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Effect of Different Gas-Solid Drag Models in a High-Flux Circulating Fluidized Bed Riser

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Circulating fluidized beds (CFBs) have applications in many industrial processes like fluid catalytic cracking, coal gasification, coal combustion, biomass gasification and chemical looping. Consequently, the process have been studied intensively for many researchers seeking to understand the complex gas-solid flow encountered in circulating fluidized beds. In this sense, the Computational Fluid Dynamics (CFD) tools are very useful to study gas-solid flows, but this approach directly depends on the correct choice of the mathematical models. There are many numerical studies on CFBs at low solids fluxes and only a few studies for high solids flux, which is very common in many applications, therefore, this regime was chosen to conduct the simulations in this work. The results were compared with experimental data on a riser with an internal diameter of 76 mm and a height of 10 m. Radial and axial profiles were computed using a two-phase 3-D computational fluid dynamics model, with four different correlations for the drag between the phases, Gidaspow, Syamlal-O'Brien, and other two models that account for particle clusters, the energy-minimization multi-scale (EMMS) and the Four-Zone model. The results indicates that all the correlations predicts the solids concentration, found experimentally, in the dilute and developed flow regions but, in the region of highest solids concentration, especially at the level close to the inlet, the Gidaspow and Syamlal-O'Brien correlations not properly represented the solids concentration. The EMMS and Four-Zone models improved the results on these regions showing the influence of these models especially at the bottom of the riser, where the solids concentration is higher.

1. Introduction

Circulating fluidized beds (CFBs) have applications in many industrial processes like fluid catalytic cracking, coal gasification, coal combustion, biomass gasification and chemical looping, consequently, the process have been studied intensively for many researchers in recent years. The CFBs are normally used to promote the contact between gas and solid phases but, the gas-solid flow encountered in this kind of process is very complex because the dynamic behaviour of the individual phases coupled with their interaction. In this sense, an alternative approach to study, understand, and improve the process are the Computational Fluid Dynamics (CFD) tools, capable to simulate the system. The study using CFD techniques depends directly on the correct choice of mathematical models, like the drag model that equate the momentum transfer between phases. The drag model is the most important correlation to describe the interaction between the phases, but most correlations found in the literature were derived from homogeneous systems, like the correlation of Syamlal and O'Brien (1987). Another approach, widely used in the literature that also was derived with experimental results from homogeneous systems is the correlation of Gidaspow (1994). However, according to Li et al. (1993) the fluidization of a gas-solid system is definitely heterogeneous, with regions of low concentration of particles and high particle concentration regions that create particle aggregates called clusters. According to many authors in the literature, the models should be derived taking into account the reduction in drag of the

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particles due the formation of these clusters structures (Agrawal et al. 2001). In this regard, two approaches that were highlighted in the literature in recent years were the Energy-Minimization Multi-Scale or EMMS (Yang et al. 2003) and the Four-zone model (Li et al. 2009). The EMMS model considers two types of structures in circulating fluidized beds, one characterized by a dense phase and one by a dilute phase. After simplification of some terms and the introduction of others, Yang et al (2003) finally managed to integrate the EMMS approach to CFD simulation techniques. The Four-Zone model, originally derived for fluidized beds, considers a dense phase, a sub-dense phase, a sub-dilute phase and a dilute phase to calculate the drag coefficient. The present study investigates four different correlations for the drag between the phases, two models that account for particle clusters, EMMS and Four-Zone, and two models that not, Gidaspow and Syamlal-O'Brien. The simulations were conducted in a high-flux circulating fluidized bed, were the formation and influence of the clusters is higher, in an attempt to show the effects of the different drag correlations.

