Engineering Conferences International
ECI Digital Archives

10th International Conference on Circulating Fluidized Beds and Fluidization Technology - CFB-10

Refereed Proceedings

Spring 5-2-2011

Numerical Simulations of a Circulating Fluidized Bed with a Square Cross-Section

Tingwen Li
National Energy Technology Laboratory

S Pannala
Oak Ridge National Laboratory

C. Guenther
National Energy Technology Laboratory

NUMERICAL SIMULATIONS OF A CIRCULATING FLUIDIZED BED WITH A SQUARE CROSS-SECTION

Tingwen Li[1,2], Sreekanth Pannala[3], Chris Guenther[2]
1. URS Corporation, Morgantown, WV 26505, U.S.A.
2. National Energy Technology Laboratory, Morgantown, WV 26505, U.S.A.
3. Oak Ridge National Laboratory, Oak Ridge, TN 37831, U.S.A.

ABSTRACT

In this study, both 2D and 3D numerical simulations of a well-documented circulating fluidized bed with a square cross-section were conducted. With some assumptions, a series of 2D simulations was first carried out to study the influence of grid resolution, initial flow field, and boundary condition on the flow hydrodynamics. It was found that 2D simulations under-predicted the solids inventory even with the finest grid (10-particle-diameter grid size). On the other hand, a 3D simulation with relatively coarse grid was found in better agreement with the experimental data. Differences between 2D and 3D simulations were briefly discussed.

INTRODUCTION

Circulating fluidized beds (CFBs) have been widely utilized in a variety of industrial applications including coal combustion, gasification, fluid catalytic cracking, etc. To accomplish successful and reliable design and operation of CFBs, numerous investigations pertaining to different hydrodynamic aspects of CFBs have been undertaken over the past few decades e.g. (1, 2). Among various research tools, computational fluid dynamics (CFD) is playing an increasingly important role in studying the complex flow hydrodynamics in CFBs. Numerical simulation of gas-solids flow in CFBs, usually with two-fluid model (TFM) based on kinetic theory of granular flow, requires a very fine mesh (typically 10~100 particle diameters), and consequently, very small time steps (typically 0.1~1.0 milliseconds). However, due to the high computational cost of multiphase flow simulations of usually very long CFBs, such a high resolution simulation is prohibitive.

An appropriate simplification of the computational domain is necessary to achieve a good balance between speed and accuracy of the CFB simulations. Axi-symmetric assumption of the flow was employed mainly in the steady flow simulations as this assumption is likely to result in unphysical accumulation of particles along the axis in unsteady simulations (1). Alternatively, most unsteady numerical studies were carried out with a two-dimensional flow assumption in which a cut plane along the axis of a cylindrical column was simulated. Two-dimensional flow assumption is a rough assumption of the flow in a cylindrical column as the transient riser flow has significant angular movements despite its wide applications in the literature and successes in predicting certain flow hydrodynamics, for example, the core-annular pattern in riser flows. Undoubtedly, a 2D numerical simulation is not able to accurately account for the 3D effects resulting from geometry and operation. In addition, comparing ratios of wall area to column volume, 2D simulations inherently under-estimate the wall effects that are usually important in lab-scale riser flows. Hence, it is necessary to quantify the differences between 2D and 3D simulations in order to conduct efficient numerical modeling.

In this study, the gas-solids flow in a well-documented circulating fluidized bed of square cross-section has been simulated. The influences of initial conditions and grid resolution on 2D simulations were investigated mainly with respect to solids loading to seek a way to accelerate numerical modeling. After that, a 3D numerical simulation was conducted to evaluate the differences between 2D and 3D simulations.

NUMERICAL SIMULATION

Numerical Model

An open source software, Multiphase Flow with Interphase eXchanges (MFIX), was used to conduct the numerical simulations. In MFIX, a multi-fluid, Eulerian-Eulerian approach, with each phase treated as an interpenetrating continuum, was employed. Mass and momentum conservation equations were solved for the gas and solid (particulate) phases, with appropriate closure relations (3). Constitutive relations derived based on the granular kinetic theory were used for the solid phase. More information on MFIX as well as detailed documentation on the hydrodynamic model equations can be found in (4).

Simulation Setup

A cold-model CFB riser of 146×146 mm square cross-section and total height of 9.14 m was simulated. Sand of mean diameter 213 µm, particle density 2640 kg/m^3 and loosely packed bed void fraction of 0.43 was used as the bed material. In this study, a superficial gas velocity of 5.5 m/s and a solids circulating flux of 40 kg/m^{2}s were simulated. Detailed information on the experimental setup and measurements on void fraction and solids velocity profiles were provided in the literature (5, 6).

