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Modelling of Three Phase System with Non-Newtonian Liquid Using Computational Fluid Dynamics Model

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Abstract: A 2 dimensional numerical simulation was used to describe the flow behaviour and circulation pattern of three phase system inside an isothermal slurry bubble column using a finite volume technique. The three phase system consists of; air as the gas phase, non-Newtonian solution of poly acryl amid (PAA) as the liquid phase, and alumina catalyst as the solid phase. To experimentally validate the code, local gas hold-up and bubble characteristics have been measured using a modified electroconductivity probe. The model was based on the principle of continuity and momentum equations. The gas and liquid velocity were prescribed numerically and the gas velocity simulated agrees with experimental observation. The experimental results as well as the numerical results show that the gas velocity decreases with increasing the non-Newtonian behaviour of the system and this may due to the increasing in bubble coalescence.

Key words: Three phase, CFD, modelling, non-Newtonian liquid, slurry bubble column

INTRODUCTION

Gas-liquid-solid three phase sparged reactor have been widely used in petrochemical, metallurgical, environmental and cool liquefaction process. They are the preferred reactor type of synthesis gas conversion. They are flexible and may be tailored to produce high quality transportation fuel and a verity of products. Thus it is essential to improve its performance through the understanding of its hydrodynamic properties. Several empirical correlations have been proposed for the estimation of these hydrodynamic parameters but they are restricted in their application to the geometry of which they were determined (Chen *et al*., 1995; Wang *et al*., 2003; Majumder *et al*., 2006).

Recently, many publications have established the potential of Computation Fluid Dynamic (CFD) to describe the hydrodynamic characteristics of two phase system like (Pfleger *et al*., 1999; Sokolichin and Eigenberger, 1999) and some searchers reported modeling of pilot plant size bubble column (Krishna *et al*., 2000; Krishna and Van Beter, 2002; Van Beter *et al*., 2003; Mitra-Majumdar *et al*., 1999; Padial *et al*., 2000 ; Gamw *et al*., 1999). But still most of these researches are limited to two and three phase system for Newtonian liquid and little of them used to study CFD simulation with non-Newtonian liquid.

The aim of this research is to study the gas flow structure inside a pilot plant size slurry reactor with non-Newtonian liquid. The model system used and especially the solid material have chosen to resemble the flow situation inside a bubble column bioreactor.

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THEORETICAL MODEL

The stress deformation behavior of non-Newtonian fluid can be represented by the general Herschel-Bulkley model (Carreau *et al*., 1997).

$$\tau = \tau_0 + k\ \gamma^n \qquad \text{for } |\ \tau\ | < \tau_0 \tag{1}$$

$$\gamma = 0 \qquad \text{for } |\ \tau\ | < \tau_0 \tag{2}$$

For power, low model it was commonly used the Ostwald-Dewaele constitutive equation which is the simplification of the Herschel-Bulkley relationship in the absence of shear stress:

$$\tau = k\ \gamma^n \tag{3}$$

$$\mu_{eff} = k(\gamma)^{n-1} \tag{4}$$

Note that the above equations restore the Newtonian low of viscosity when the yield stress is zero or when the power low index is unity.

In this model it's assumed that, for three phase slurry reactor, the liquid phase is the continues phase while gas and solid are the dispersed phases, according to their volume fraction. The continuity and momentum conservation equations for gas and liquid phases in the Eulerian form are applied.

The global assumptions involved are: isothermal steady state, axisymetric, incompressible flow, the added mass and lift forces contributions were both ignored and the drag force contribution between the continuous and the dispersed phases had been included in keeping with studies of Sanyal *et al*. (1999) and Sokolichin and Eigenberger (1999).

The conservation Eq:

$$\varepsilon_g + \varepsilon_l + \varepsilon_S = 1 \tag{5}$$

The continuity Eq. for k phase:

$$\nabla(\varepsilon_K \rho_K V_K) = 0 \tag{6}$$

Momentum Eq. for gas phase:

$$\nabla\left(\varepsilon_g \rho_g V_g V_g\right) = \nabla P + \nabla \varepsilon_g \tau_g + \varepsilon_g \rho_g g - F_{gL} \tag{7}$$

Momentum Eq. for liquid phase

$$\nabla(\varepsilon_l \rho_l V_l V_l) = \nabla P + \nabla \varepsilon_l \tau_l + \varepsilon_l \rho_l g + F_{gL} - F_{ls} \tag{8}$$

The momentum balance equation for liquid phase is appropriate for Newtonian liquid. It has been successfully determined that the momentum balance equations for Newtonian liquid also apply to non-Newtonian liquids (Liu and Masliyah, 1998) and the only difference is in the effective viscosity. So, the effective viscosity for non-Newtonian liquid will be used instead of the usual viscosity of Newtonian liquid.