2. Mathematical Model

The equations used for the gas and solid phases were developed with an Eulerian-Eulerian approach, assuming a continuous and interpenetrating representation of the phases. The behavior of the gas and solid phases are calculated by solving transport equations for mass and momentum, thus, the movement of the phases was determined by solving transport equations for velocity. The turbulent character of the system is characterized according to Reynolds, as the appearance of instabilities in the laminar flow. For the operating conditions used in the equipment studied in this work, the choice of adequate models to describe the turbulent effects is necessary. Therefore, the turbulence was simulated by the k-ω model because it offers good agreement between numeric effort and computational accuracy. The k-ω model is an empirical model based on model transport equations for the turbulence kinetic energy and the specific dissipation rate. For the closure of the conservation equations some constitutive equations need to be specified to predict the exchange between the continuum phases. For the momentum transfer we used in this study four different equations to simulate the drag coefficient, Gidaspow detailed in Gidaspow (1994), Syamlal-O'Brien detailed in Syamlal and O'Brien (1987), EMMS detailed in (Yang et al. 2003) and Four-Zone detailed in (Li et al. 2009). Finally, fluctuations in particle velocity were modelled using the kinetic theory of granular flow. More details about the equations and models used in this study can be found in Ansys Fluent 14.0 Theory Guide (2011).

3. Simulation Conditions

The simulations were conducted with three-dimensional models because of its importance to correctly predict the flow (Lopes et al., 2011). In order to compare the simulations with experimental data, a geometry having the same dimensions of the riser presented by Parssinen and Zhu (2001) was created through the ICEM software. Details of the riser geometry with an internal diameter of 0.076 m and height of 10 m are illustrated in Figure 1.

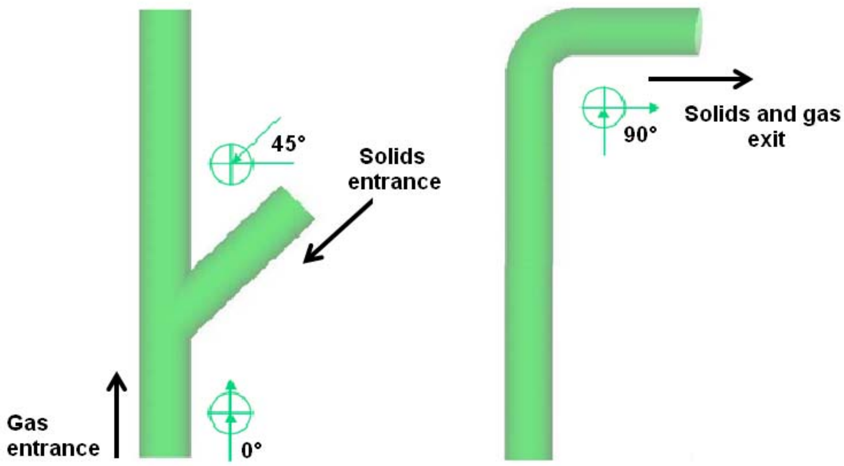

Figure 1: Entrances and exit of the analysed riser

The operation conditions used by Parssinen and Zhu (2001) also provided the basis for the boundary conditions used in the simulations. As initial conditions, the superficial gas velocity was set as 8 m/s and the solids flow as 300 kg/m^{2}s. The particles were considered spherical, with an average diameter of 67 µm and density of 1,500 kg/m^3. For the gas phase, the density and viscosity were defined as 1.225 kg/m^3 and 1.78 x 10^{-5} Pa s respectively, furthermore, the gas-phase pressure, treated as incompressible, was defined at the exit, assuming atmospheric pressure. Finally, for wall boundary conditions, the gas phase was set with the no-slip condition and the solid-phase with free-slip condition, as recommended in literature (Karcz et al., 2011). The commercial code Ansys Fluent 14.0, which is based on the finite volume method, was used to solve the model equations and user-defined functions were developed to implement the EMMS and Four-Zone drag correlations, which are not included directly in the simulator. Second order upwind discretization was used for momentum solutions and a Courant number less than one was chosen to ensure good results. The time step used in all simulations was 0.0001 seconds and the calculation was considered to be convergent when all residuals were less than 0.0001. Finally, all the data presented in this study were computed after the system reaches the statistical steady state regime, judged by the solid mass flux at the riser outlet. The operating conditions used in the simulations are summarized in Table 1.

Table 1: Operating conditions used in the simulations

Parameter	Value
Particle diameter	67 µm
Particle density	1,500 kg/m^3
Gas density	1.225 kg/m^3
Gas viscosity	1.78 x 10^{-5} Pa s
Superficial gas velocity	8 m/s
Solid flux	300 kg/m^{2}s
Maximum solid volume fraction	0.63
Restitution coefficient	0.9

4. Results and discussion

The numerical mesh is of extreme importance to avoid numerical errors (Bastos et al. 2008). Initially six meshes were tested progressively increasing the number of control volumes and a mesh with 590,000 control volumes proved to be numerically independent and adequate to conduct the remaining simulations. The details of its refinement, both at the entrances and at the exit, are presented in Figure 2.

