THREE-DIMENSIONAL GAS-SOLID FLUIDIZED BED SIMULATION USING A LATTICE BOLTZMANN BASED DRAG CORRELATION.

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ABSTRACT

From the pool of industrial gas-solid fluidization processes those using circulating fluidized bed (CFB) technology are implemented in a wide variety of fields, including fluid catalytic cracking (FCC), combustors, powder generation and mineral processing. As this process requires a huge economical investment for building a new or upgrading an existing unit, there is an especial interest in understanding the fluid dynamic behavior of CFBs. Unfortunately there is no sufficiently accurate analytical model that describes all the complex phenomena that occur in such units. In this context the computational fluid dynamic (CFD) is a very promising tool, allowing the simultaneous modeling and numerical solution of mass, energy and momentum transfer as well as the hidrodynamics and collisional phase interactions even on very complex geometries. This work has as aim to study the implementation of a drag force correlation in three-dimensional gas-solid CFD simulations, performed with a commercial CFD code (Ansys CFX 10.0), in a laboratory scale. This correlation was developed by [4], which was obtained not by the usual empirical data, but was instead formulated on lattice Boltzmann simulations data and later extended by [2]. A Fortran subroutine was developed in order to include in the commercial CFD code a set of drag correlations, based on data from lattice-Boltzmann simulations. The numerical results were compared with the laboratory scale CFB experimental work of [10]. The apparatus consist of a 1 m vertical column with an internal diameter of 0.032 m. For the numerical mathematical modeling, the Eulerian-Eulerian approach was used to describe the gas-solid flow in a CBF. For the gas phase the k-epsilon model was applied to represent the turbulence, and a laminar model was used for the particles phase. Also, the results of this work were compared with simulations carried out by [8] using the hybrid drag correlation suggested by [3].

Keywords: gas-solid fluidization, CFD, lattice Boltzmann drag correlation

1. INTRODUCTION

The main hydrodynamic phenomena to be accounted for in a gas-solid fluidization process in order to correctly model it , is the thorough contact between the solid particles and the fluid phase. A large number of experimental and numerical researches have been conducted and reported in the literature [1,7,9,10,11,12]. The reason for such an interest in this process is due to its large application in several branches of industries, including chemical, petrochemical, metallurgical and food industries, taking advantage of the favorable mass and heat transfers properties of such units. Still, their design and scale-up remains very difficult not only because of the complex hydrodynamic, but also of the other phenomena that may be involved. Even so, only the modeling of the multiphase flow is by itself a challenging accomplishment.

Different approaches have been developed considering specific spatial scales for these problems. As described by [5], three approaches are commonly used for the mathematical modeling, these being the lattice Boltzmann method (LBM), the Eulerian-Lagrangean or Discrete Particle Model (DPM) and the Eulerian-Eulerian or Two-Fluid Model (TFM) approach. The lattice Boltzmann is the most elementary methodology, describing the fluid-particle interaction at a microscopic scale, where both the fluid and the solids are represented as finite particles. According to [6], the LBM is based on a discrete particle kinetic, which involves collision and propagation of particles in a lattice. As an advantage, the simplicity of the algorithm and the accuracy of the mass and momentum conservations are cited. Recent articles [4,5] made use of this method to derive a drag law for gas-solid flow, since by doing so there is no need for empirical data to be used in order to formulate a drag correlation. The DPM calculates the fluid phase through the Navier-Stokes equations and the particles through Newton's law of motion. This method can produce very precise results for the particulate phase although it requires great computational processing and data storage capability, which depending on the amount of particles to be simulated, becomes prohibitive. The third approach, TFM, considers that the solid phase can be modeled as a fluid, resolving thus both phases through the Navier-Stokes equations. This is a very popular CFD methodology, requiring less computational effort, even though generating quite accurate results for a variety of multiphase flows.