In this study, both 2D and 3D simulations as schematically shown in Figure 1 were conducted. The simple geometry of square riser was discretized by Cartesian grid with uniform grid size in each direction. Uniform inflow boundary conditions were imposed at the bottom gas distributor and the solids side inlet and a constant pressure at the outlet was imposed. A partial slip wall boundary condition was applied for the solids phase and a no-slip wall boundary condition was used for the gas phase.

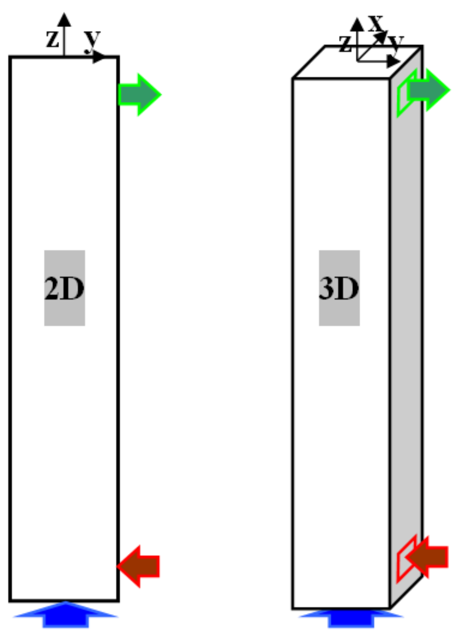

Figure 1. Schematic plots of 2D and 3D simulations.

RESULTS AND DISCUSSIONS

A series of 2D simulations is first presented to evaluate the effects of grid resolution and initial flow condition. This is followed by the 3D simulation and the differences between 2D and 3D numerical simulations are briefly discussed. Finally, comparisons between numerical results and experimental data are presented.

Grid Resolution

Different grid resolutions of 15×456, 30×456, 30×912, 60×912, 60×1824 and 60×3648 were tested in the 2D simulations. The finest grid resolution (dy≈dz≈2.5 mm) corresponds to 12-particle-diameter grid size which is very close to the 10-particle-diameter criterion for grid independence in gas-solids flow simulations (1, 7). The simulation has been typically performed for 100 seconds of real-time for most grid resolutions reported here. The solids inventory inside the system was monitored in form of the overall solids holdup to characterize the flow development as shown in Figure 2. It can be seen from the plot that solids loading decreases with time and finally reaches a near-stationary value indicating the fully developed state. The grid resolution affects the history of solids loading inside the riser at the initial stage but has no significant influence on the solids inventory after reaching the fully developed state except for the coarsest grid. Compared to an estimation of solids holdup, which is greater than 0.08, based on the experimental measurements of cross-sectional void fraction (5), the current 2D simulations substantially under-predict the solids inventory. It seems that the under-prediction cannot be overcome by decreasing grid size even to 10-particle-diameter, at least for the current case. Similar finding was reported by Lu et al. (8) in their 2D simulations of CFB riser with FCC particles although the grid sizes in their study were greatly larger than 10-particle-diameter. Consistent to their study, refinement of grid does affect the predicted transient flow behavior for example the spatial distribution of solids. The transient flow fields suggest that a finer grid tends to predict higher gradient of concentration and lower void fraction in the clusters.

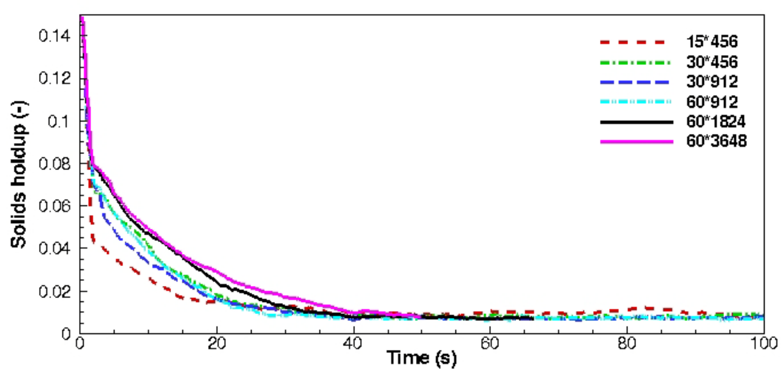

Figure 2. Temporal variation of the overall solids holdup predicted by the 2D simulations with different grid resolutions.

