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Numerical simulation of horizontal jet penetration using filtered fluid model in gas–solid fluidized bed

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The influence of horizontal jet on flow behavior of gas and FCC particles is predicted using a filtered two-fluid model proposed by Sundaresan's group in a cylindrical fluidized bed. The distributions of velocity and solid volume fraction along lateral direction are investigated by analyzing the transient simulation results at the different height of the fluidized bed. The jet penetration lengths of different jet velocities have been obtained and compared with published experimental data as well as with predictions of empirical correlations. The predicted air jet penetration length by several empirical correlations is discussed in the gas–solid bubbling fluidized bed. An agreement between the numerical simulation and experimental results has been achieved.

1. Introduction

Fluidized beds are widely applied in coal combustion and gasification, chemical and petrochemical industries because of the advantage of high mass and heat transfer coefficients. In fluidized bed reactors with chemical reactions, reactant gases are often introduced from lateral nozzles at a certain height above the distributor plate, for different purposes: to supplement the reactant, enhance mixing and control NO_x emission. Understanding the hydrodynamics of the gas and solids resulting from the introduction of gas jets is essential in improving reactor design and process optimization.

The effect of horizontal injection of gas into fluidized beds on flow behavior of gas and particles is widely investigated [1–3]. When gas with high velocity is injected into the fluidized bed from a horizontal nozzle, a permanent jet plume with bubbles will be formed in the bed. Chen and Weinstein [4] measured the penetration and shape formed by a horizontal jet in a rectangular fluidized bed. Measured results showed the horizontal jet formed three regions in the fluidized bed: a coherent void, i.e., the jet, bubble trains, and a surrounding compaction zone. Several correlations for predicting the penetration lengths of horizontal gas jets have been developed based on experimental data [5–9]. These studies show that the jet penetration length increases with increasing velocity of gas injection in gas–solid fluidized beds.

With the improvements in computational power, numerical modelling has become an attractive tool to model hydrodynamics in fluidized beds. Hong et al. [6] performed two dimensional simulations with an Eulerian–Eulerian model to study the formation of a jet through an inclined nozzle into a fluidized bed. Simulated jet penetration length was reported in agreement with their experimental measurements. Simulation of a single horizontal round gas jet issuing into a gas–solid fluidized bed of FCC particles was performed by Li et al. [10] using McKeen and Pugsley drag model [11] which is a non-uniform scale factor taking the effect of agglomerates on fine particles flow into account. The successful validation against experimental results demonstrates the validity of this scaled drag model in the simulation of an FCC fluidized bed. This indicates an adequate modeling of the unresolved part of the drag that is essential to predict the correct hydrodynamics of gas and particle in the fluidized beds. Wang et al. proposed the cluster structure-dependent (CSD) drag coefficient model based on the minimization of energy dissipation by heterogeneous drag [12]. The model describes the basic physical mechanisms in the interactions between the gas and solid phases. The model predicts the cluster effect by analyzing the local heterogeneous flow field. The energy minimization multiscale approach (EMMS) developed by Li et al. [13,14] was used to predict flow behavior of particles in fluidized beds. The EMMS model assumes that the heterogeneous gas–solid system is composed of three homogeneous sub-systems: dense phase, dilute phase and interphase. The clusters of dense phase and the dispersed particles of dilute phase consist themselves of homogeneously distributed particles enabling the application of a homogenous drag correlation to these structures. Zhou and Wang proposed the modified EMMS-based two-

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fluid model [15], where the particle-rich dense phase and gas-rich dilute phase were treated as the two interpenetrating continua, and were used to simulate the hydrodynamics of high-density CFB risers. An effective drag correlation accounting for unresolved scales was proposed by Schneiderbauer et al. [16] based on the assumption of the formation of subgrid heterogeneities inside fluidized beds. They assumed that the solid volume within the dilute phase is negligibly small leading to a closed set of equation for the heterogeneity index. However, in the models mentioned above the effect of heterogenous structures on solid viscosity and particle pressure is not considered in the gas–solid two-fluid model of fluidized beds. On the other hand, Ozel et al. proposed an appropriate modelling approach accounting for the influence of unresolved structures [17]. The sub-grid drift velocity is taken into account for obtaining the correct drag. The filtering meso-scale structures yield to sub-grid scale (SGS) stress tensors which increase the effective viscosity and normal stresses of the particulate phase. Simulations indicate that the grid resolution may be necessary to fully demonstrate the accuracy of two-fluid model in predicting gas–solids flows because the coarse grid simulation without considering the effect of unresolved sub-grid scale structure results in a qualitatively incorrect conclusion.