In the present work the drag correlation developed by [4] and later extended by [2] was used in a turbulent gas-solid riser CFD simulation. The results were compared to experimental data from the work of [11] and to the CFD simulation of [8].

2. MODEL DESCRIPTION

All the numerical simulations were carried out using the commercial ANSYS CFX 10.0 CFD code. This code is based on the Finite Volume Method for the discretization of groups of partial differential equations. The well known k-epsilon turbulence model was applied for the gas phase. The particulate phase was modeled using a laminar approach. The multiphase flow was modeled with the two-fluid model, for which formulation and mathematical details can be found elsewhere [1,10]. The main closure equations, which defined this work, were briefly described.

Closure Equations:

The drag law applied was presented by [2]. The Friction Coefficient β is given by

$$\beta = \frac{3}{4}\frac{Cd(1-\phi)\rho_g\phi\left|\vec{v_g}-\vec{v_s}\right|}{d_s} \tag{1}$$

where ρ_g is the gas density, $\emptyset$ is the solid volume fraction, $\vec{v}_g$ is the gas velocity vector, $\vec{v}_p$ is the solid velocity vector, d_s is the particle diameter and the adimensional drag coefficient *Cd* can be expressed as

$$Cd = 12\frac{(1-\phi)^2}{Re}F \tag{2}$$

where *Re* is the Reynolds number (Equation 3) and *F* is the drag force coefficient (Equation 4)

$$Re = \frac{\rho_g(1-\phi)\left|\overrightarrow{v_g}-\overrightarrow{v_s}\right| d_s}{2\mu_g} \tag{3}$$

here μ_g is the gas phase viscosity.

$$F = \begin{cases} 1+\frac{3}{8}Re \;\; for \;\; \phi \leq 0.01\,, \;\; Re \leq \frac{(F_2-1)}{(3/8-F_3)} \\ F_0 + F_1 Re^2 \; for \;\; \phi > 0.01\,, \;\; Re \leq \frac{F_3+\sqrt{F_3^2-4F_1(F_0-F_2)}}{2F_1} \\ F_2+F_3 Re \;\; for \;\; \begin{cases} \phi \leq 0.01 \;\;, \;\; Re > \frac{(F_2-1)}{(3/8-F_3)} \\ \phi > 0.01 \;\;, \;\; Re > \frac{F_3+\sqrt{F_3^2-4F_1(F_0-F_2)}}{2F_1} \end{cases} \end{cases} \tag{4}$$

The Coefficients F_0, F_1, F_2, F_3 in the equations above are given by

$$F_0 = \begin{cases} (1-w)\left[\frac{1+3\sqrt{\frac{\phi}{2}}+\left(\frac{135}{64}\right)\phi ln(\phi)+17.14\phi}{1+0.681\phi-8.48\phi^2+8.16\phi^3}\right]+w\left[10\frac{\phi}{(1-\phi)^3}\right], 0.01 < \phi < 0.4 \\ 10\frac{\phi}{(1-\phi)^3}, \phi \geq 0.4 \end{cases} \tag{5}$$

$$F_1 = \begin{cases} \frac{\sqrt{\frac{2}{\phi}}}{40}, 0.01 < \phi \leq 0.1 \\ 0.11+0.00051e^{11.6\phi}, \phi \geq 0.4 \end{cases} \tag{6}$$

$$F_2 = \begin{cases} (1-w)\left[\dfrac{1+3\sqrt{\frac{\phi}{2}}+\left(\frac{135}{64}\right)\phi ln(\phi)+17.89\phi}{1+0.681\phi-11.03\phi^2+15.41\phi^3}\right]+w\left[10\dfrac{\phi}{(1-\phi)^3}\right], \phi < 0.4 \\ 10\dfrac{\phi}{(1-\phi)^3}, \phi \geq 0.4 \end{cases} \tag{7}$$

$$F_3 = \begin{cases} 0.9351\phi + 0.03667, \phi < 0.0953 \\ 0.0673 + 0.212\phi + \dfrac{0.0232}{(1-\phi)^5}, \phi \geq 0.0953 \end{cases} \tag{8}$$