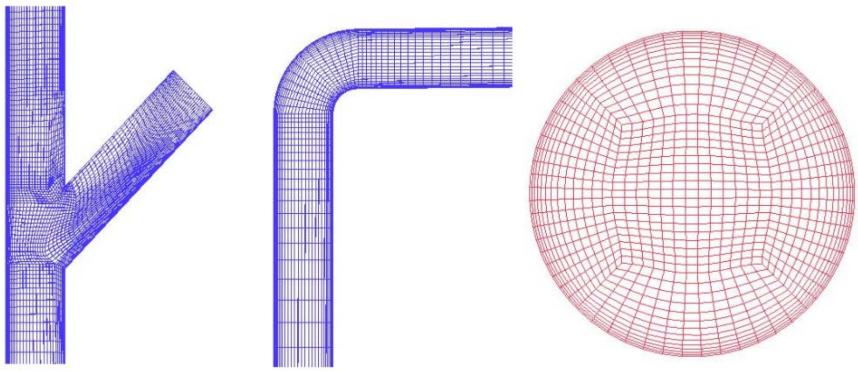

Figure 2: Numerical mesh details at the entrances and the exit of the equipment

The simulated results were taken in accordance with the experimental data of Parssinen and Zhu (2001), i.e., at the same axial levels and radial positions. Figure 3 shows the time-averaged values of the solid volume fraction in axial planes located at 3 m, for each of the drag models tested, Gidaspow, Syamlal-O'Brien, EMMS and Four-zone.

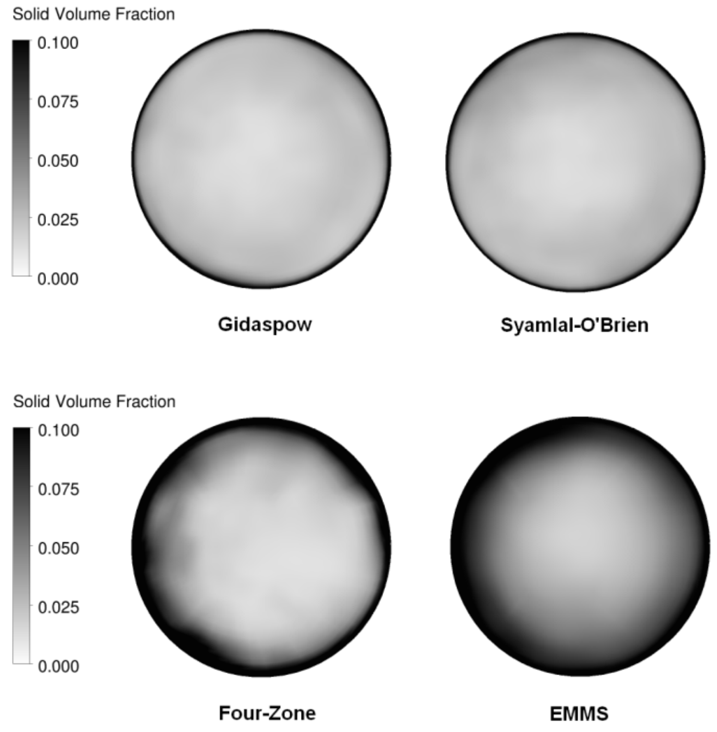

Figure 3: Solid volume fraction profile obtained with Gidaspow, Syamlal-O'Brien, Four-Zone and EMMS models for drag coefficient

As can be seen, all drag models used in this study showed qualitatively correct radial flow profiles, described in literature as core-annulus. The radial flow, defined as *core-annulus*, has a dilute central solids region and high solids concentration near the walls. However, the results showed a clear influence of the drag models in the simulations. Near the base of the riser, the correlations of Gidaspow and Syamlal-O'Brien showed very similar results, while the Four-zone and EMMS correlations showed higher concentrations of solid in the transversal sections. To quantitatively evaluate each model, the simulated results were compared with the experimental data reported by Parssinen and Zhu (2001). Figure 4 shows the axial profile of solid along the riser height.

