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Fine-grid two-fluid modeling of fluidization of Geldart A particles

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ABSTRACT

A series of fine-grid simulation with two-fluid model (TFM) is performed for bubbling, turbulent and circulating fluidized beds (CFB) with Geldart A particles. The results show that the fine-grid TFM with homogeneous drag seems feasible for simulation of low-velocity, bubbling fluidized beds. However, the fidelity of fine-grid TFM declines with the increase of gas velocity. In particular, the solids flux predicted deviates much from the experimental data of CFB though the clustering phenomenon can be captured with refinement of grid. In contrast, the structure-dependent approach as exemplified by the energy-minimization multi-scale (EMMS)-based multi-fluid model gives better agreement with experimental data. This discrepancy raises the question of the applicability of the local equilibrium assumption underlying the TFM. It also sheds light to the necessity of meso-scale modeling and the critical role of solids flux to evaluate the simulation of CFB.

1. Introduction

The two-fluid model (TFM) has been widely used for simulation of gas–solid fluidization. In the TFM, the collective behavior of solid particles is simplified with a pseudo-fluid, whose strain–stress relation can be closed with constitutive models such as the kinetic theory of granular flow (KTGF) [1]. As to the interphase drag force, several classic correlations have been widely cited in literature. These correlations are normally derived from experimental data based on fixed beds, homogeneous fluidization or sedimentation, including, e.g., Ergun [2], Richardson and Zaki [3] and Wen and Yu [4].

In its early stage of development, the TFM was applied mainly to simulate bubbling fluidization and dilute pneumatic transport [5–7]. When a dense circulating fluidized bed riser is simulated, however, the situation is quite different, as the high-velocity, dense gas–solids flow is characterized by heterogeneous, dynamic clusters on the meso-scale [8,9], and these meso-scale structures can be smaller than the grid size used in computational fluid dynamics (CFD) simulations [10]. Li and Kwauk [8] indicated that the effects of these unresolved, meso-scale structures are remarkable, resulting in several orders of magnitude difference in drag and mass transfer coefficients, and hence "combination of the EMMS model and the pseudo-fluid model may yield a comprehensive understanding of both the heterogeneous structure and the time-dependent behavior of particle-fluid two-phase flow". As a result, the meso-scale modeling became a hot issue of CFD for fluidized bed simulation in recent years [11–21].

For simulation of bubbling fluidized beds, some argued if the grid is fine enough to the size of 10 times the particle diameter, then the conventional TFM with closures derived from homogeneous systems may well predict the flow behavior [11,22]. Cloete et al. [23] found that the aspect ratio of grid should be smaller than one and the second order implicit time stepping might be needed to reach grid independent solutions. Xie et al. [24,25] found that 2D and 3D simulations coincide with each other for bubbling fluidization of Geldart B particles, but deviation grows for turbulent fluidized bed even when the computational grid is fine enough to reach its grid-independent solution. Lu et al. [26] indicated that the effects of meso-scale structure decay with increasing particle diameter, or, the Archimedes number, so, it is easier to reach grid-independent solution for low-velocity, coarse particle fluidization.

As to circulating fluidized bed (CFB), Zhang and VanderHeyden [27] performed high-resolution, 3D simulations of a riser containing Geldart B particles and found that the fine-grid results coincide with the experimental data. However, Gidaspow et al. [28] argued that their dilute flow conditions shed no light on the behavior of a real CFB. In their simulation of circulating fluidized beds, Li et al. [29] showed that the grid convergence depends on the flow field variables chosen for verification but no general rule for grid size is available to guarantee the grid-independent results for axial pressure gradient. In addition, the inlet and outlet configuration was found to have significant impacts on the grid convergence in their 2D simulations whereas the 3D simulations were found to have better grid convergence and quantitative prediction. Cloete et al. [30] and Li et al. [31] also suggested 3D simulation for quantitative prediction of bubbling fluidized beds.

In fact, dispute exists as to whether the fine-grid TFM simulation is feasible to capture CFB flow behavior [17,26,32]. For the so-called fast

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fluidization with Geldart A particles, say, fluid catalytic cracking (FCC) catalyst, Lu et al. [33] pointed out that the fine-grid simulation may improve the results but it is not sufficient to predict correctly the solids flux. Following the work of Lu et al. [33], Benyahia [34] refined the grid size further to 1 mm (about 18 times the particle diameter) and found that the refinement of grid helps to predict the S-shaped axial profile, though the predicted solids flux is still much higher than experimental data. Syamlal and Pannala [32] pointed out that it is possible that there are sub-grid structures that cannot be captured even with high resolution simulations. Obviously, such dispute concerns the basis for two-fluid modeling of a fluidized bed, and its clarification deserves more efforts.

In this article, we will try to give a comprehensive evaluation of the fine-grid two-fluid modeling of gas fluidized beds over a wide range of flow regimes. The particle property discussed here is restricted into Geldart A [35], though more precise description should be defined with Archimedes number [36,37]. 3D TFM simulation is believed to have better quantitative prediction, whereas direct use of it with fine-grid resolution is computationally demanding. As a substitute, we will perform 3D, coarse grid simulations with sub-grid closure laws derived either from fine-grid two-fluid modeling or the energy-minimization multi-scale (EMMS) model [8]. Comparison to experimental data is provided and the effects of the inlet/outlet and boundary conditions are also discussed.

