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Interphase Momentum Study in a Slurry Bubble Column

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Eulerian three-dimensional transient simulations have been conducted to study the hydrodynamics of threephase flow inside a slurry bubble column with intermediate and high concentration of solid particles. The present work evaluated the influence of interactions among phases, in the time-averaged numerical results. Predictions were compared with experimental data available in the literature. Analysis of drag models for the liquid-solid and gas-solid interactions plays an important role in the dynamic behavior of a gas-solid-liquid slurry bubble column. The CFD models simulated was capable to predict gas holdup and (gas velocity) x (gas holdup) profiles similarly to that found experimentally.

1. Introduction

Slurry bubble columns are widely used in industries, as chemical reactors, due the simplicity in its construction and operation, as well as, its compactness and absence of moving parts. Despite all the previous advantages, bubble columns are also known a complex flow. In order to design and scale up a bubble column effectively, it requires a detailed description of the bubble characteristics, mass and heat transfer parameters (Kantarci et al., 2005) and is widely accepted that characteristics are dependent on the hydrodynamics prevailing in this system.

A successful way of studying complex flows has been made through the Computational Fluid Dynamics (CFD), and these models are able to achieve numerical results with good agreement compared to experimental data. Here are still a large number of controversial theories around the interphase forces that govern momentum transfer between system phases. It is well-known that interphase forces and turbulence play a crucial role in the correct modeling of hydrodynamics in bubble columns (Tabib et al., 2008).

In this sense, the main objective of the present work is to present a CFD code that is capable of simulating a three-phase flow with intermediate and high concentrations of solids in laboratorial scale slurry bubble column. For this purpose, different empirical correlations to represent the interactions among phases are adopted in the simulations in a time-averaged approach. The commercial code ANSYS CFX 14 is used in all CFD simulations.

2. Mathematical model

The Eulerian approach is based on ensemble-averaged mass and momentum transport equations for each of the three phases. The mass and momentum conservation transport equation can be written in a general form for the three phases as:

$$\frac{\partial}{\partial t}(\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k U_k) = 0$$

(1)

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$$\frac{\partial}{\partial t} (\alpha_k \rho_k U_k) + \nabla \cdot (\alpha_k (\rho_k U_k U_k)) = -\alpha_k \nabla P + \nabla \cdot (\alpha_k \mu_{k,eff} (\nabla U_k + (\nabla U_k)^T)) + M_k + \rho_k g$$
(2)

where ρ is the density, α is the phase holdup, U is the velocity vector, μ is the viscosity, the subscript *eff* denotes the effective viscosity, g is the gravitational acceleration and M is the total interfacial force acting between the phases and the subscript k indicates the phase (g=gas; I=liquid; s=solid). The momentum transport equation of solid phase presents an additional term due to solids pressure, and can be written as $\alpha_s \zeta_s (\nabla \cdot U_s) + \nabla P_S$ where ζ is the bulk viscosity and P_s represent the additional pressure due to presence of particulate solid. These terms were considered only in simulation with Kinetic Theory of Granular Flow (KTGF). The KTGF with $e_{ss} = 0.9$ was considered in our analysis. The drag force can be described as:

$$M_{k} = M_{D} = \frac{3}{4} \frac{C_{D}}{d_{d}} \rho_{c} \alpha_{d} | U_{d} - U_{c} | (U_{d} - U_{c})$$
(3)

where C_D is the non dimensional drag coefficient, *d* is phase diameter. The subscript *c* indicates the continuous phase and *d* stands for dispersed phase. The drag model correlation applied to gas-liquid contact was the Ishii-Zuber model, based on the good results obtained by Silva et al. (2011). The drag models for liquid-solid and gas-solid interactions used in this work are presented in the next sections.

2.1 Liquid-solid drag force correlations

a) Wen-Yu Model: The Wen-Yu model considers a swarm of particles flowing is a function of solid holdup. The model modified by Jia et al. (2007) is mathematically represented as:

$$C_{D,ls} = \alpha_s^{-1.65} max \left(\frac{24}{\alpha_s Re_s} \left(l + 0.15 (\alpha_s Re)^{0.687} \right), 0.44 \right)$$
(4)

b) Gidaspow Model: The Gidaspow model is usually recommended for densely distributed solid particles systems and it can be represented by:

$$C_{D,ls} = C_D(Wen - Yu)if \ \alpha_s < 0.20 \ , \ M_{D,ls} = \left(150 \frac{\alpha_{S^2} \mu_l}{\alpha_l d_p^2} + \frac{7}{4} \frac{\alpha_s \rho_l |U_s - U_l|}{d_p}\right) |U_s - U_l| \ if \ \alpha_s > 0.20 \ (5)$$

