R&D NOTES

Fine-Grid Simulations of Gas-Solids Flow in a Circulating Fluidized Bed

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DOI 10.1002/aic.13826
Published online May 11, 2012 in Wiley Online Library (wileyonlinelibrary.com).

Keywords: circulating fluidized beds, computation fluid dynamics (CFD), fluidization, multiphase flow, particle technology

Introduction

This research note demonstrates that more accurate predictions of a two-fluid model for the riser section of a circulating fluidized bed are obtained as the grid size is equally refined along all the directions of the gas-particle flow. However, two-fluid simulations of large-scale fluidized beds with such a fine mesh are currently computationally prohibitive. Alternatively, subgrid models can significantly reduce the simulation time of multiphase flow by using coarse mesh, whereas maintaining a high level of accuracy.

Fine heterogeneous structures in the form of clusters and streamers are known to increase the slip velocity in gas-driven flows of small particles.[1] Studies have shown that accurate prediction of solids segregation and flux profiles,[2] as well as axial pressure gradient profiles[3] in circulating fluidized beds with coarse-grid simulations require the inclusion of subgrid scale closures.

Fine-grid simulations of a small-scale bubbling fluidized bed of Geldart type A powder showed that a grid size in the order of few particle-diameters is essential to predict the correct bed expansion due to the formation of small bubbles that were not resolved with coarse-grid simulations.[4] In addition, refined two-fluid simulations of gas–solids flows in a small-scale hypothetical riser were shown to yield essentially the same results as those obtained with coarse-grid simulations using a subgrid model.[5] In that study, wall corrections to the subgrid model obtained in the fine-grid simulations were included in the coarse simulation.

This study demonstrates that two-fluid models can capture basic experimental observations without any subgrid corrections. In particular, grid refined computations are conducted on a much larger riser section of a circulating fluidized bed[3,6] to demonstrate accurate predictions of continuum (two-fluid) models with respect to gas pressure drop and solids holdup measurements. A previous claim in the literature by Lu et al.[6] that two-fluid models cannot capture these basic experimental observations was found in this study to be probably due to insufficient grid resolution along the vertical flow direction.

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The simulations in this effort use a standard homogeneous drag law without any subgrid corrections. Simulations using three different grid resolutions are investigated. The most refined mesh employs approximately one million computational cells, translating into a grid size of 1 mm with a grid-size ratio of one. The results clearly show improvement in the two-fluid model predictions of the gas pressure drop vertical profiles with grid refinement. A major hurdle in conducting these large-scale transient simulations is the requirement for long-time-averaged numerical data to compare with experimental measurements.

Description of physical and numerical parameters

The two-fluid model based on granular kinetic theory and the well-known Wen and Yu drag correlation has been described in detail in a previous publication[3] and is not repeated here for brevity. The geometry of the riser section of a circulating fluidized bed with a constant particle inventory, which is simulated here, has also been described in previous studies.[3,6] The mass of small catalyst particles (Geldart type A particles) used in this study remained constant because the solids exiting the two side-outlets at the top of the riser are recycled through the two side-inlets (see Benyahia[3] for more information).

The Multiphase Flow with Interphase eXchanges Computational Fluid Dynamics (MFIX CFD) code (https://mfix.netl.doe.gov) is used to discretize the governing equations with the finite volume technique, and solves these equations on a staggered grid using a second-order discretization scheme.[3] Three grid sizes were used to discretize the 0.09-m wide by 10.5-m high geometry of the riser. The results of the coarse-grid of 60×450 simulations were obtained in our previous study.[3] The medium-grid of $60 \times 4{,}500$ and the fine-grid of $90 \times 10{,}500$ simulations were conducted as part of this study. Thus, the fine-grid simulation consists of a grid size of 1 mm or about 18 particle-diameters. This fine-resolution simulation required a very small time-step of the order of 10^{-5}s to converge, and a 1 s of simulation time required about 9 days of wall-clock time on 24 Intel Xeon 2.83 GHz processors. In addition to requiring large CPU times, the fine resolution simulation had some convergence problems. The issue was tracked to severe gas back-flow at the two-side pressure outlets. More specifically, as the grid is refined some computational cells in the pressure-outlet exhibit large-gas velocity

Figure 1. Time-averaged (20-25 s) solids-volume fraction contour profiles in the 2-D riser geometry (not to scale), where blue and red indicate dilute and dense (30% and higher) flow regions, respectively.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

entering the domain, which subsequently prevented the simulation from converging. Traditionally, this issue is resolved by extending the geometry of the pressure outlet so that a fully-developed flow is obtained. However, this is an expensive solution for such a fine grid. Instead, a cheaper solution was adopted wherein the size of the outlets was temporarily reduced by 35%. Note that even with the size reduction the area of the two pressure outlets is still double that of the riser, ensuring that the flow does not accelerate near the outlet. Once the gas back-flow diminished, which usually took no more than 0.01 s, the geometry of the pressure outlet patches were returned to their original size. This issue occurred several times during a simulation and each instance was addressed as described. The simulations were run for 10 s, after which data was collected for time-averaging at a rate of 100 Hz for 20 to 25 additional seconds.