The drag force exerted on the gas phase Fgl is a result of relative motion between the flowing phases to oppose slip, neglecting the force between the two dispersed phases gas and solid. The forces exerted on liquid phase involve; the drag forces Fls experienced by the liquid due to shear, nearby, the liquid-solid boundary and Fgl the gas-liquid interfacial force.

$$F_{gl} = \frac{3}{4}\frac{C_D}{d_b}\rho_g\left|V_g - V_l\right|\left(V_g - V_l\right)\varepsilon_g \tag{9}$$

$$F_{sl} = \frac{3}{4}\frac{C_D}{d_p}\rho_s\left|V_s - V_l\right|\left(V_s - V_l\right)\varepsilon_s \tag{10}$$

Drag coefficient of gas phase was calculated depending on (Mpandelis and Kelessidis, 2004) for non-Newtonian system as:

$$C_D = \frac{24}{Re}\left(1 + 0.14Re^{0.601}\right) + \frac{0.211}{1 + 0.42Re} \tag{11}$$

To avoid the complexities of turbulent in our model at higher superficial velocity, only the laminar flow will be considered.

The slip velocity between liquid and gas velocity was also used in this model.

$$u_S = V_g - V_l \tag{12}$$

For non-Newtonian liquid and for low gas hold up slip velocity can be calculated depending on Clark and Flememer (1985).

$$u_S = V_b(1 - \varepsilon_g)^n \tag{13}$$

NUMERICAL SOLUTION

Numerical solution of the form of equations listed before was made using a finite volume technique with appropriate initial and boundary condition. The mesh cells are fixed in two dimensional spaces. The scalar variables are located at the cell and the vector variables at the cell boundary.

The momentum equation is solved using staggered mesh. The geometrical method assumed an axial symmetry and the vessel was divided into 82×82 computation cells.

EXPERIMENTAL WORK

Experiments were carried out in a QVF vessel with 0.5 m inside diameter and 1 m total height (Fig. 1) with static clear height to vessel diameter of 1.1.

A stationary solid of alumina (Al_2O_3) with particle size 500 μm and solid loading 2 kg were used and a continues flow gas of compressed air that passed through two calibrated flow meters and distributed to the vessel through a single ring distributor made from copper.

The liquid phase is a non-Newtonian solution of polyacrylamide (PAA) with different concentrations (0.01, 0.03, 0.05 and 0.07 wt%). Different solutions were prepared by dissolving highly

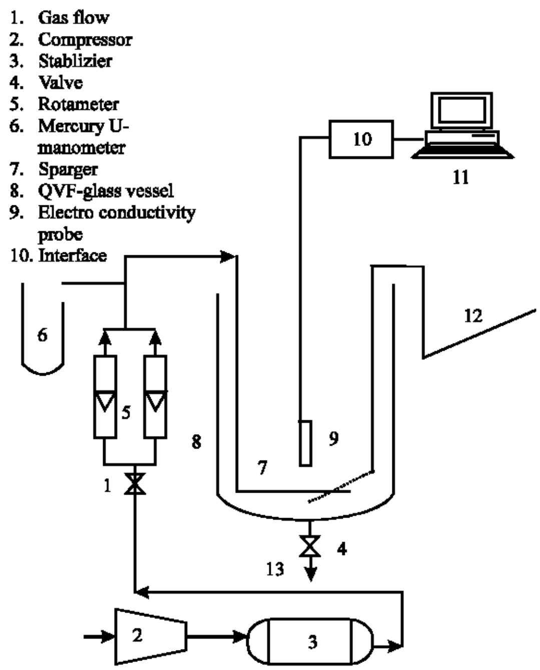

Fig. 1: Experimental approach

Table 1: The physical properties of liquid

Liquid concentration of PAA (wt%)	Flow behavior index (n)	Consistency Index (k , Pa.s^n)	Density at 303K ρ_L (kg m^{-3})	Surfacetension, (σ, N m^{-1})
0.01	0.800	0.0062	1000.2	0.0208
0.03	0.720	0.0139	1000.5	0.0214
0.05	0.651	0.0289	1000.7	0.0232
0.07	0.594	0.0589	1001.01	0.0245