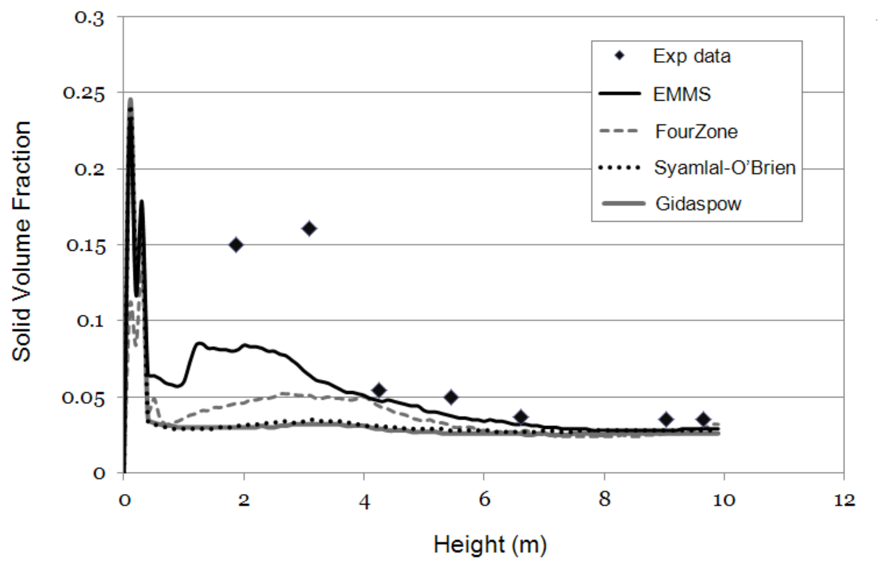

Figure 4: Axial profile of solid volume fraction along the riser height obtained with Gidaspow, Syamlal-O'Brien, Four-Zone and EMMS models for drag coefficient

The amount of solids along the height was calculated by the average of solids in each of the transversal sections. In all models, at the beginning of riser, it can be seen that the amount of solids increases very rapidly due the position of the solids entrance in the equipment. However after 0.5 m, where the models gain more influence on the riser, some differences can be noted. The Gidaspow and Syamlal-O'Brien correlations showed good agreement with experimental results after 6 m in the height of the riser, where the flow is dilute and developed. But in the dense region, close to the inlet, the simulation with these two models underestimated the solid volume fraction, showing the deficiency of these models in properly simulate the system studied in this work. In the simulations with the EMMS and Four-Zone models, it can be seen an increased amount of solids near the entrance of the equipment. The higher concentration of solids is because these models take into account the decrease in the drag coefficient due to the presence of clusters or aggregates of particles. With this reduction, the transfer of momentum between the phases decreases, decreasing the influence of the gas phase in the dispersed phase, which concentrates at the bottom of the riser. Finally, comparing Four-Zone and EMMS models, it can be seen that in this case, the EMMS presented better agreement with the experimental data.

5. Conclusions

Research dealing with circulating fluidized beds, especially for high solids fluxes, is very important because of the multiple industrial processes which utilize this system. Using a two-phase 3-D computational fluid dynamics model, this work compared four different correlations for the drag coefficient between the phases, two very traditional models in literature, Gidaspow and Syamlal-O'Brien, and other two models that account for particle clusters, Four-Zone and EMMS models. The correlations were verified by comparing the simulated results with the experimental data reported by Parssinen and Zhu (2001). The results showed that all correlations predicted the solids concentration in the dilute and developed flow region of the riser but at the level close to the inlet, where the solids concentration is higher, the Gidaspow and Syamlal-O'Brien models failed to represent the solid volume fraction found experimentally. The Four-Zone model and the EMMS models, improved the results showing the influence of these models especially close to the inlet, where the flow is more heterogeneous, with regions of low concentration of particles and high particle concentration regions. Between the four models tested, the EMMS showed the best results when compared with the experimental data. It is worth mentioning the importance of numerically calculate the correct amount of solids to validate the simulations of various industrial processes that use CFBs. Underestimating the amount of solids, other parameters are underestimated, as the pressure drop, the reaction products between the phases, and other factors analysed in industrial cases. Although the models based on clustering presents better results than traditional models for the drag correlations, it is verified that more studies are needed to correctly modelling the drag between the phases.

Acknowledgements

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