In Equations (5) and (7) w is a weighting factor

$$w = e^{\left(\frac{\frac{-10}{0.4-\phi}}{\phi}\right)} \tag{9}$$

The drag relation used in the work of [8], for dense (Equation 10) and dilute (Equation 11) as functions of solid volume fractions

$$\beta = 150\frac{\phi^2}{(1-\phi)}\frac{\mu_g}{d_s^2} + 1.75\phi\frac{\rho_g\left|\overrightarrow{v_s}-\overrightarrow{v_g}\right|}{d_s}, \phi > 0.2 \tag{10}$$

$$\beta = \frac{3}{4}\frac{Cd(1-\phi)\rho_g\phi\left|\overrightarrow{v_g}-\overrightarrow{v_s}\right|}{d_s}(1-\phi)^{-2.65}, \phi < 0.2 \tag{11}$$

$$Cd = (1-\phi)^{-1.65} max\left[\frac{24}{Re(1-\phi)}\left(1+0.15\left(Re(1-\phi)\right)^{0.687}\right), 0.44\right] \tag{12}$$

Physical Description

The experimental setup reported by [11] consisted of a 1.0 m long riser with an internal diameter of 0.032 m. At 0.05 m of its heights there is a secondary entrance with a diameter of 0.008 m. The density of the particles was 1600 kg/m^3 with a Sauter mean diameter of 0.06 mm. Three different superficial gas velocities were used in the experiment, 0.36 m/s, 0.71 m/s and 1.42 m/s, all at 25 ºC. A constant velocity of 0.05 m/s was held at the secondary entrance. The initial bed height of the solids was 0.05 m. Results for radial profiles of axial velocity were reported for three different heights of the column, namely 0.16 m, 0.32 m, 0.48 m.

An overview of the geometry design and numerical mesh can be seen in Figure 1.

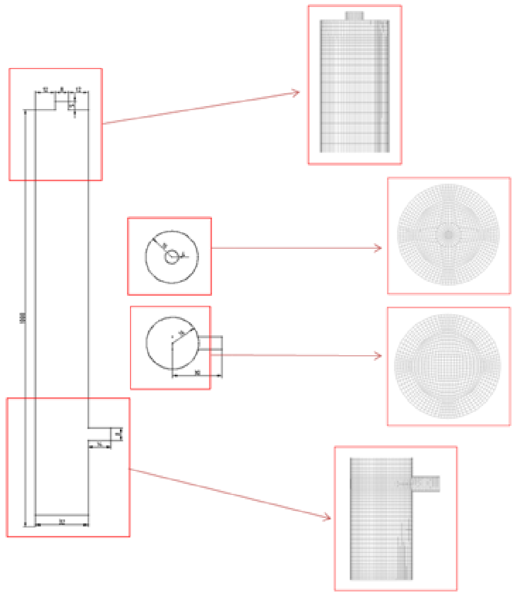

Figure 1: Geometry and details of the *Riser*'s mesh.

Initial and Boundary Conditions

No velocity profile was applied to the primary entrance due to the presence of the distributor in the experimental column. The constant velocity for each case, 0.36 m/s, 0.71 m/s and 1.42 m/s, was set at this boundary. For the secondary entrance a function that represented the recirculation of the solids was necessary. It was set as equal to the mass flux of the solid at the exit. Also, a constant air entrance velocity of 0.05 m/s was fixed there. An opening condition for the exit was preferred over an outlet due to numerical stability. The conditions at the walls were no slip for the gas phase and free slip for the solid phase. As an initial condition, the bottom of the column was filled with a bed height of 0.05 m. The time step of the numerical solver ranged from $1x10^{-5}$ s to $1x10^{-3}$ s. The RMS convergence criterion for the mass and momentum equations was set to $1x10^{-4}$. Higher order discretization schemes were selected.