purified and highly viscous polyacrylamide powder in water. The resulting solutions exhibited a pseudoplastic rehological behavior which was well represented by means of simple power low Ostwald De-Waels model. The consistency index k and power low index n fitted for each process and shown in Table 1.

In order to measure the bubble characteristic of bubble rise velocity, bubble diameter, and gas hold up a bubble monitoring and analytical system was used which consists of a modified electroconductivity probe (tips). It was similar to that of (Burgress and Calderbank, 1975) but it consists of four tips instead of two.

RESULTS AND DISCUSSION

Figure 2 shows the steady state radial velocity profile from 2D simulations of the gas and liquid phases are shown in. All these steady state values were determined at a position 20 cm above the distributor and reported below. The flow structures that developed in three phase bubble column far away from sparger is expected to mainly consists of a parabolic radial profile of axial liquid and gas velocity. This is due to the fact that large bubbles are rising quickly in the center of the column dragging

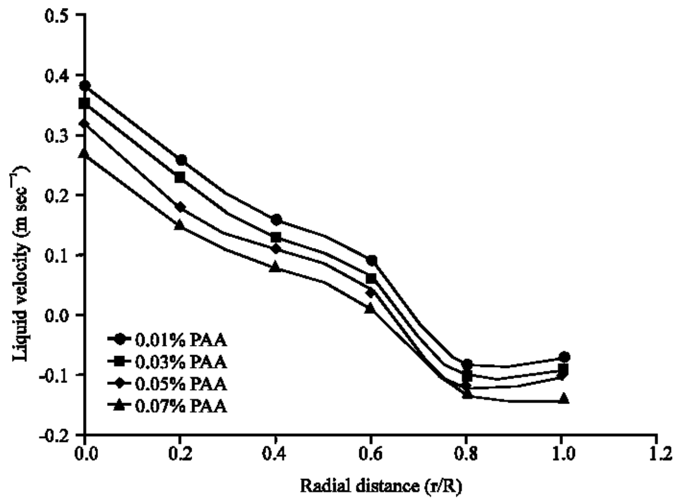

Fig. 2: Radial liquid velocity distribution

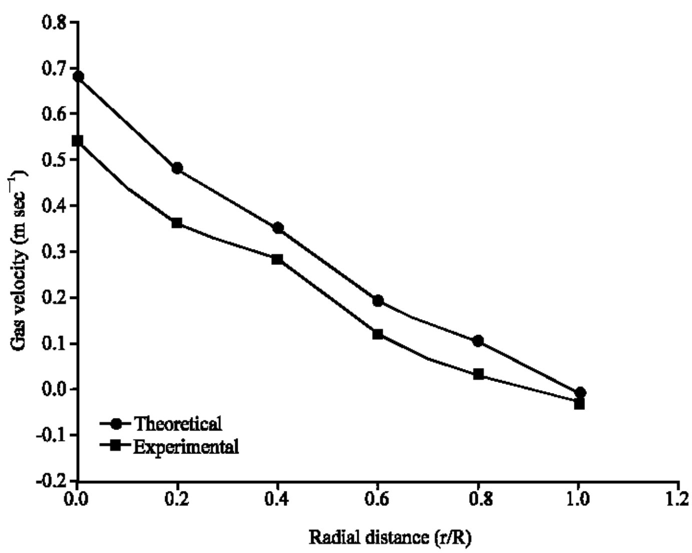

Fig. 3: Radial distribution of gas velocity with 0.01% of PAA

liquid with them, continuity consideration them lead to down flow area close to the reactor wall, as it shown in Fig. 2.