The groups of Sundaresan derived filtered drag, solid pressure and viscosity correlations from filtering highly resolved simulations. Igci and Sundaresan argued that neglecting their unresolved contribution produces quantitative changes in the predicted results in fluidized beds [18]. They pointed out a contribution to the solid stresses arising from subgrid-scale Reynolds-stress-like velocity fluctuations, which appear to be much larger than the particle stresses from kinetic theory [19]. Recently, it has been shown that the filtered two-fluid model simulations are able to predict the Reynolds-stress-like velocity fluctuations appropriately. The study of Milioli et al. reveals that these fluctuations follow a Smagorinsky-like sub-grid scale model [20]. The objective of this study is to simulate the horizontal gas injection into a fluidized bed of FCC particles using filtered two-fluid model proposed by Sundaresan's group. Different jet velocities have been simulated and the results of these simulations are validated against the available experimental data.

2. Filtered gas-particles two-fluid model equations

In general, the two-fluid model (TFM) equations for gas and particles phases are derived by translating the Newton's equation of motion for a single particle directly into continuum equations representing the momentum balances for the solid phase. Keep in mind that this gas–solid two-fluid model is derived from data of nearly homogeneous systems as the microscopic two-fluid model equations coupled with constitutive relations. However, gas-particles flow in riser reactors that are inherently unstable, and manifest inhomogeneous structures over a wide range of length and time scales. Thus, if one sets out to solve the microscopic two-fluid model equations, the fine grid is used to resolve the unresolved small-scale spatial structure. To resolve inhomogeneous structures, the filtered two-fluid model is needed to account for the effects of unresolved scale structure through residual correlations appearing in the filtered models. The filtered two-fluid model equations are obtained by performing a spatial average of the microscopic two-fluid model equations [18,20]. As a result of the filtering procedure, the effect of the fine-scale gas-particle flow structure occurring on length scales smaller than the filter size is captured through residual terms that must be constituted from theoretical considerations or from filtering the results of fine-grid two-fluid model simulations. Filtered models have been shown to yield quantitatively similar macroscopic behavior to that observed in fine-grid simulations of the same [21].

The two-fluid model consists of balance equations for mass and momentum of gas phase and particle phase. The filtered continuity balances of gas phase and particle phase without chemical reactions proposed by Igci et al. are

$$\frac{\partial}{\partial t}\left(\overline{\varepsilon}_g\rho_g\right)+\nabla\cdot\left(\overline{\varepsilon}_g\rho_g\overline{\mathbf{u}}_g\right)=0 \tag{1}$$

$$\frac{\partial}{\partial t}\left(\overline{\varepsilon}_s\rho_s\right)+\nabla\cdot\left(\overline{\varepsilon}_s\rho_s\overline{\mathbf{u}}_s\right)=0 \tag{2}$$

where ρ_s and ρ_g denote the densities of particles and gas phase. $\overline{\mathbf{u}}_s$ and $\overline{\mathbf{u}}_g$ are the filtered velocity of particles and gas phase. $\overline{\varepsilon}_s$ and $\overline{\varepsilon}_g$ are the filtered volume fractions of particles and gas phases (which add up to unity).

The momentum balances of gas phase and particle phase without chemical reactions proposed by Igci et al. are

$$\frac{\partial}{\partial t}\left(\overline{\varepsilon}_g\rho_g\overline{\mathbf{u}}_g\right)+\nabla\cdot\left(\overline{\varepsilon}_g\rho_g\overline{\mathbf{u}}_g\overline{\mathbf{u}}_g\right)=-\overline{\varepsilon}_g\nabla\overline{p}_g+\nabla\cdot\overline{\boldsymbol{\tau}}_g+\overline{\varepsilon}_g\rho_g\mathbf{g}+\overline{\beta}_{gs}\left(\overline{\mathbf{u}}_s-\overline{\mathbf{u}}_g\right) \tag{3}$$

$$\frac{\partial}{\partial t}\left(\overline{\varepsilon}_s\rho_s\overline{\mathbf{u}}_s\right)+\nabla\cdot\left(\overline{\varepsilon}_s\rho_s\overline{\mathbf{u}}_s\overline{\mathbf{u}}_s\right)=-\overline{\varepsilon}_s\nabla\overline{p}_g+\nabla\overline{p}_s+\nabla\cdot\overline{\boldsymbol{\tau}}_s+\overline{\varepsilon}_s\rho_s\mathbf{g}+\overline{\beta}_{gs}\left(\overline{\mathbf{u}}_g-\overline{\mathbf{u}}_s\right) \tag{4}$$