Initial Condition

For the cases shown above, a uniform solids concentration of 0.15 was assumed throughout the domain as the initial flow condition. It is expected that the initial flow condition has no influence on the final results when the flow is fully developed. However, it is still meaningful to evaluate if different initial conditions affect the duration for the flow to fully develop so that the computation time can be shortened. For this purpose, two additional cases with initial conditions of a partial filled packed bed with the same loading (solids holdup of 0.15) and a uniform solids concentration of 0.05 were conducted. Figure 3 presents the temporal variation of the overall solids holdup for cases with different initial conditions. As expected, the initial condition does not affect the solid inventory when the flow is fully developed. However, it does affect the time needed to reach the stationary state. These simulations indicate that it is helpful to set the solids loading closer to that at the developed state to decrease the simulation time and accelerate convergence through the initial transients. For real process simulations, this is possible since the solids inventory can be roughly estimated based upon the overall pressure drop.

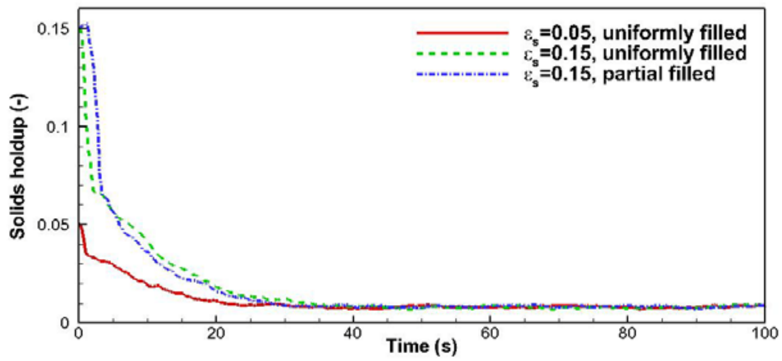

Figure 3. Temporal variation of the overall solids holdup for the cases with different initial flow conditions (grid resolution: 30×456).

Inflow Condition

The yz plane cutting along the side inlet and outlet was simulated in the 2D simulations. Constant solids feed rate at the side inlet was set based on the whole column cross-sectional solids flux reported in experiments. An alternate way was also evaluated to set the solids inflow rate based on the solids flux at the side inlet along the intersection of the yz plane. With this method, the solids circulating rate was higher than that based on the riser cross-section. For example, the resulting cross-sectional solids flux of 51 kg/m^{2}s was 25% higher than that of 40 kg/m^{2}s reported experimentally. As shown in Figure 4, the solids holdup at the fully developed state increases with the solids circulating rate. However, this adjustment of inflow condition in the 2D simulations cannot overcome the significant under-prediction of solids loading.

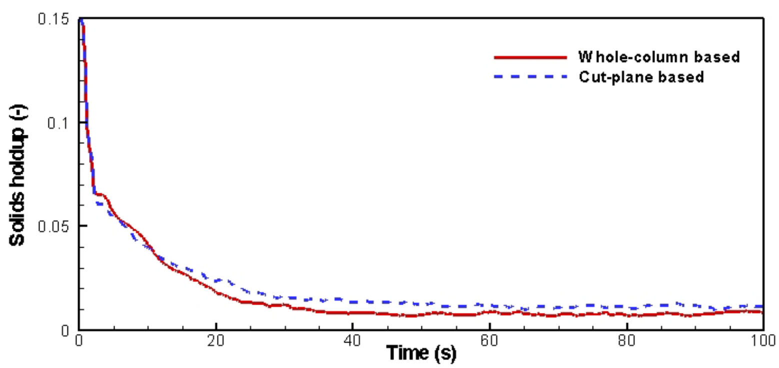

Figure 4. Time variations of the overall solids holdup for cases with different solids inflow rates based on column solids flux and side inlet flux (grid resolution: 30×456).