2.2 Gas-solid drag force correlations

There are few works in literature which considered the gas-solid drag in three-phase flows. In this work, the importance of this momentum transfer was evaluated using two correlations:

a) Schallenberg et al. Model: Mathematically, the correlation proposed by Schallenberg et al. (2005) is given as:

$$C_{D,gs} = 80, \min[1, \max(0, (-15\alpha_g + 1.8))]$$
(6)

b) Syamlal-O'Brien Model: The model proposed by Syamlal and O'Brien (1989) is based on the classical drag correlation of Dalla Valle:

$$C_{D,gs} = \left(0.63 + \frac{4.8}{\sqrt{Re_{gs}/V_r}}\right)^2, V_r = \left(A - 0.06Re_{gs} + \sqrt{(0.06Re_{gs})^2 + 0.12Re_{gs}(2B - A) + A^2}\right)$$

$$Re_{gs} = \frac{\rho_g |U_s - U_g| d_p}{\mu_g}, \quad A = \alpha_g^{4.14}, \quad B = 0.8\alpha_g^{1.28} \text{ if } \alpha_g \le 0.85 \text{ and } \alpha_g^{2.65} \text{ if } \alpha_g > 0.85$$
(7)

where V_r is the ratio of the terminal settling velocity of a multiparticle system to that of an isolated single particle, proposed by Garside and Al-Dibouni (1977).

2.3 Turbulence

The turbulence is described by the two-equation RNG k- ε model, add the Dispersed Phase Induced Turbulence. As a result, the sum of all these contributions determines an effective viscosity (μ_{eff}). In this sense comes:

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$$\mu_{eff,l} = \mu_l + \mu_{t,l} + \mu_{b,l}, \quad \mu_{eff,g} = \mu_g + \mu_{t,g} \quad \text{and} \quad \mu_{eff,s} = \mu_s + \mu_{ss}$$
(8)

where, μ_t is the turbulent viscosity, which was considered for the gas phase by Zero-Equation model, μ_{bi} is the bubble induced turbulence calculated by the Sato and Sekoguchi (1975) model, μ_{ss} is the shear viscosity induced by solids collisions, considered only in the simulations with KTGF.

2.4 Numerical procedure

The numerical results are validated with experimental data from the literature Wu et al. (2008) in a column with a diameter of 10.2 cm and height of 1.05 m. The Euler model is applied to all three phases. The initial condition is fill the column with the liquid and solid phase (the respective concentration) to the operating height equal 0.9 m, as in physical experiments. Is imposed atmospheric pressure at the top of the column, non-slip condition for the liquid and free slip to the gas and solid phase in the walls. The gas enters to the column with a constant velocity by an area equivalent to 70 % the total cross section. The liquid and solid phases are not load/leave the domain. The gas and solid phases are treated as a dispersed fluid, where, it is assumed that all the bubbles have the same diameter, 4.5 mm (8.5 mm to high gas flow) and 75 μ m to solid phase. The slurry bubble column is considered to be operated at 25 °C and 1 atm at isothermal conditions. No heat and mass transfer occurs. The apparent alumina suspension viscosity can be estimated through empirical correlations from simple parameters is given by a Krieger and Dougherty model:

$$\mu_s = \mu_l \left(1 - \frac{\alpha_s}{\alpha_{s,max}} \right)^{-2.5 \ \alpha_{s,max}} \tag{9}$$

where, μ_s is the apparent viscosity of suspension, $\alpha_{s,max} = 0.62$ and α_s is the solid holdup in the system. A well distributed hexahedral mesh is used to 3D and transient simulations with the commercial CFD code ANSYS CFX 14. A time step of 0,01 s was used along all the simulations, and a real time of 200 s was simulated, where the first 30 s was used to establish a pseudo-stationary condition. A high-order interpolation scheme was used for the hydrodynamics equations and upwind for the turbulence equations, with a convergence criteria of RMS set to 10^{-4} . The pressure-velocity coupling was obtained using the SIMPLEC algorithm. Four test cases conditions are shown in Table 1. The numerical results are compared with experimental data, in a plane located at 56.1 cm from the bottom of the bubble column.