3. RESULTS AND DISCUSSION

A mesh test was carried out in order to obtain an acceptable numerical accuracy with the smallest computational cost.The results showed that a mesh with about 300000 hexahedral volumes of control was suitable for this geometry.

The computational results obtained in the present work correspond to a time average of the last 7 s of simulation, hence assuming the initial bed expansion would have no influence on the results and that a pseudo-stationary state was achieved. The velocity profiles were presented in Figures 2, 3 and 4.

All the numerical results using the drag law presented by [3] were obtained by [8]. Both simulations showed the typical core-annulus flow, where a low solid volume fraction region moves upward in the center of the flow and a ring region with a higher particle volume fraction falls downward near the walls.

For the 0.36 m/s inlet velocity case, the current simulations showed that a strong internal particle re-circulating pattern was present. Due to this pattern the predicted radial particle velocity profiles were higher for the 0.16 m and 0.32 m height and lower for the 0.48 m measurement, as seen in Figure 2. Just as reported by [11] the profiles were not symmetric, especially near the secondary entrance.

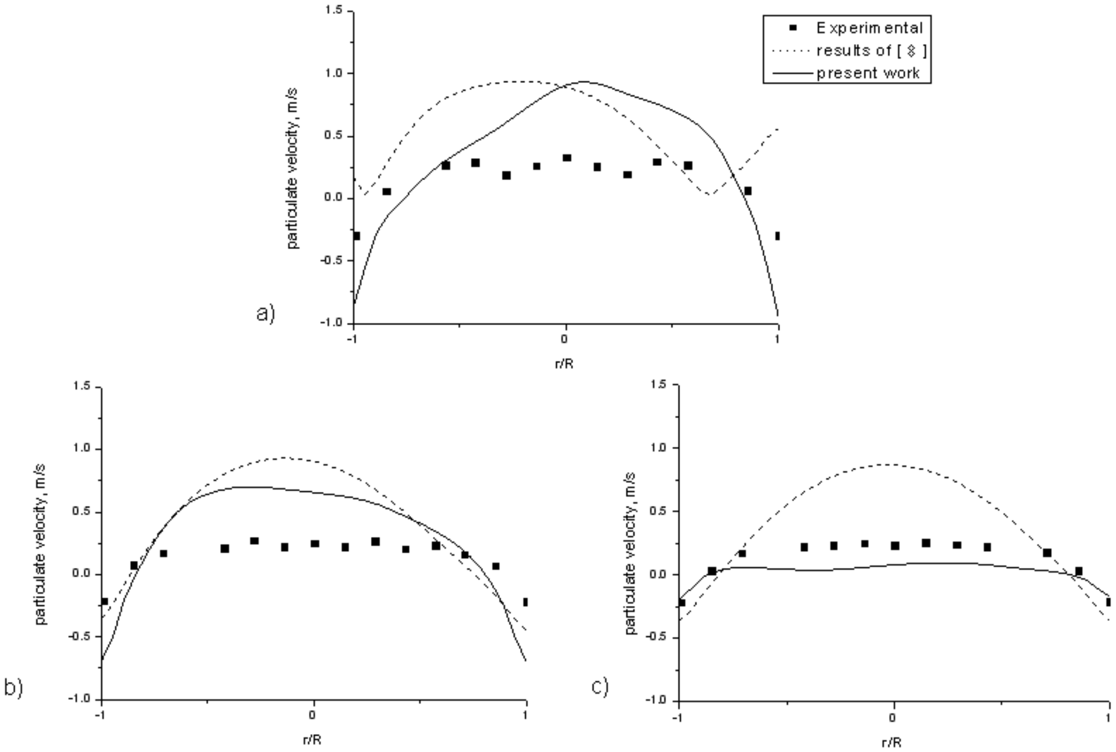

Figure 2: Experimental and simulated radial particle velocity for $v_{sup} = 0.36$ m/s, at heights of a) 0.16 m; b) 0.32 m; c) 0.48 m.