3D Simulation

A case with grid resolution of 30×30×456 is conducted for which 150 seconds simulation was completed to address the differences between 2D and 3D simulations. Temporal variation of the overall solids holdup predicted by both 2D and 3D simulations with comparable grid sizes is presented in Figure 5. There is a substantial difference between 2D and 3D simulations with respect to the solids loading. Differences in 2D and 3D simulations for both cylindrical and rectangular fluidized beds operated in bubbling, slugging, and turbulent fluidization regimes have been systematically discussed by Xie et al. (9, 10). Their results demonstrated that a 2D Cartesian simulation can be used to successfully study a bubbling fluidization regime close to U_{mf} (minimum fluidization velocity) but needs extra caution for modeling other fluidization regimes with higher gas velocity. The substantial differences presented here indicate that 3D simulation should be used for modeling CFBs. Of course, this inevitably leads to an extremely large number of computational cells for a grid-independent simulation. Due to the prohibitively expensive computational cost, not many 3D unsteady simulations of CFB riser flows were reported. To overcome high computational cost, a coarse grid three-dimensional numerical simulation with appropriate sub-grid closure models is necessary, which has been addressed by many researchers, e.g. (8, 11). Nevertheless, 2D simulations might be used as an effective tool to conduct qualitative study.

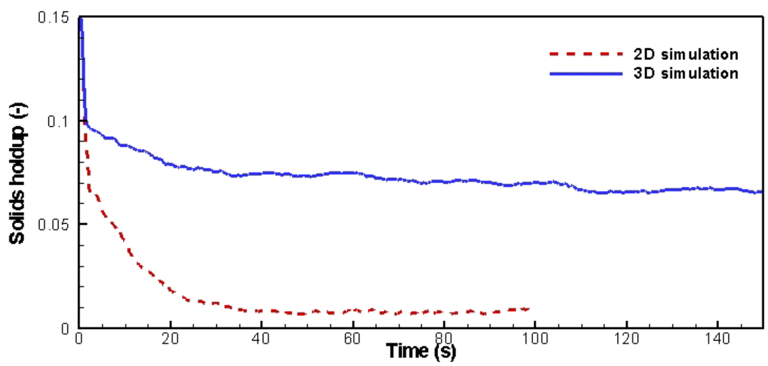

Figure 5. Time variations of the overall solids holdup predicted by 2D (30×456) and 3D (30×30×456) simulations.

Due to the computational cost of 3D simulation, no sensitivity study on the grid resolution and initial conditions was conducted so far. However, in future it might be helpful to conduct sensitivity studies on grid resolution, wall boundary conditions, and other physical and operational parameters in 3D unsteady simulations.

Comparison with Experimental Data

Figure 6 presents axial profiles of mean void fraction at different lateral positions predicted by the current numerical simulations when the flow is fully developed as well as the experimental data measured by a fiber optic probe (5). General profiles of low void fraction at the bottom of the riser and gradually increasing towards the top are predicted by the 3D simulation. However, the trend is not correctly predicted by the 2D simulation and the void fraction is substantially over-predicted almost everywhere. The results clearly indicate that 3D effects in a CFB riser are important in the case studied and assuming 2D flow can lead to under-prediction of solids inventory. Under-prediction of solids inventory with a fixed solids mass flux or over-prediction of solids flux with a fixed solids inventory has often been reported in the literature for 2D numerical simulations of CFB riser flows with fine FCC particles by using traditional inter-phase drag correlations. It is usually attributed to the unresolved meso-structure or clustering phenomena by insufficient grid resolution. The current results likely suggest that the three-dimensional effect is another reason for the discrepancies owing to the inherent differences between 2D and 3D simulations as stated before.