2. Fine-grid TFM simulation without sub-grid modeling

Four lab-scale systems were selected in the following simulations. High-resolution schemes were used only for 2D cases. Fig. 1 shows the 2D geometries of the relevant fluidized beds. The bubbling fluidized bed of Mckeen and Pugsley [38] is 1.0 m in height and 0.14 m in inner diameter. Its initial height of bed material is 0.5 m with solids packing fraction of $\varepsilon_s = 0.55$. For the turbulent fluidized bed of Venderbosch [39], it is 0.75 m in height and 0.05 m in inner diameter. The initial height of bed material is 0.2 m with solids packing fraction of $\varepsilon_s = 0.5625$. For the circulating fluidized bed of Horio et al. [40], the riser is 2.79 m in height and 0.05 m in diameter. Initially, the particles are uniformly distributed across the riser with $\varepsilon_s = 0.086$. For the circulating fluidized bed of Li and Kwauk [8], the riser is 10.5 m in height and 0.09 m in diameter. Initially, the particles are uniformly distributed across the riser with $\varepsilon_s = 0.09$.

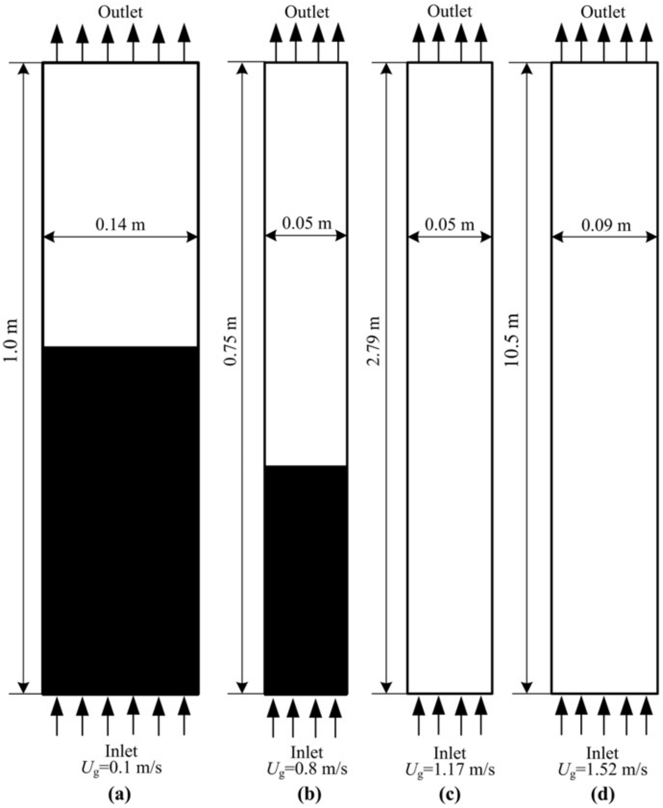

Fig. 1. Schematic 2D geometries of four fluidized beds: (a) bubbling fluidized bed of Mckeen and Pugsley [38], (b) turbulent fluidized bed of Venderbosch [39], (c) circulating fluidized bed of Horio et al. [40] and (d) circulating fluidized bed of Li and Kwauk [8].

2.1. Numerical settings

The Eulerian multiphase flow model, or, the two-fluid model, of FLUENT® 6.3.26 was used in fine-grid simulations. The solids stress was closed with the algebraic form instead of the partial differential equation (PDE) formulation of the kinetic theory of granular flow (KTGF). Such an approximation is helpful to save run time and allows reasonable agreement with experimental results of bubbling fluidized bed[41]. The algebraic formulation of KTGF has also been applied in our simulations of circulating fluidized beds[33,42]. Compared to the full PDE formulation, we found it enables better numerical convergence in particular with fine grid resolution and reasonable agreement with experimental data. A combination of Wen and Yu [4] and Ergun [2] correlations was used to close the drag coefficient [1]. For all the four cases, the gas was assumed to flow uniformly into the bottom inlet and leave from the top outlet, where the atmospheric pressure boundary was prescribed. The initial velocities of the gas and solids inside the beds were assumed to be zero. To ensure constant solids inventory inside the bed, the entrained solids were recirculated into the solid inlet. The no-slip boundary condition was prescribed for the gas phase, whereas the partial-slip boundary condition developed by Johnson and Jackson [43] was used for the solid phase. The values for the restitution coefficient and specularity coefficient were chosen in line with the relevant literature [44–46]. Simulations were first performed for 10 s, and then the time-averaged analysis was carried out for another period of 10 s. Different grid resolutions were tested for each fluidized bed while the highest resolutions for the three cases in Fig. 1(a), (b) and (c) used grid size smaller than 10 times the particle diameter, which is widely recommended as the criterion for reaching grid-independent prediction [11,22]. In the last case of Li and Kwauk [8], the finest grid size is about 20 times the particle diameter due to limitation of computing cost and difficulty in convergence. The turbulence is not included in this work, as it is widely believed to be of minor importance compared to the drag and gravity for such dense gas–solids flow in fluidized beds [6,11,33,47]. Table 1 summarizes the relevant parameters and simulation settings. It should be noted that all these cases were limited to particles of Geldart group A, for which the effects of meso-scale structure are significant. For coarser particles, or rather, larger Archimedes number, the clustering effects are of minor importance [26].

2.2. Results and discussion

2.2.1. Bubbling fluidized bed

Fig. 2 gives snapshots of the distribution of solids volume fraction in the bubbling fluidized bed under different grid resolutions. In general, more resolved flow structure and lower bed expansion are captured with smaller grid size. As the uniform gas inlet is used at the bottom to simulate the perforated air distributor, irregular voids instead of spherical bubbles are found being dispersed in the emulsion phase. In our experience, such simplified inlet will not affect the prediction of bed expansion, which is of our major concern for quantitative comparison in following discussions.

Fig. 3 shows the effect of grid size on the time-averaged solids distribution and axial profiles. The bed expansion height decreases gradually with increasing grid resolution and approaches the experimental data (about 0.6 m). From the results with grid sizes of 0.75 mm and