Case	Superficial gas velocity (Ug, cm/s)	Gas flow (Q _g , m ³ /s)	Solid Concentration (α_s , %v/v)
A	2.0	0,000163	9.1
В	13.0	0,00106	9.1
С	2.0	0,000163	25.0
D	13.0	0,00106	25.0

Table 1: Studied cases

3. Results

3.1 Influence of liquid-solid interaction

The influences of different drag laws for liquid-solid interaction are shown in Figure 1. Starting with qualitative analyses of case C (critical case), analyzing the alumina holdup fields, all simulations shows that alumina is in suspension, agreement with the experimental visualization reported by Wu et al. (2008). The numerical radial profiles of gas holdup are shown in Figure 1a and 1c. This profile has a parabolic shape and agrees with the experimental behavior. When increase the superficial gas velocity, increases the gas holdup and gas velocity maximal value in central core of column. In this sense, the numerical simulation represents this feature. It is possible to note in simulation results that the modified Wen-Yu drag model provides better predictions for the radial profiles of gas holdup and (gas velocity) x (gas holdup), while the Gidaspow drag model overestimates the experimental data in the region near the column center.

3.2 Influence of gas-solid interaction

Simulations results for all cases (A to D) are show in Figure 2. It can be observed in that the inclusion of gassolid drag did not promote any improvement as compared to the results obtained when only KTGF model is considered. The results using gas solid interaction become worse for (gas velocity) x (gas holdup) profiles showed in Figure 2b. The KTGF model with shows a good agreement almost in all the radial extension. Nevertheless, when gas-solid interaction is included the numerical profiles in the center underestimated and showed worse predictions with experimental data.



Figure 1: Radial profile of gas holdup and (gas velocity) x (gas holdup). Liquid-solid interaction analysis.

Figures 2c and 2d show the radial profiles obtained from case B. It is noted in Figures 2c and 2d that the gassolid interaction improvement the results. It can be due the interactions gas-solid in high gas velocity is needed to be considered. The model proposed by Schallenberg promoted a good agreement with experimental data for both fluid dynamic variables investigated. The Syamlal-O'Brien model underestimated the product between bubble velocity and gas holdup and overestimated gas holdup.

In Figures 2e and 2f, it could be pointed out that for this operating flow regime the gas-solid interaction can be neglected. The better prediction for this case is showed by G-L + L-S + No G-S interaction + KTGF. Since in this case we are dealing with high concentration of solids and the solid-solid interaction plays an important role as observed from several research works in the past.

Figures 2g and 2h show the numerical profiles for case D with high solid concentration and high gas superficial velocity. It can be seen that a better prediction against the experimental data was obtained without gas-solid interaction (G-L + L-S + No G-S interaction + KTGF). However, all models showed similar behavior for the gas holdup profile.

In this sense, the gas-solid interaction improves the results only to an intermediate solid concentration. In the case of high solid concentration will increase the size of bubbles inside the column and damped the gas circulation, and will decrease the gas volume fraction (Kantarci et al., 2005).

For a final comparison, Figure 3 shows for all cases liquid-solid and gas-solid interphase momentum transfer rates. It is noted that gas-solid momentum exchange increased with gas superficial velocity and solids concentration. The gas-solid drag force in Figure 3 showed for all cases lower rates of momentum exchanges. For case D (high gas superficial velocity and solid concentration) higher values of momentum exchange were observed.

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Figure 2: Radial profile of gas holdup and (gas velocity) x (gas holdup). Gas-solid interaction analysis.

Analyzing the liquid-solid drag momentum fields obtained in the simulation it is possible to see that low gas superficial velocities promoted more homogeneous fields, since the solid particles are well distributed throughout the slurry, in contrast for high gas superficial velocities the particles tend towards the wall, promoting a dense particle concentration in this region. The liquid-solid momentum for case C presented higher rates than in case D, which operates with high gas superficial velocity.



Figure 3: Momentum transfer countour plots for liquid-solid and gas-solid interactions considering G-L, L-S, KTGF and G-S by Schallenberg model.

4. Conclusions

A CFD code was capable of simulating intermediate and high solid concentration inside a slurry bubble column. In addition, the simulations presented show a good agreement with experimental indicating a good numerical consistency with the experimental operating condition. For the liquid-solid phase drag force the modified Wen-Yu model gave a better prediction of the alumina in suspension inside the system. The Kinetic Theory of Granular Flow (KTGF) promoted a better agreement with experimental data for all cases, except for intermediate solid concentration and high gas velocity (case B), in which the model proposed by Schallenberg et al. (2005) resulted in a better prediction of experimental data.

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