

CFD simulations of gas-solid flows in a CFB riser: Effect of inlet boundary conditions

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Abstract: In this study, the effect of types of inlet and wall boundary conditions on the gas-solid flow fields in circulating fluidized bed risers was investigated using Eulerian-Eulerian simulations in both 2D and 3D domains. The 2D simulations were conducted using 3 different inlet configurations: (a) solids entering in radial direction from a two-sided inlet and gas entering axially from the bottom inlet, (b) solid entering axially from two-sided bottom inlet near the wall and gas entering axially from a bottom inlet at the centre, and (c) gas phase entering axially from two-sided bottom inlet near the wall and solids entering axially from a bottom inlet at the centre. From the 2D simulations, it was found that both the time-averaged axial velocity and solids volume fraction radial profiles were functions of the inlet kinetic energy profiles and gas-solid mixing patterns of each of the inlet configurations. Whilst 2D simulations using boundary conditions (a) and (c) showed significant deviations from experimental profiles, the boundary condition (b) as well as full-scale 3D simulations gave reasonable agreements with experimental observations.

Keywords: *Gas-solid flows, Circulating fluidised bed Riser, Eulerian-Eulerian, Boundary conditions*

1. INTRODUCTION

A circulating fluidized bed (CFB) reactor has many advantages over conventional chemical reactors due to its enhanced heat and mass transfer characteristics. For these reasons CFB reactors are widely applied in several unit operations such as fluid catalytic cracking, catalytic reforming, coal combustion and polymerization. The most important section of a CFB unit is the riser where chemical reactions take place, which may be either catalysed by the solids such as fluid catalytic cracking or occurring between the gas and fluidized solids such as combustion of pulverised coal. The gas-solid flow in the riser plays a dominant role in governing conversions of chemical reactions, and in turn performance of the CFB unit. Therefore, an in-depth understanding of the hydrodynamics of multiphase flow in riser is required to minimize any errors in designing and scaling-up of CFBs (Dudukovic, 2009). Recently, computational fluid dynamics has been extensively used to study the hydrodynamics of risers (Benyahia *et al.*, 2001; Vaishali *et al.*, 2007; Almuttahir and Taghipour, 2008). Typically, an Eulerian-Eulerian approach has been applied, with most previous studies assuming 2D domains of riser to make the simulation tasks computationally manageable.

Since a 2D domain cannot directly capture the asymmetric entry of solids to a continuously flowing riser, simulations in previous studies have been conducted using different types of boundary conditions for the inlets and outlets. For example, Pita and Sundaresan (Pita and Sundaresan, 1993) examined three different boundary conditions: (i) uniform, (ii) core-annulus flow, and (iii) circumferential injection of secondary gas at the inlet. They found that for the uniform and core-annulus cases the segregation of particles towards the wall caused widespread internal recirculation of solids and gas. For the circumferential injection of secondary gas, the authors noted that the segregation of particles towards the wall occurred more slowly and resulted in a substantial reduction in the recirculation of solids. Neri and Gidaspow (Neri and Gidaspow, 2000) used uniform and trapezoidal profiles of gas and solid velocities at the U-tube inlet which was smaller in diameter than the riser. They found that the simulations using trapezoidal inlet profiles predicted denser flows in both core and annular regions than those using the uniform profiles. Moreover, their results for both types of inlet boundary conditions only showed qualitative agreement with the experimental data. Benyahia *et al.* (Benyahia *et al.*, 2001) compared simulations with experimental measurements for both single one- and two-sided inlets. The simulations using the one-sided inlet predicted the gas to be flowing towards the opposite side of the solid inlet, which in turn created a non-symmetric radial distribution of solids throughout the full height of the riser. The core-annular flow regime, which has been widely observed experimentally (Knowlton *et al.*, 1995) was not produced in the simulations for the one-sided single inlet, but it did appear in the simulations for the two-sided inlet. Vaishali *et al.* (Vaishali *et al.*, 2007) also used a two-sided inlet in their riser simulations, which were in qualitative agreement with experimental data (Bhusarapu *et al.*, 2005) under dilute phase flow conditions. Almuttahir and Taghipour (Almuttahir and Taghipour, 2008) simulated a 2D geometry of the inlet section of a riser. They found that a core-annulus inlet having solids entering vertically upward along the walls and the air entering in the core of the riser gave reasonable qualitative and quantitative agreements between simulations and experimental measurements of solids volume fraction and radial profiles of solid velocities.