Results and Discussion

Time-averaged results of solids-volume fraction profiles in the riser are presented in Figure 1 for the three computational grid densities examined. The results of the coarsest mesh size show a homogeneous flow along the height of the riser without any distinct structures except at the bottom section where solids are fed through the two side-inlets. This homogeneous flow results in the transport of large amounts of solids that is continuously recycled at the two side inlets. An order of magnitude increase in the grid density along the height of the riser (60 $\times$ 4,500) reveals distinct structures not previously seen with the coarse grid. As the grid is refined a core-annulus flow regime becomes apparent where higher solids concentration occurs near the walls and more dilute flow occurs at the core of the riser. This behavior is especially apparent at the mid-bottom section of the riser. With the finest grid size of 1 mm, corresponding to a grid density of 90 $\times$ 10,500, the core-annulus flow regime is apparent throughout the riser height. Accordingly, a more dilute flow is revealed at the top section of the riser. From a qualitative point of view, this flow regime is expected under these conditions and has been widely reported in the literature.[7]

The quantitative results of time-averaged solids circulation rate taken at the outlet (or inlet) of the riser are presented in Table 1. A large circulation rate, or solids mass flux, compared to the experimentally measured values is computed with the coarse and medium mesh sizes used in this study. Lu et al.[6] used similar mesh sizes and concluded that the two-fluid model fails to predict the experimentally measured solids circulation rates. In this study, however, the grid is refined a step further. Specifically, the simulation using a 1 mm grid size predicts a much lower solids-mass flux illustrating a clear improvement of the two-fluid model predictions with grid refinement. However, these results are still larger than the experimental measurements, indicating that further grid refinement may be necessary to achieve a grid-independent solution of the two-fluid model. This claim is not unreasonable given that a previous study[4] demonstrated that a grid size as small as few particle diameters was necessary to predict the correct bed expansion height in a small-scale bubbling fluidized bed.

Figure 2 shows the time-averaged void fraction deduced from computed gas pressure gradient (see Benyahia[3] for more details) for the three grid densities used in this study compared with the experimental measurements. As evident, a large solids holdup at the top section of the riser is computed with the coarsest mesh. In this region, a flat profile of solids holdup or pressure gradient is an indication of a ‘‘fully-developed’’ flow region. The predictions of large solids holdup with the coarsest mesh can easily be understood given the large solids-volume fraction computed throughout the riser (see Figure 1). As the grid is refined a lower solids holdup or pressure-gradient is computed in the upper flow region in better agreement with the experimental measurements. Here

Table 1. Solids-Mass Flux Predicted at Outlet of Riser for Different Grid Resolutions

Grid resolution	60×450	60×4500	90×10500	Experimental
Solids mass flux (kg/m^{2}s)	205	200	130	14.3

again, the conclusion of Lu et al.[6] that the two-fluid model fails to predict the characteristic S-shape of void fraction was misled by the fact that the authors did not refine the mesh sufficiently along the height of the riser (although they did refine the mesh along the width of the riser). With the finest mesh, not only is the fully-developed flow region better predicted, but the typical S-shape of pressure-gradient profile is in better agreement with the experimental measurements. Note that the fluctuations in the void fraction profiles can be reduced for the medium- and fine-grid densities at a significant cost of CPU time. So while further time-averaging of the numerical data may be necessary to obtain smoother curves it will not change the basic quality of the plotted profiles.

The time-averaged, horizontal profiles of solids-volume fraction and mass flux at the midsection of the riser are plotted in Figure 3. The predictions with the fine mesh exhibit the core-annulus flow regime with higher-solids concentrations near the wall region of the riser. However, the coarse grid predictions exhibit an opposite behavior with high-solids concentration at the core of the riser, which is qualitatively inaccurate from experimental data published in fluidization textbooks.[7,8] Note that direct comparison with experimental data was not possible as such information was not obtained. The solids mass flux predictions are also plotted in Figure 3. All resolutions show a large solids-mass flux at the core of the riser that becomes flatter in this flow region as the grid is resolved. The lower solids circulation rate obtained with the finest mesh (see Table 1) is due to the large downflow of solids near the walls of the riser (see Figure 3). This can be traced directly to the larger solids concentration in the annulus region of the riser as the grid is refined.