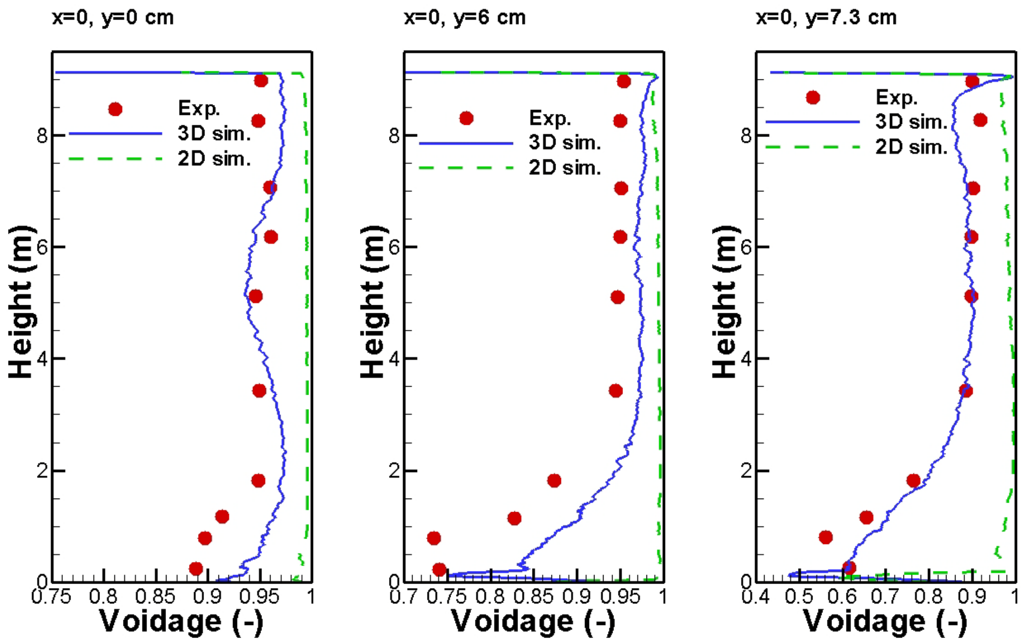

Figure 6. Axial profiles of mean voidage at different lateral positions.

Lateral profiles of mean void fraction at two heights are shown in Figure 7. Again, results of the 3D simulation shows better agreement with the experimental data than the 2D simulation. Offset of the void fraction maxima from the axis of the column is predicted. The asymmetric lateral distribution of void fraction caused by the side exit is reasonably captured. By examining the cross-sectional distribution of void fraction and solids velocity, a core-annulus flow structure is observed for this riser of square cross-section similar to risers of circular cross-section. Different lateral profiles of the mean vertical solids velocity at z=5.13 m above the distributor predicted by the numerical simulations are also compared to the experimental data in Figure 8. Numerical predictions are consistent with the experimental measurements, with most particles traveling downwards close to wall and upwards in the central region except that the rising velocity in the core region is under-predicted. Overall, the 3D numerical simulation shows reasonably good agreement with the experimental data.

Although the 3D simulation produces much improved results, there are some discrepancies in void fraction and velocity profiles between simulation and experiment. For example, good agreement is obtained for the axial voidage profiles near the wall, but relatively poor agreement is predicted along the central axis. One possible reason can be the coarse nature of the grid (much larger than the

10-particle-diameter thumb-rule for grid independence) and probably a sub-grid correction for the inter-phase drag is needed to account for clusters. Another possible reason is the simplification of solids inlet and outlet configurations. For instance, the effect of solid side inlet cannot be accurately modeled by the simple uniform inflow condition upon entering the system. Fluctuations in solids concentration and velocity at the inlet have been predicted by numerical simulations with a short L-valve (12). While, the simplification of the horizontal duct connecting the riser exit to cyclone into a simple pressure outlet is not capable of predicting the solids accumulation in the duct and its influence on the riser flow observed in the experiments. Closer agreement with the experimental data is expected if more accurate inlet and outlet conditions are assigned for the simulations.

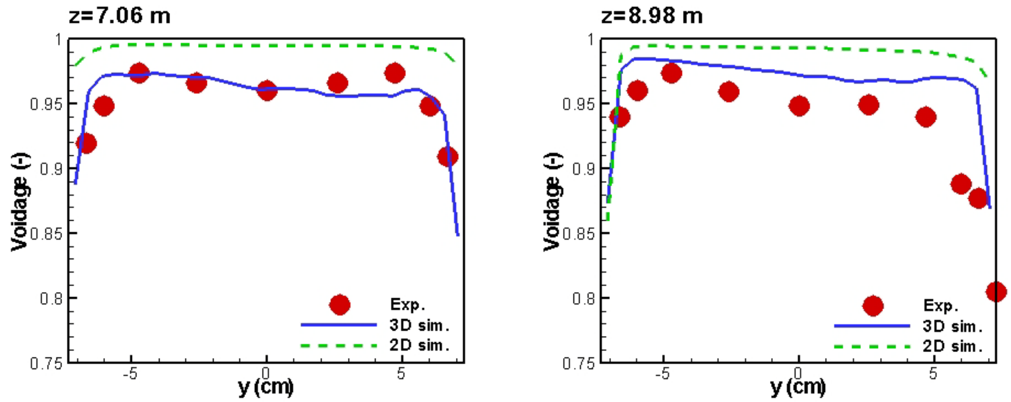

Figure 7. Lateral profiles of mean voidage at z=7.06, 8.98 m and x=0 cm.