Figure 3 shows the 0.71 m/s inlet velocity case. These simulations were more consistent with the experimental data. However there was an overprediction of the core velocity, which was compensated by higher downflow velocities near the walls. The comparison of the two drag correlations showed only small differences between them, having both generated higher velocity profiles than those obtained experimentally.

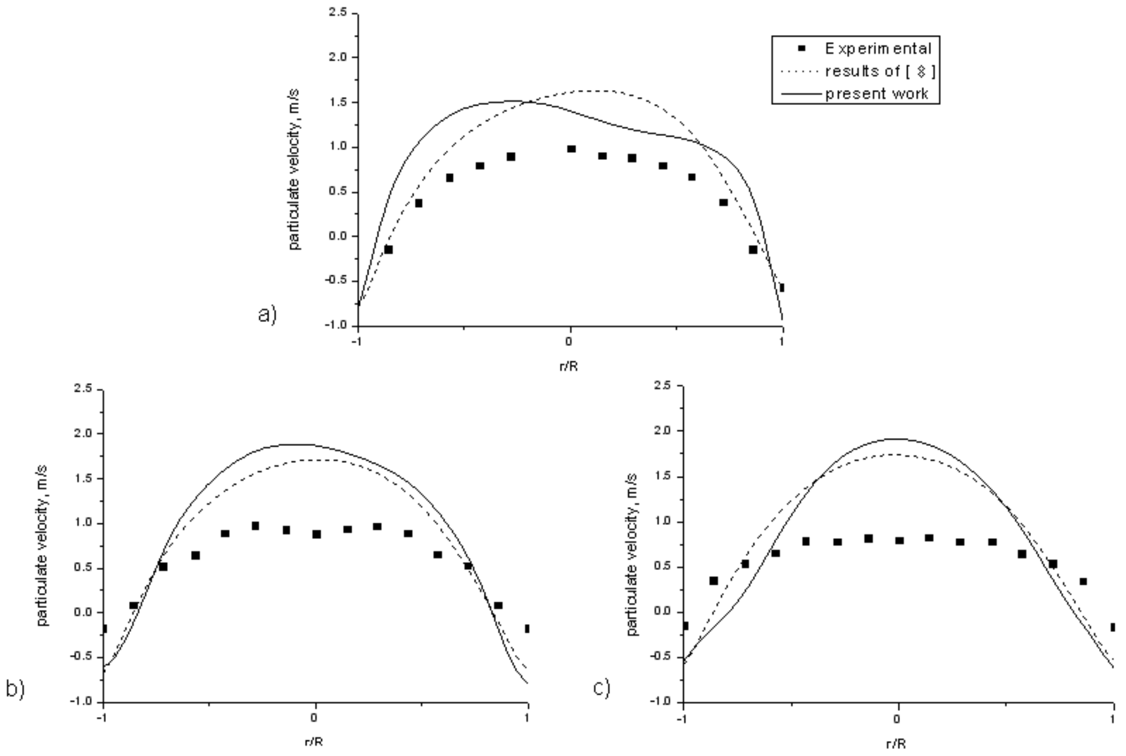

Figure 3: Experimental and simulated radial particle velocity for $v_{sup} = 0.71$ m/s, at heights of a) 0.16 m; b) 0.32 m; c) 0.48 m.

The 1.42 m/s inlet velocity case, Figure 4, also shows a similar solid velocity profile, when comparing the two drag correlations. Both have the same characteristics, producing a steeper profile at the center, especially at 0.32 m and 0.48 m, but a closer approximation with experimental data at the annulus region. At a hight of 0.16 m the predicted radial solids velocities showed good agrement with the measurements in both the core and annulus regions for the present work simulation.