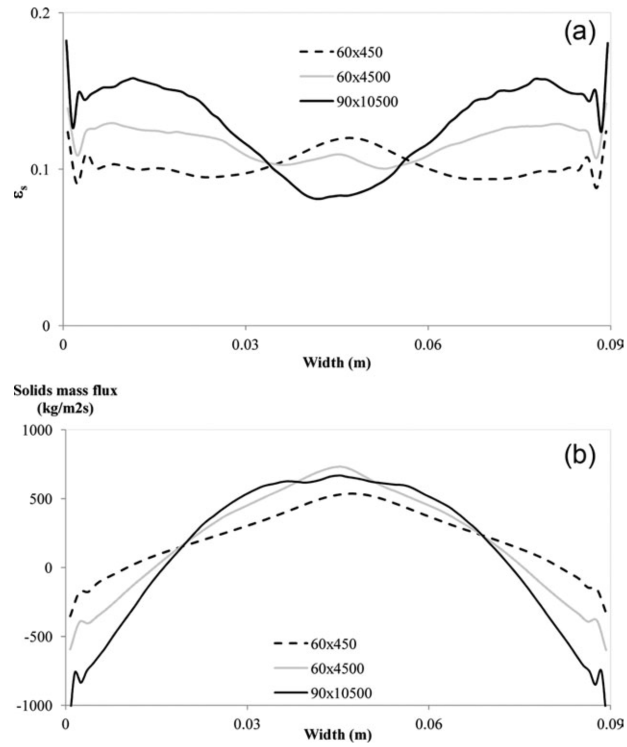

Figure 3. Time-averaged (10–30 s) solids-volume fraction and mass-flux profiles at the middle section (ca. 5.25 m above the gas distributor) of the riser for the three different grid resolutions used in this study.

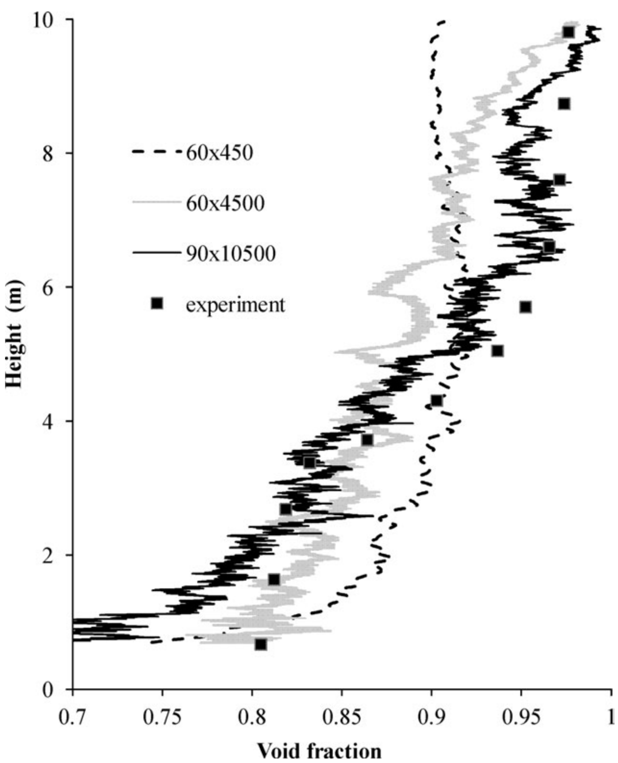

Figure 2. Time-averaged (10–30 s) void fraction vertical profiles (deduced from computed pressure gradient) obtained with three different grid resolutions and compared with experimental data.

Summary

This study demonstrates that more accurate predictions of the two-fluid model can be obtained in the riser section of a circulating fluidized bed as the grid is resolved. Insufficient grid resolution in the vertical direction of the riser was probably the cause of an opposite conclusion presented earlier in the literature.[6] Further grid resolution may be necessary to fully demonstrate the accuracy of two-fluid model in predicting gas–solids flows in the riser section of circulating beds. This work underscores the need to include subgrid corrections to predict the flows in large-scale reactors cheaply yet accurately.

Acknowledgment

The author gratefully appreciates the useful discussions and comments received from Janine Galvin (NETL, Albany) during the course of this study.

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Manuscript received Dec. 8, 2011, and final revision received Apr. 18, 2012.