Figure 2 shows that the predicted liquid velocity distribution decreased with increasing of PAA concentration (and thus liquid viscosity). At the center of the column, for example, the liquid velocity is 0.32 m sec^{-1} in 0.01% PAA concentration; this value decreased to 0.27 m sec^{-1} in 0.07% PAA concentration. This can be attributed to that increasing of PAA concentration means an increase in effective viscosity, i.e., increasing in liquid viscous force, also it can be attributed due to the increase in bubble diameter (size), these large bubbles don't generate sufficient liquid circulation.

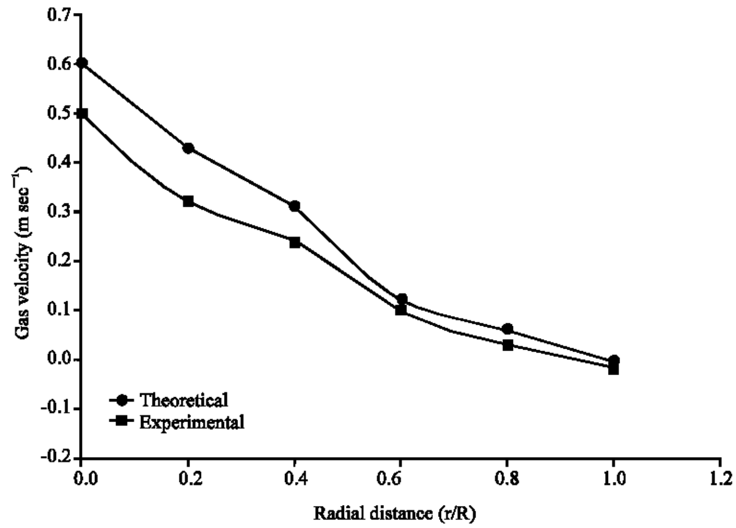

Fig. 4: Radial distribution of gas velocity with 0.03% of PAA

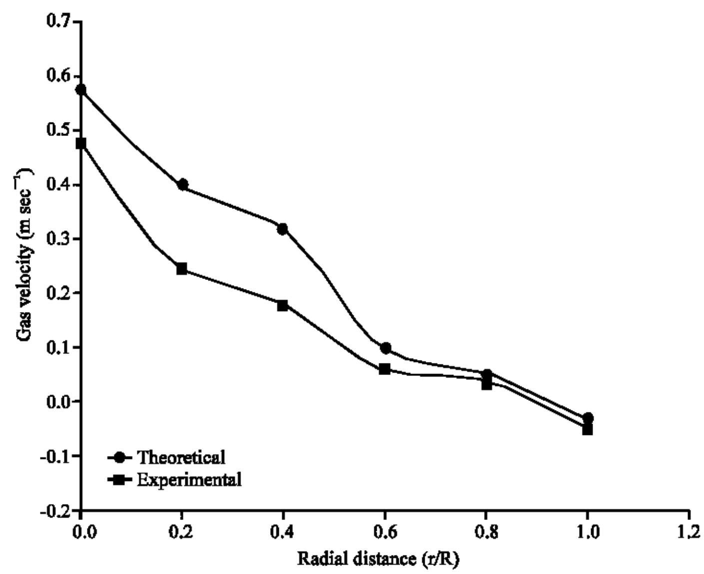

Fig. 5: Radial distribution of gas velocity with 0.05% of PAA

Table 2: The experimental results of gas velocity at different axial position and PAA concentration

Position	PAA concentration (%)			
(r/R)	0.01	0.03	0.05	0.07
0.2	0.35	0.32	0.25	0.24
0.4	0.27	0.25	0.18	0.20
0.6	0.11	0.10	0.075	0.07