Proceeding discussion clearly indicates that there is a lack of agreement on type of boundary conditions in 2D domains, and more research is therefore required into the selection of inlet boundary conditions for riser simulations. In this study, three different types of boundary conditions in 2D simulations have been investigated and compared with the experimental results of Bhusarapu *et al.* (Bhusarapu *et al.*, 2005) as well as transient 3D simulations. The influence of both no- and partial-slip wall boundary conditions has also been investigated.

2. GAS-SOLID FLOW MODEL

Gas-solid flow models can be broadly classified into two approaches, namely Eulerian-Eulerian (EE) and Eulerian-Lagrangian (EL). Majority of CFB riser simulations have adopted the EE approach as it is more amenable to large-scale geometries having a high solid inventory. In the EE approach, both phases are treated as an interpenetrating continuum and the ensemble averaging of local instantaneous mass, momentum and energy balances for each phase are used in formulating the governing equations. Due to the continuum assumption the stress tensor for the solid phase is not explicitly defined and the kinetic theory of granular flow (Lun and Savage, 1984), which is based on the kinetic theory of gases, is applied to determine the motion of the particles. In adopting this approach the stress tensor requires additional closure for several other properties such as the granular viscosity, solid pressure, frictional viscosity and frictional pressure. The governing equations for both phases are coupled with the inter-phase exchange drag coefficient. A comparative study of the different solid phase closures is discussed in van Wachem *et al.* (Van Wachem *et al.*, 2001), following their recommendations the model equations used in this study.

3. SIMULATION APPROACH

The commercial CFD package FLUENT v 6.3 was used for transient CFD simulations. 2D simulations were conducted using a time step size of 0.0005 s which was found to be small enough for accurate 2D simulations in several previous studies (Benyahia *et al.*, 2001; Yang *et al.*, 2003; Vaishali *et al.*, 2007; Almuttahir and Taghipour, 2008). 3D simulations were conducted with time step of 0.0002 s considering their computational intensity and limitations of computational resources. It should be noted that a use of cluster of eight high speed computers took more than three weeks for each 3D simulation to complete. A second order discretisation scheme was used for the momentum equation and the QUICK scheme was applied for the volume fraction. The turbulence in the gas phase and its effect on the dispersed secondary phase was modelled using the standard k-ε model. The pressure-velocity coupling was resolved using the SIMPLE algorithm. The physical properties of the gas and solid phases are listed in Table 1. Also included in the table are the simulation parameters, which correspond to the experimental study of Bhusarapu *et al.* (Bhusarapu *et al.*, 2005).

Phase properties		Simulation parameters	
Gas phase	Air	Riser diameter	152 mm
Air density	1.12 kg/m ³	Riser height	7.9 m
Air viscosity	1.18e-05 kg/m.s	Inlet boundary	Velocity inlet
Air velocity	4.5 m/s	Outlet boundary	Pressure outlet
Solid phase	Glass beads	Discretisation	Second order
Particle diameter	150 μm	Turbulent model	k-ε model
Solid density	2550 kg/m ³	2D simulation	
Solid flux	37 kg/m ² s	Grid size	9.5 x 25 mm
Restitution factor		Time step	5 × 10 ⁻⁴ s
Particle-particle	0.95	C/s area of riser	1 × 0.152 m ²
Particle-wall	0.9	Mass flow rate of solids	5.624 kg/s
Max. packing limit	0.6	3D simulation	
		Time step	2 × 10 ⁻⁴ s
		C/s area of riser	0.01814 m ²
		Mass flow rate of solids	0.6714 kg/s