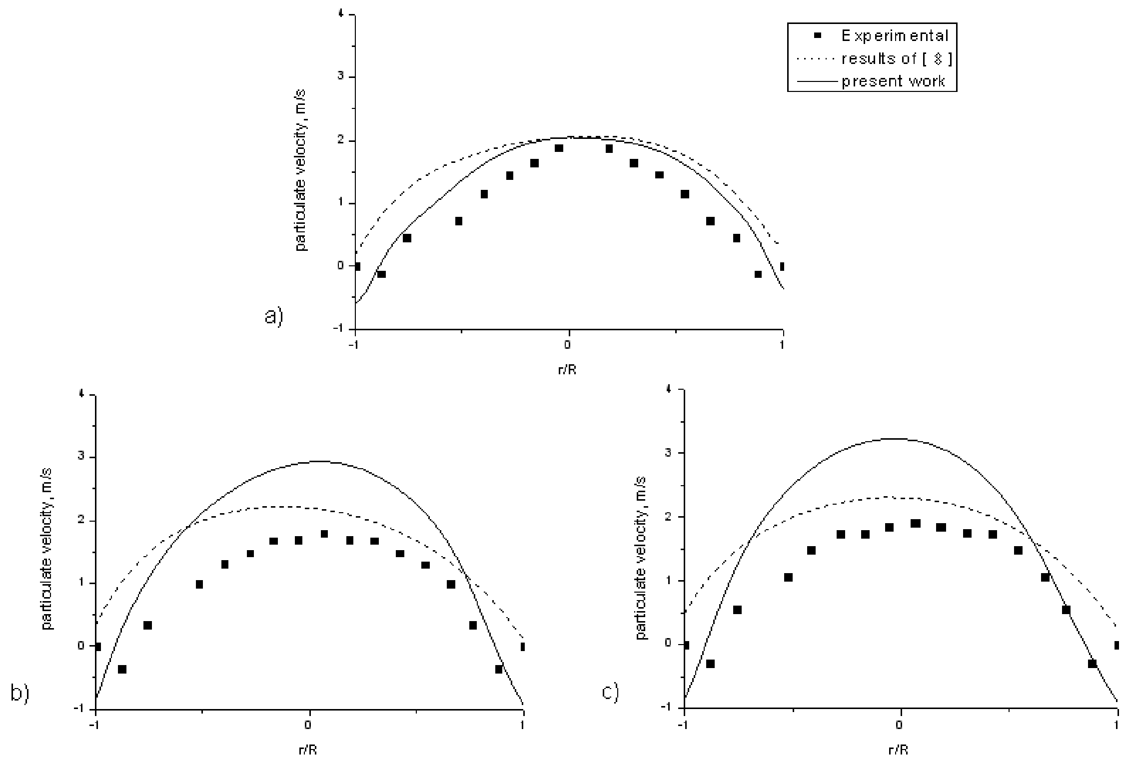

Figure 4: Experimental and simulated particle velocity for $v_{sup} = 1.42$ m/s, at heights of a) 0.16 m; b) 0.32 m; c) 0.48 m.

4. CONCLUSION

The study of a lattice Boltzmann based drag correlation was accomplished trough the transient 3D CFD simulations of a gas-solid CFB Riser. The results of these simulations were compared to the experimental work of [11] and the CFD simulation reported by [8]. The predicted radial solids velocities at the hights of 0.16 m and 0.48 m and the superficial velocities of 1.42 m/s and 0.36 m/s, respectively show good agreement with the measuments in both the core and annulus regions. For other cases studied, the results overpredicted the core flow region, but a set of drag correlations, based on data from lattice-Boltzmann simulations showed, in the regions near the wall, similar profiles to those found experimentally.

NOMENCLATURE

Cd	drag coefficient
d_s	particle diameter, m
F	drag force coefficient
μ_g	viscosity of gas phase, kg/m.s
$\rho_{g,p}$	density of gas or particulate phase, kg/m^3
Re	Reynolds number
$\vec{v}_{g,p}$	velocity vector gas or particulate phase, m/s
$\emptyset$	volume fraction of particulate phase

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