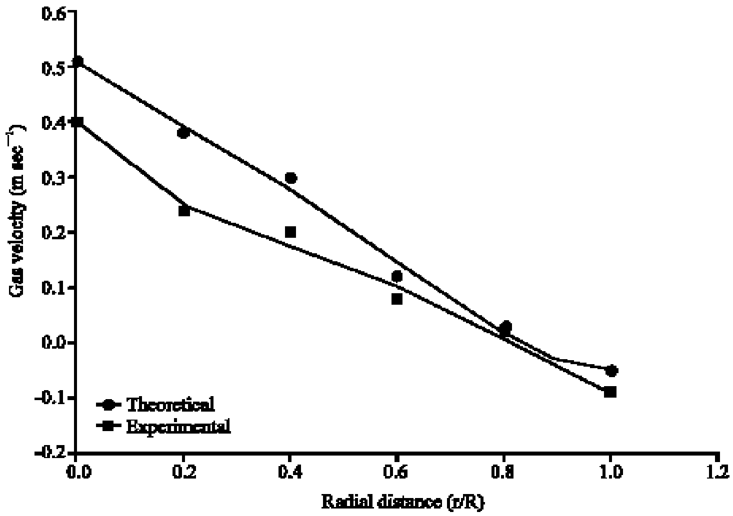

Fig. 6: Radial distribution of gas velocity with 0.07% of PAA

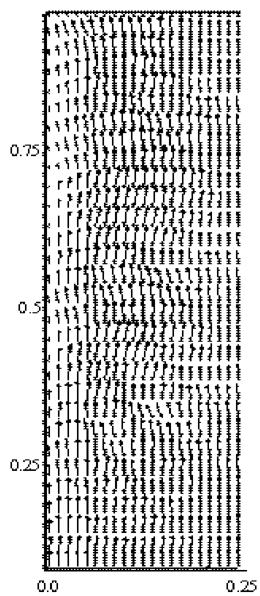

Fig. 7: Gas flow pattern

The experimental results of gas velocity at different axial positions and different gas concentration are shown in Table 2. It could be noticed from this table that gas velocity increases with increasing PAA concentration. This Increasing is coupled with decreasing in gas hold up. The later decreasing can be explain on the basis of hindered gas bubble motion in viscous fluid, in which at very height drag forces will be height enough to cause bubble coalescence. This means increasing PAA concentration causes an increase in its viscous force that will depress bubble breakup.

The ability to compare the model prediction results with the corresponding experimental data obtained with gas non-Newtonian solid system could be shown in Fig. 3- 6. These figures show the radial gas velocity, experimentally and theoretically. It can be seen that the curves corresponding well to the measured local gas velocity and the largest difference simulation and experimental are detected in the region close to the center of the column. This large difference may be due to the symmetry assumption and to the absence of the continuity balance of the solid phase as well as to the absence of third dimension .

The simulated gas flow pattern can shown in Fig. 7, representing the central up flow and down flow at the wall. Also, in agreement with experimental observation the model predicts that for a given gas velocity an increasing in PAA concentration caused a decrease in its value, for example at the center of the column the gas velocity in 0.01% PAA concentration is 0.54 m sec^{-1} and the predicted one is 0.68 m sec^{-1} these values decrease to 0.4 and 0.51 m sec^{-1}, respectively in 0.07% PAA concentration and this is due to the height viscous force of the liquid.

CONCLUSIONS

In this study, a two dimensional model of CFD technique has been used to describe the gas and liquid velocity distribution in slurry bubble column for three phase reactor containing a non-Newtonian liquid. This model based on the continuum and momentum equations and it seems to predict reasonable radial profiles of velocity for gas and liquid.

The simulated liquid velocity was found to have the parabolic shape. It decreases with increasing PAA concentration due to the increase of viscous force.

The distribution of gas velocity also has the parabolic shape with increasing in its value with increasing of flow consistency.

NOMENCLATURE

CD : Drag coefficient
db : Bubble diameter (m)
dp : Particle diameter (m)
Fgl : Gas-liquid interfacial force (N m^{-1})
Fsl : Solid-liquid interfacial velocity (N m^{-1})
g : Gravity acceleration (N m^{-1})
k : Consistency index (kg /ms^{2}-n)
n : Flow behavior index
P : Pressure
Re : Reynold number
uS : Slip velocity (m sec^{-1})
Vb : Bubble rise velocity (m sec^{-1})
VG : Gas velocity (m sec^{-1})
VL : Liquid velocity (m sec^{-1})

GREEK SYMBOLS

γ : Shear rate (sec^{-1})
ε_g : Gas hold up

ε_L : Liquid hold up
ε_S : Solid hold up
μ_{eff} : Effective viscosity (kg/ms)
ρ_G : Gas density (kg m^{-3})
ρ_L : Liquid density (kg m^{-3})
ρ_S : Solid density (kg m^{-3})
σ : Surface tension (N m^{-1})
τ : Shear stress (Pa)
τ_0 : Yield stress (Pa)

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