Simulations were conducted in both 2D and 3D domains of riser. The 3D simulations were performed using the cylindrical riser with actual dimensions in all three co-ordinates. In the 2D simulations, only a rectangular slice of the cylindrical riser was used with the conservation equations being solved in only two co-ordinates. In the FLUENT code the neglected co-ordinate is assumed to be a unity, resulting in a cross sectional area being numerically equivalent to the diameter of the riser. Consequently, the solid mass flow rates for the 2D and 3D simulations are often significantly different (See Table 2) for a given solid flux.

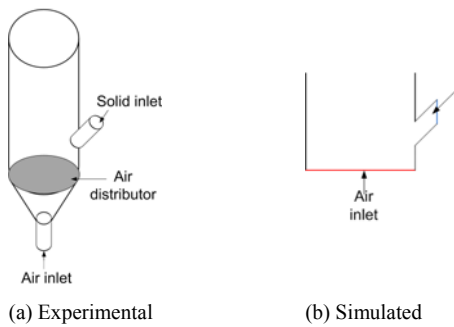


Figure 1: Experimental and simulated (Benyahia *et al.*, 2001) solid inlet configurations.

The inlet arrangement configurations were selected to best represent the experimental study of Bhusarapu *et al.* (Bhusarapu *et al.*, 2005), where the gas entered at the bottom of the riser through a distributor while the solids were introduced via an inclined pipe (see Figure 1a).

Previous 2D simulation studies (Benyahia *et al.*, 2001) have shown, however, that by having a single solid inlet, such as that shown in Figure 1(b), it was not possible to produce the experimentally-observed core annulus solids density profile. Consequently, inlet arrangements for 2D have been widely tweaked to get desired comparisons with 3D experimental data. Therefore, the following three inlet configurations in

2D domain as shown in Figure 2 were investigated in this study:

BC-A: (Figure 2a) Solid entering in radial direction from a two-sided inlet and gas entering axially from the bottom inlet (Benyahia *et al.*, 2001; Vaishali *et al.*, 2007).

BC-B: (Figure 2b) Solid entering axially from two-sided bottom inlet near the wall and gas entering axially from a bottom inlet at the centre (Pita and Sundaresan, 1993; Almuttahir and Taghipour, 2008).

BC-C: (Figure 2c) Axial solid entry from a single bottom inlet at the centre and gas entry from two bottom inlets near the walls.

The experimental setup of (Bhusarapu *et al.*, 2004; Bhusarapu *et al.*, 2005) comprised a single outlet at the top of the riser through which the gas-solid flow entered into the disengagement section. Therefore, a single top outlet was adopted for this study.

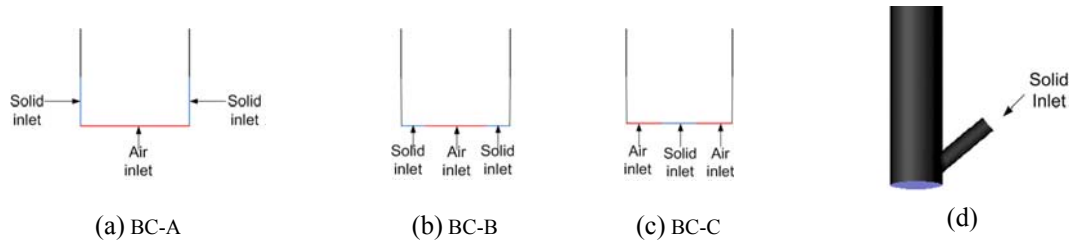


Figure 2: (a), (b) and (c) Inlet arrangements used in 2D simulations. (d) Inlet arrangement in 3D geometry