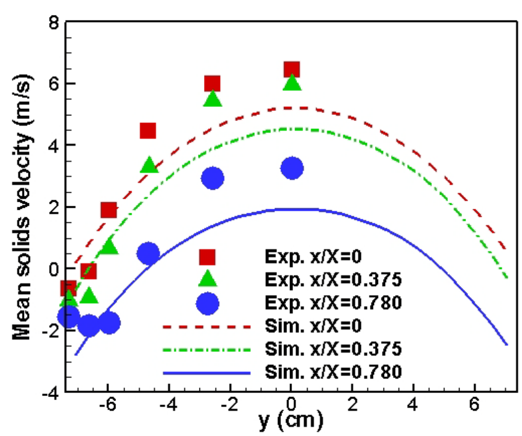

Figure 8. Lateral profiles of mean solids velocity at z=5.13 m.

CONCLUSIONS

In this study, both 2D and 3D numerical simulations of a well-documented circulating fluidized bed of square cross-section were conducted. Effects of grid resolution and initial flow condition were studied in 2D simulations. It was found that the time needed by numerical simulations to reach the stationary state can be reduced by carefully choosing the initial bed loading. However, it was demonstrated that the 2D simulations under-predicted the solids inventory even with very high grid resolution (~10-particle-diameter grid size). A 3D simulation predicted a considerably higher solids inventory compared to the 2D simulation. Profiles of void fraction and solids velocity predicted by the 3D simulation were in reasonable agreement with the experimental data. Clearly, three-dimensional simulations are required to accurately represent a circulating fluidized bed system, at least for the system simulated. With this in mind, some conclusions obtained through 2D simulations might need further verification in 3D simulations.

ACKNOWLEDGMENT

This research was sponsored by the Fossil Energy, U.S. Department of Energy. The work was partly performed at the Oak Ridge National Laboratory, which is managed by UT-Battelle, LLC under Contract No. DE-AC05-00OR22725. The authors thank Drs. Sofiane Benyahia, Tom O'Brien, and Madhava Syamlal at National Energy Technology Laboratory. This research was also supported in part by an appointment to the National Energy Technology Laboratory Research Participation Program, sponsored by the U.S. Department of Energy and administrated by the Oak Ridge Institute for Science and Education.

REFERENCES

1. Guenther, C.; Syamlal, M.; Shadle, L.; Ludlow, C. A numerical investigation of an industrial scale gas-solids CFB, Proceedings of the 7th International Conference on Circulating Fluidized Beds, Falls, Ontario, Canada, 2002.
2. De Wilde, J., G.B. Marin, and G.J. Heynderickx. The effects of abrupt T-outlets in a riser: 3D simulation using the kinetic theory of granular flow. Chemical Engineering Science 2003, 58: 877-885.
3. Syamlal, M., W. Rogers, and T. J. O'Brien. MFIX documentation: Theory guide. Morgantown, West Virginia, U.S. Department of Energy (DOE), Morgantown Energy Technology Center, 1993.
4. Benyahia, S., M. Syamlal, and T.J. O'Brien. Summary of MFIX Equations 2005-4. 2007.
5. Zhou, J., J.R. Grace, S. Qin, C.M.H. Brereton, C.J. Lim, and J. Zhu, Voidage profiles in a circulating fluidized bed of square cross-section, Chemical Engineering Science, 1994, 49: 3217-3226.
6. Zhou, J., J. R. Grace, C. J. Lim, and C. M. H. Brereton, Particle velocity profiles in a circulating fluidized bed riser of square cross-section, Chemical Engineering Science, 1995, 50: 237-244.
7. Andrews, A. T., P. N. Loezos, and S. Sundaresan. Coarse-grid simulation of gas-particle flows in vertical risers. Industrial & Engineering Chemistry Research, 2005, 44(16): 6022-6037.
8. Lu, B., W. Wang, and J. Li, Searching for a mesh-independent sub-grid model for CFD simulation of gas-solid riser flows. Chemical Engineering Science, 2009, 64: 3437-3447.
9. Xie N, Battaglia F, Pannala S. Effects of using two- versus three-dimensional computational modeling of fluidized beds: Part I, hydrodynamics. Powder Technology, 2008; 182:1-13.
10. Xie N, Battaglia F, Pannala S. Effects of using two- versus three-dimensional computational modeling of fluidized beds: Part II, budget analysis. Powder Technology, 2008; 182:14-24.
11. Igci, Y., A. T. Andrews, S. Sundaresan, S. Pannala, and T. O'Brien, Filtered tow-fluid models for fluidized gas-particle suspensions. AIChE Journal, 2008, 54: 1431-1448.
12. Li, T., J. Dietiker, and M. Shahnam, Numerical modeling of NETL challenge problem 3. Poster at CFB10, Oregon, USA, May 1-5, 2011.