where $\mathbf{g}$ is the gravitational acceleration, and $\overline{\beta}_{gs}$ is the filtered drag coefficient. $\overline{\boldsymbol{\tau}}_s$ and $\overline{\boldsymbol{\tau}}_g$ are the stress tensors of particles and gas phase. The stress tensor of gas phase is calculated by a Newtonian-type approximation with a constant viscosity. For particle phase, the stress tensor is expressed as a function of filtered viscosity as follows

$$\overline{\boldsymbol{\tau}}_s=\overline{\mu}_s\left\{\left[\nabla\overline{\mathbf{u}}_{ss}+\left(\nabla\overline{\mathbf{u}}_s\right)^{\mathrm{T}}\right]-\frac{1}{3}\left(\nabla\cdot\overline{\mathbf{u}}_{ss}\right)\mathbf{I}\right\}. \tag{5}$$

The filtered viscosity of particle phase is

$$\frac{\overline{\mu}_s g}{\rho_s v_t^3}=\begin{cases}\dfrac{\overline{\mu}_{kin}g}{\rho_s v_t^3}+F_\mu\left(\overline{\varepsilon}_s-0.59\right)\left(-1.22\overline{\varepsilon}_s-0.7\overline{\varepsilon}_s^2-2\overline{\varepsilon}_s^3\right), & \overline{\varepsilon}_s\le 0.59\\ \dfrac{\overline{\mu}_{kin}g}{\rho_s v_t^3}, & \overline{\varepsilon}_s>0.59\end{cases} \tag{6}$$

$$F_\mu=0.37\left(Fr_f^{\;-1.22}\right)\left(0.28Fr_f^{\;-0.43}+1\right)^{-1}\text{and } Fr_f^{-1}=g\Delta_f/v_t^2 \tag{7}$$

where v_t is the terminal velocity of particles and $\triangle_f$ is the filtered size. The kinetic model term is

$$\frac{\overline{\mu}_{kin}g}{\rho_s v_t^3}=\begin{cases}1720\overline{\varepsilon}_s^4-215\overline{\varepsilon}_s^3+9.81\overline{\varepsilon}_s^2-0.207\overline{\varepsilon}_s+0.00254, & \overline{\varepsilon}_s\le 0.0200\\ 2.72\overline{\varepsilon}_s^4-1.55\overline{\varepsilon}_s^3+0.329\overline{\varepsilon}_s^2-0.0296\overline{\varepsilon}_s+0.00136, & 0.0200<\overline{\varepsilon}_s\le 0.2\\ -0.0128\overline{\varepsilon}_s^3+0.0107\overline{\varepsilon}_s^2-0.0005\overline{\varepsilon}_s+0.000335, & 0.200<\overline{\varepsilon}_s\le 0.6095\\ -23.6\overline{\varepsilon}_s^2+28.0\overline{\varepsilon}_s+8.3, & \overline{\varepsilon}_s>0.6095\end{cases}. \tag{8}$$

The filtered solid pressure is a function of filtered solid volume fraction, and expressed by

$$\frac{\overline{p}_s}{\rho_s v_t^2}=\begin{cases}\dfrac{\overline{p}_{kin}}{\rho_s v_t^2}+F_p\left(\overline{\varepsilon}_s-0.59\right)\left(-1.69\overline{\varepsilon}_s-4.16\overline{\varepsilon}_s^2+11\overline{\varepsilon}_s^3\right), & \overline{\varepsilon}_s\le 0.59\\ \dfrac{\overline{p}_{kin}}{\rho_s v_t^2}, & \overline{\varepsilon}_s>0.59\end{cases} \tag{9}$$

$$F_p=0.48\left(Fr_f^{\;-0.86}\right)\left(1-\exp\left(-\frac{Fr_f^{\;-1}}{1.4}\right)\right) \tag{10}$$

where the kinetic model term is

$$\frac{\overline{p}_{kin}}{\rho_s v_t^2}=\begin{cases}-10.4\overline{\varepsilon}_s^2+0.310\overline{\varepsilon}_s, & \overline{\varepsilon}_s\le 0.0131\\ -0.185\overline{\varepsilon}_s^3+0.066\overline{\varepsilon}_s^2-0.000183\overline{\varepsilon}_s+0.00232, & 0.0131<\overline{\varepsilon}_s\le 0.290\\ -0.00978\overline{\varepsilon}_s+0.00615, & 0.29<\overline{\varepsilon}_s\le 0.595\\ -6.62\overline{\varepsilon}_s^3+49.5\overline{\varepsilon}_s^2-50.3\overline{\varepsilon}_s+13.8, & \overline{\varepsilon}_s>0.595\end{cases}. \tag{11}$$

Note that we do not consider bulk viscosity in the filtered model. Parmentier et al. [22] argued that the filtered stress corrections are