4. RESULTS AND DISCUSSION

Preliminary 2D simulations were carried out using the boundary condition BC-A to determine the approximate time required for the system to attain a “dynamic” steady state. A mass flux of 37 kg/m² and superficial gas velocity of 4.5 m/s were used, which corresponded to experimental conditions of Bhusarapu *et al.* (Bhusarapu *et al.*, 2005). As shown in Figure 3(a), the solids mass flow rate at the outlet was plotted for the first 30 seconds of a simulation. It is clear that after an initial period of about 5 seconds the solids mass flow rate fluctuated around an average solid flow rate of about 5.4 kg/s. A further check on the time required for dynamic steady state was carried out by comparing the radial profiles of solids velocity and volume fraction at an arbitrary riser height of 5.5m, which were time-averaged at a sampling frequency of 2 kHz over the previous 10, 15, and 20 seconds of the 30 s simulation. This comparison is shown in Figure 3(b).

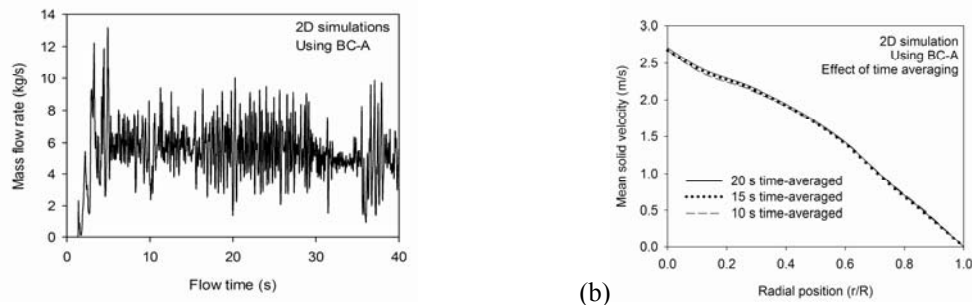


Figure 3: (a) Simulated mass flow rate at the outlet as a function of time. (b) Mean solids axial velocity. It can be seen that there was negligible difference between the solid velocity profiles for all three time-averaging periods. A maximum velocity at the centre with a zero velocity near the wall was observed that was consistent with the core-annulus flow structure reported in previous simulation studies {Nieuwland, 1996 #99; Neri, 2000 #74}. Above checks have also been performed for simulations with other boundary conditions, and it was found that averaging time of 20 seconds, corresponding to the time interval 10-30 s, was sufficient for all further quantitative analysis.

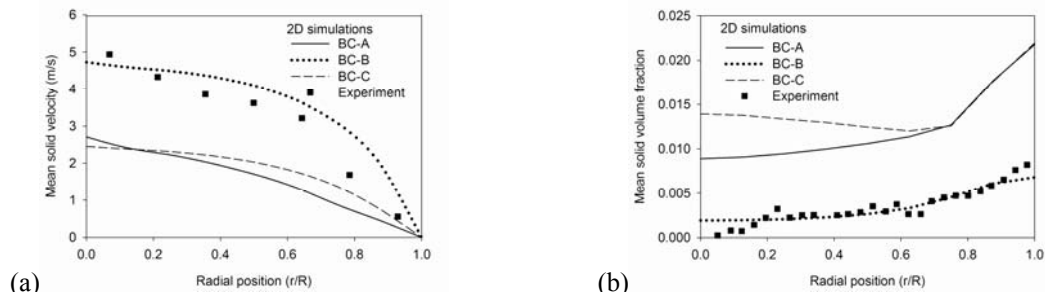


Figure 4: Time-averaged radial profiles for (a) solids axial velocity and (b) solid volume fraction.

4.1 Effect of solid inlet boundary conditions

Time-averaged radial profiles of mean solid velocity and volume fraction in the fully developed zone for the three simulation conditions were compared with the experimental measurements of Bhusarapu *et al.* (2005) as shown in Figure 4. It can be seen that the simulations using the boundary condition BC-B were in good

agreement with the experimental measurements, while simulations using both BC-A and BC-C under-predicted the mean solid velocity and over-predicted volume fraction. The differences between the simulation predictions can be attributed to differences in the mixing the gas and solid phases at the inlet as shown in Figure 5, which shows a set of time-averaged velocity vector plots (Figures. 5(a), (c), (e)) and solid volume fraction contours (Figures 5(b), (d), (f)) near the inlets for the three different inlet configurations.

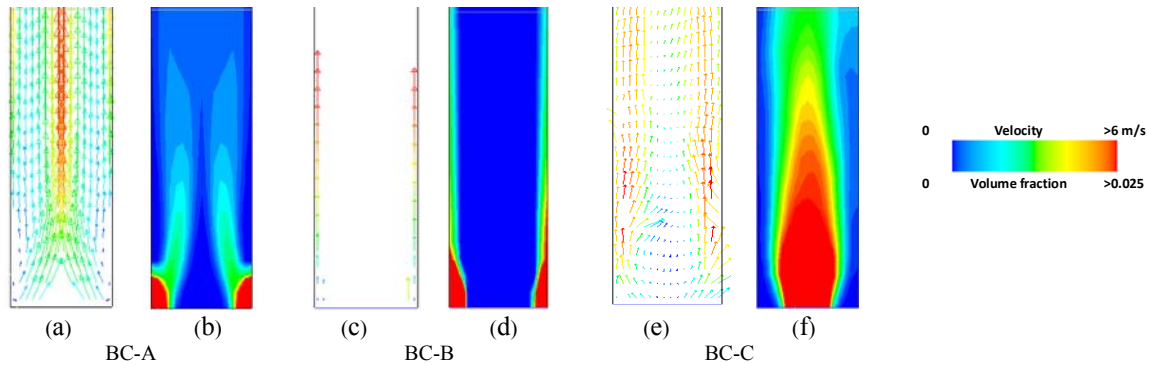


Figure 5: Solids axial velocity vector and volume fraction contours in the riser entrance region.

For the BC-A configuration (Figures 5a and 6b), it can be seen that as the solids entered in the radial direction, they were thoroughly mixed with the gas entering from the bottom in the axial direction. The mixing between the solids and gas phases led to a relatively higher dissipation of the kinetic energy, and thus a lower solids velocity than configuration BC-B (Figures 5c and 5d), where the solids moved upwards with a higher velocity and higher volume fractions near the wall, and the gas moved along the centre part. Consequently, there was less mixing between the two phases, which then rapidly assisted in the formation of a core-annular flow structure. For the boundary condition BC-C (Figures 5e and f), even the axial entry of both phases did not adequately prevent the mixing between the two phases, which then along with the rapid motion of gas along the wall prevented the formation of the core annular structure.

The kinetic energies of the solids and gas phases at the entrance for the three different inlet configurations are compared with the experimental measurements of Bhusarapu *et al.* (Bhusarapu *et al.*, 2005) in Figure 6.

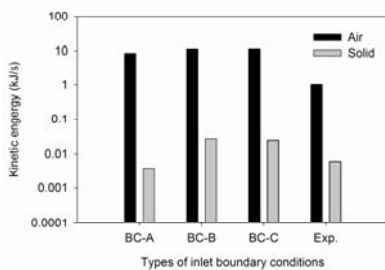


Figure 6: Kinetic energies of gas and solid phases in the riser entrance region.

It can be seen that for all three inlet configurations the simulated kinetic energies for the gas phase were approximately an order of magnitude higher than those determine for experimental inlets. For the solids phase the BC-B and BC-C simulations were similar and higher in value than the experimental results. Conversely, the BC-A simulation reported a lower value. An interesting observation is that while BC-B and BC-C have similar solids kinetic energy terms, the resultant radial profiles for the solids axial velocity and volume fraction are considerably different, as shown in Figures 4(a) and (b), respectively. Similarly, while the solids kinetic energy for BC-A is similar to the experimental results the corresponding solids axial velocity and volume fraction profiles are considerably different from the measured values (see Figure 4).

In summary, the discrepancies between 2D simulation results and experimental data, for the same mass flux and superficial gas velocity, highlights the challenges in correctly establishing the appropriate boundary conditions.

4.2 Effect of type of wall boundary condition

The effect of type of wall boundary condition was investigated by configuring the wall as either “no-slip” or “partial-slip” for the solid phase. Simulations using BC-A and BC-B inlet configurations were conducted to investigate the effect of the wall boundary conditions on the time-averaged mean solid velocity and volume fraction. The results are shown in Figure 7. For BC-A (Figures 7a and b), the partial-slip wall boundary condition resulted in poor agreement for both solids velocity and volume fraction. The higher solid segregation near the wall using the partial-slip wall can be attributed to dissipation of energy due to collisions between solids and wall, which are neglected in the no-slip wall boundary condition. Conversely, the no-slip wall boundary condition was generally in reasonable agreement with the measured solid velocity and volume

fraction profiles, especially near the wall. This improvement can be attributed to the exclusion of dissipation caused by the particle-wall collisions, which is a reasonable assumption for the dilute phase transport. Figure 7(c) and (d) shows the effect of wall type on the radial profiles using the inlet type BC-B. Unlike that for BC-A, only a minor effect of the wall boundary condition on both solids velocity and volume fractions profiles were observed.

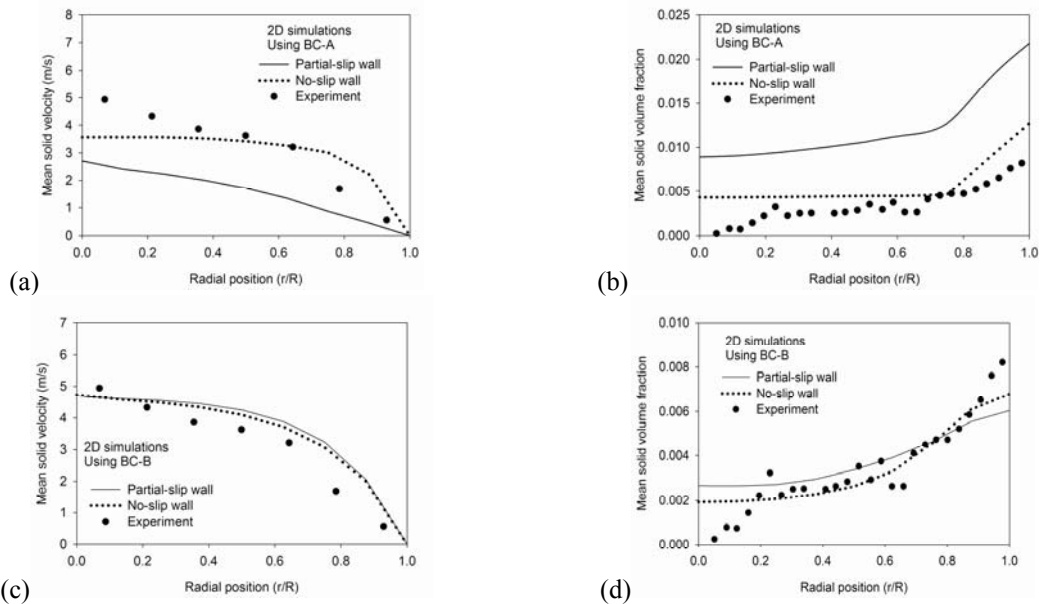


Figure 7: Effect of type of wall boundary conditions on mean (a) and (c) solid velocity and (b) and (d) fraction profiles.

4.3 3D full-scale simulations

Figure 2(d) shows a schematic of the 3D geometry of inlet of the riser, which was meshed with a total of over 210,000 cells. A cluster of eight processors was used to conduct these CFD simulations. Since a small time step size of 0.0002 s was used to carry out the simulation, it took more than three weeks for a 30s of real flow time simulation.

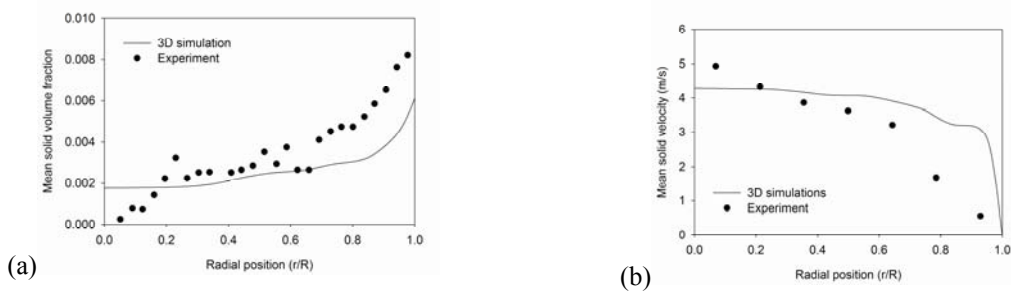


Figure 8 Time-averaged radial profiles of (a) solid volume fraction and (b) axial velocity. Figures 8(a) and (b) show the time-averaged radial profiles of the solid volume fraction and axial velocity, respectively. The predicted values showed a reasonable qualitative agreement with the experimental values. However, near the centre, the simulation slightly over-predicted solid volume fractions and under-predicted solid velocities, and an opposite trend was predicted near the wall.

A comparison between the predictions and experimental evidences in both 2D and 3D simulations of the current study consistently predicted a qualitative trend for the core-annulus flow with some quantitative discrepancies which can be removed by further simulations with different combination of closure laws and/or fine grid simulations. However, coarse-grid EE model presented in this study provides a strong basis for further improvements.

5 CONCLUSIONS

In this work, the effect of boundary conditions on gas-solid flows in riser was investigated by conducting both 2D and 3D simulations. In 2D simulations, three different types of inlet configurations: (i) BC-A (Figure 2a), (ii) BC-B (Figure 2b) and (iii) BC-C (Figure 2c) were investigated, and found to have profound effect on the radial profiles of solid velocity and volume fractions even in top section of riser which has been generally described as fully developed region and believed to be immune to any entry effect. Furthermore, boundary type BC-B gave reasonable agreement with the experimental data than BC-A and BC-C. This profound effect of inlet arrangements was attributed to two possible causes, i.e. (i) mixing and (ii) kinetic energies of two phases at the entrance. The contour plots of solid volume fractions (Figure 6) at the entrance clearly indicated that the mixing of two phases was inadequate in boundary type BC-B, which then eventually assisted the solid holdup profile to “core-annular”, whereas in the other two inlet types, the solid and gas phases got nearly completely mixed. These mixing patterns were then observed to be directly correlated to the radial distribution of the solids, even to the top part of the riser. The kinetic energies of both phases at the inlets (Figure 7) were significantly different from the 3D experimental case for either of the 2D boundary conditions. Thus, using an arbitrary boundary condition in 2D simulations, the energy balances inside the domain may not reflect the experimental values.

The effect of the type of wall boundary condition was also investigated by considering it as either partial or no-slip condition. Using BC-A type inlet boundary condition, a change in the wall condition from the partial to no-slip, gave results closer to the experimental data (figure 8). This could be attributed to exclusion of the dissipation caused by particle-wall collisions. Interestingly, the effect of wall configuration on the radial profiles using the BC-B was negligible. This could also be attributed to predicted lower solid volume fractions using this boundary condition. Thus, the effect of type of wall boundary conditions was strongly dependent on the inlet configurations. Therefore, the selection of boundary conditions in 2D simulations was found to be challenging, and the use of an arbitrary type of boundary conditions could mislead in judging the validation of the EE model.

3D full-scale simulations were conducted by implementing the inlet and outlet boundary conditions similar to the experimental setup. The 3D simulations qualitatively agreed reasonably well with the experimental data, but quantitatively there were disagreements (figure 9) near the centre and walls.

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