and its possible contacts with other particles and wall boundaries. In this technique, the fluid phase is usually described as a continuum and solved on Eulerian grid and exchanging momentum/heat/mass based on known correlations that can be derived empirically, computationally or theoretically. These interphase transfers are still carried out at the scale of the CFD grid so that grid resolution can influence the fluid-particle flow behaviors. Thus, fine grid simulations are also needed within the CFD-DEM method as well [9]. Another major issue with CFD-DEM is the large computational cost that makes it nearly infeasible when simulating industrial reactors although the DEM can be accelerated by GPUs [20]. A practical way to circumvent this tremendous cost by several orders of magnitude is to lump several real particles into a computation parcel. To distinguish from CFD-DEM, this method is usually called coarse grained particle method (CGPM) [21–25]. In CGPM, the collision diameter of the computational parcel can be much larger than that of a real particle. To ensure the accuracy of inter-phase transfer mechanisms by computing correct void fraction, the grid size for the fluid phase is usually larger than collision diameter of parcels. However, coarsening the grid results in the loss of the small-scale structures and reduces/degrades the accuracy of the simulations. Thus, the sub-grid models used in TFM may also be used in CGPM to improve their accuracy. In fact, several previous researchers have used sub-grid drag models with parcel-based methods. For example, Li et al. [26] simulated a lab-scale CFB riser using coarse grid MP-PIC with EMMS drag model. Also, Lu et al. [27] simulated a lab-scale and pilot-scale CFB riser using CGPM on coarse CFD grids with EMMS drag model. Finally, Ozel et al. [28] simulated gas-solids flow in a 3D periodic domain on a coarse grid MP-PIC with corrected drag model filtered from fine-grid simulations of the same system. Besides the strong effect of grid size and drag model, the parcel size can also influence the simulation results. As indicated by Lu et al. [27] the parcel size should be small enough to resolve the cluster evolutions in CFB riser.

In this study, we attempt an optimization of CGPM simulation in terms of parcel and grid sizes while using different drag correlations. For this purpose, a bubbling fluidized bed is simulated with different grid resolutions and parcel sizes, and with three drag models: an empirical correlation [29], a correlation obtained by fitting direct numerical simulation data [30] and a sub-grid correlation for bubbling fluidized bed [31]. To quantitatively analyze the bubbling behavior, we propose an efficient method to identify and track bubbles in a fluidized bed. Bakshi et al. [32] proposed a method to analysis bubble properties, that we found can easily be achieved by using connected component labeling algorithm (CCL) [33]. The CCL is one of the basic algorithms widely used in computer vision to detect objects in figures. Since this general method can be used to analysis bubble and cluster properties in simulation or experiment research of gas-solids flow, the 2D C++ source code of this algorithm is shared in this study. It can easily be extended to 3D by using 3D connected component labeling algorithm.

2. Method

The CGPM reduces simulation cost by lumping W real particles into a computation parcel. The equivalent diameter of the parcel is $d_p W^{1/3}$ and the collision forces are calculated at that scale as similarly calculated at the real particle scale with the DEM [34]. Other forces like drag, gravity, and pressure gradient forces are calculated at real particle scale. In this section, the fluid and parcels equations of motion are briefly introduced, while the three different drag models used in this study are explained in more detail.

2.1. Fluid governing equations

The volume-averaged Navier-Stokes equations are used to describe the motion of fluid phase [35],

$$\frac{\partial(\varepsilon_f \rho_f)}{\partial t} + (\nabla \cdot \varepsilon_f \rho_f \mathbf{u}_f) = 0 \tag{1}$$

$$\frac{D(\varepsilon_f \rho_f \mathbf{u}_f)}{Dt} = \nabla \cdot \bar{\bar{S}}_f + \varepsilon_f \rho_f \mathbf{g} - \mathbf{I} \tag{2}$$

where ε_f is the volume fraction of fluid, ρ_f is the density of the fluid, $\mathbf{u}_f$ is the velocity of the fluid, and $\mathbf{I}$ is the drag source term. $\bar{\bar{S}}_f$ is the fluid phase stress tensor given by

$$\bar{\bar{S}}_f = -P_f \bar{\bar{I}} + \bar{\bar{\tau}}_f \tag{3}$$

where P_f is the fluid phase pressure and $\bar{\bar{\tau}}_f$ is the fluid phase shear stress tensor

$$\bar{\bar{\tau}}_f = 2\mu_f \bar{\bar{D}}_f + \lambda_f \nabla \cdot tr(\bar{\bar{D}}_f)\bar{\bar{I}} \tag{4}$$

$$\bar{\bar{D}}_f = \frac{1}{2}\left[\nabla \mathbf{u}_f + (\nabla \mathbf{u}_f)^T\right] \tag{5}$$

where $\bar{\bar{D}}_f$ is the strain rate tensor. μ_f and λ_f are the fluid dynamic and bulk viscosities.

The inter-phase momentum transfer term on fluid cell c can be calculated as

$$\mathbf{I}^c = \frac{1}{v_c}\sum_{i=1}^{N_p} \frac{1}{6}\pi d_p^3 W_p \left(\nabla P_f(\mathbf{x}^i) + \frac{\beta^i}{1-\varepsilon_f}(\mathbf{v}_f(\mathbf{x}^i) - \mathbf{v}_p^i)\right) K(\mathbf{x}^i, \mathbf{x}_c) \tag{6}$$

where v_c is the volume of cell c and N_p is number of particles influence cell c. W_p is statistic weight of particle p, β^i is drag coefficient of particle i in cell c. $\mathbf{v}_f(\mathbf{x}^i)$ is the fluid velocity interpolated at particle i and K is the interpolation weight of particle i to cell c. The divide particle volume method is used to interpolate data from particle to cell and vice-verse. The implementation details of this method can be found elsewhere [36].

2.2. Drag models for gas-solids flow

In fluidization, the motion of a particle is mainly driven by the drag force countering a constant pull of the gravitational force. Thus, the calculation of this drag force is critical to accurately model the fluidization behavior. The current state of the art drag correlations can be divided into three categories: the empirical or semi-empirical-based models such as the Gidaspow drag model; the Direct Numerical Simulations-based correlations such as BVK drag model; and those including effects of unresolved mesoscale structures such as EMMS drag model. The first two categories are similar and represent homogeneous drag correlations. The third category includes the effect of heterogeneities such as small bubbles and clusters of particles. To quantitatively compare these three types of drag correlations, dimensionless drag forces are obtained as shown below: