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Axial and Radial Gas Holdup in Bubble Column Reactor

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Bubble column reactors are considered the reactor of choice for numerous applications including oxidation, hydrogenation, waste water treatment, and Fischer-Tropsch (FT) synthesis. They are widely used in a variety of industrial applications for carrying out gas-liquid and gas-liquid-solid reactions. In this paper, the computational fluid dynamics (CFD) model is used for predicting the gas holdup and its distribution along radial and axial direction are presented. Gas holdup increases linearly with increase in gas velocity. Gas bubbles tends to concentrate more towards the center of the column and follows a wavy path.

Key Words : Bubble column, Gas holdup, Radial gas distribution, Hydrodynamics, CFD

Introduction

Bubble column reactors are of considerable interest in industrial processes and various biochemical processes. They are used for processes involving oxidation, polymerization, waste water treatment, Fischer-Tropsch (FT) and environmental friendly biomass/coal/gas-to-liquid fuels production. For reactions occurring in gas-liquid/slurry reactors, the gas liquid mass transfer rate is important. The mass transfer depends largely on the gas holdup and the interfacial area, which are also inter dependent. Effective mixing as well as high gas holdup and interfacial area between the phases leads to improved heat and mass transfer characteristics.

Bubble columns are cylindrical vessels filled with water, wherein gas is sparged at bottom *via* a distributor, in the form of bubbles, into liquid or liquid-solid suspension (slurry bubble columns). The liquid inside column begins to expand as soon as gas is introduced. Bubble column offer advantages of good heat and mass transfer characteristics. Ease to construct and operate, absence of moving parts, low maintenance cost and relatively cheap to install are some of the factors that render the bubble columns an attractive choice as reactors for the described processes.

The potential of Computational Fluid Dynamics (CFD) for describing the hydrodynamics of bubble column has been established by several publications in the past (Baten and Krishna, 2005; Wang and Wang, 2007). What happens quantitatively, when fluids flow, how fluid flow, how are the velocity vectors, how the pressure contours are predicted by the CFD simulations. Thus CFD can successfully be used to study the hydrodynamics of bubble column reactor. In the present paper CFD simulations have been carried out to predict gas holdup and its distribution along the column in axial and radial direction.

Development of CFD Model

Geometry. FLUENT preprocessor GAMBIT is used as geometry and mesh generator. A two dimensional bubble column of length 1 m and diameter 0.1 m is used which gives a length to diameter (L/D) ratio of 10. Mesh size of 0.005 m × 0.001 m is used in L/D directions. Bottom face contain 0.002 m diameter inlet for air at the center. Velocity inlet and pressure outlet boundary condition is used. The computational grid details are shown in the Figure 1.

Solver Settings. Commercial CFD software package FLUENT is used to solve the equations of continuity, turbulence and volume fraction. Pressure velocity coupling is obtained using SIMPLEC algorithm.

Simulations were carried out for 0.003 m bubble diameter with air water system, operating at superficial gas velocities ranging from 0.001 m/s to 1 m/s. Initial volume fraction of water was taken zero for all the simulations. Rake was defined from 0.5 m to 1 m at the interval of 0.01 m counting to 50 in numbers. Computational grid details are shown in Figure 1. The time stepping strategy used in all simulations

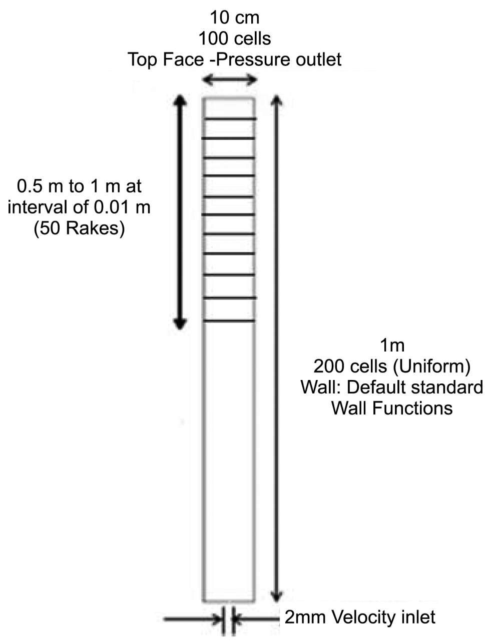

Figure 1. Computational grid details.

is 5000 time steps with 0.0001 time step size, next 2000 steps at 0.001 and remaining steps at 0.01 until steady state was achieved. The steady state was achieved in about 9000 time steps, but simulations were run until 60 seconds *i.e.* 12750 time steps. Steady state was indicated where all the variables remained constant. 2D simulations were carried out on Windows 7 platform, running on Intel Core (TM) I3 processor with 3.2 GHz CPU frequency. Each simulation was completed in about a day.

Equations. The governing equations are given below:

1. Continuity equation for gas phase

$$\frac{\partial}{\partial t}(\alpha_1\rho_1) + \nabla.(\alpha_1\rho_1\bar{v}_1) = 0 \qquad (1)$$

2. Continuity equation for liquid phase

$$\frac{\partial}{\partial t}(\alpha_2\rho_2) + \nabla.(\alpha_2\rho_2\bar{v}_2) = 0 \qquad (2)$$

3. Volume fraction sum

$$\alpha_1 + \alpha_2 = 1 \qquad (3)$$

4. Conservation of momentum for gas phase

$$\frac{\partial}{\partial t}(\alpha_1\rho_1\bar{v}_1) + \nabla.(\alpha_1\rho_1\bar{v}_1\bar{v}_1) = -\alpha_1\nabla p + \alpha_1\rho_1\bar{g} \qquad (4)$$

5. Conservation of momentum for liquid phase

$$\frac{\partial}{\partial t}(\alpha_2\rho_2\bar{v}_2) + \nabla.(\alpha_2\rho_2\bar{v}_2\bar{v}_2) = -\alpha_2\nabla p + \alpha_2\rho_2\bar{g} \qquad (5)$$

6. k-€ Turbulence model

$$\frac{\partial}{\partial t}(\rho_m k) + \nabla.(\rho_m\bar{v}_m k) = \nabla.\left(\frac{\mu_{t,m}}{\sigma k}\nabla k\right) + Gk_m - \rho_m € \qquad (6)$$

$$\frac{\partial}{\partial t}(\rho_m €) + \nabla.(\rho_m\bar{v}_m €) = \nabla.\left(\frac{\mu_{t,m}}{\sigma €}\nabla €\right) + \frac{€}{k}(C_1 € Gk_m - C_2 € \rho_m €) \qquad (7)$$

The Eulerian multiphase model (two phase) available in Fluent 6.3 was chosen to carry out computer simulation. Heat and mass transfer were not activated. The equation requires time averaged continuity and conservation equations for each phase.

Volume fraction of gas and liquid phase is calculated from Eqs. (1) and (2) respectively, with the condition that the volume fraction of phases sums to one. Eqs. (4) and (5) describe momentum balance for gas and liquid phases respectively. The k-€ turbulence model is used and solves the standard k-€ equations. The standard k-€ model is a semi empirical model based on model transport equations for turbulent kinetic energy (k) and the dissipation rate (€). The mixture density and velocity, ρm and $\bar{v}_m$ are computed from:

$$\rho m = \Sigma_{i=1}^{N} \propto i\ \rho i \qquad (8)$$

$$\bar{v}_m = \frac{\Sigma_{i=1}^{N} \propto i\ \rho i \bar{v}_i}{\Sigma_{i=1}^{N} \propto i\ \rho i} \qquad (9)$$

Turbulent viscosity $\mu_{t,m}$ in Eqs. (6) and (7) is written as:

$$\mu_{t,m} = \rho_m C\mu\frac{k^2}{€} \qquad (10)$$

It is obtained from the prediction of the transport equations for the k and € given in Eqs. (6) and (7). Gk is the rate of production of turbulent kinetic energy. The model constants are Cμ, C_1€, C_2€, σk and σ€ and their respective values are: 0.09, 1.44, 1.92, 1.0 and 1.3.

Results and Discussion

Overall Gas Holdup. The cross sectional area averaged and volume averaged gas holdup values is shown in Figure 2(a) and (b) for low uperficial gas velocity (0-0.01 m/s) and for higher superficial gas velocity (0-1 m/s) respectively. The gas holdup increases almost linearly with the superficial gas velocity. Similar results have been reported by Baten and Krishna (2005), Cachaza *et al.* (2009). As the gas velocity increases, the amount of gas introduced per unit time increases and so also the gas holdup increases.

Radial Distribution of Gas Holdup. The radial distribution for time averaged local gas holdup for varying superficial gas velocity at a height of 0.5 m from the gas distributer is shown in Figure 3. With increasing gas velocities, gas holdup increases. This is because gas bubble tend to concentrate more and more in the central core of the column (Baten and Krishna, 2005). This concentration of bubbles in the central core causes a substantial increase in the liquid circulation.

Gas Holdup Distribution along Column Height. Cross sectional area averaged values of gas holdup at different

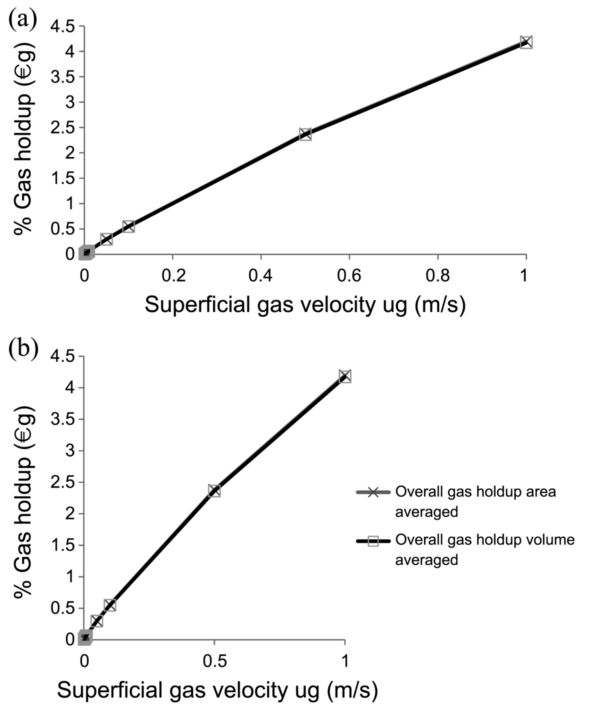

Figure 2. (a) Cross sectional area averaged and column volume average gas holdup as a function of low superficial gas velocity. (b) Cross sectional area averaged and column volume average gas holdup as a function of high superficial gas velocity.

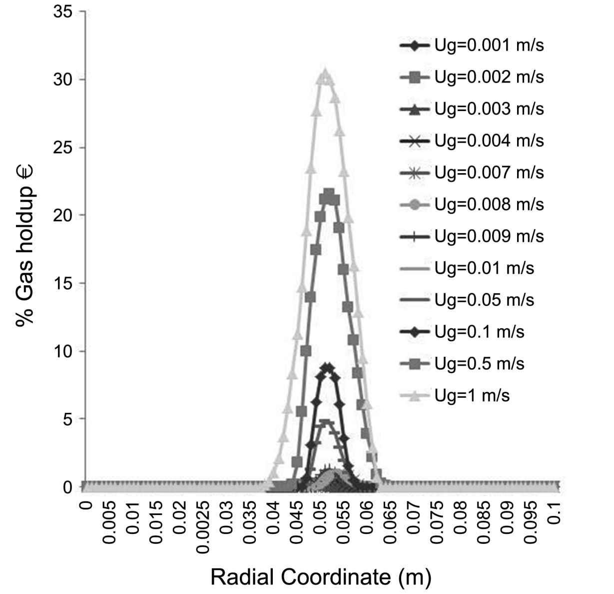

Figure 3. Radial distribution of gas holdup. Values measured at a height of 0.5 m from the gas distributor.

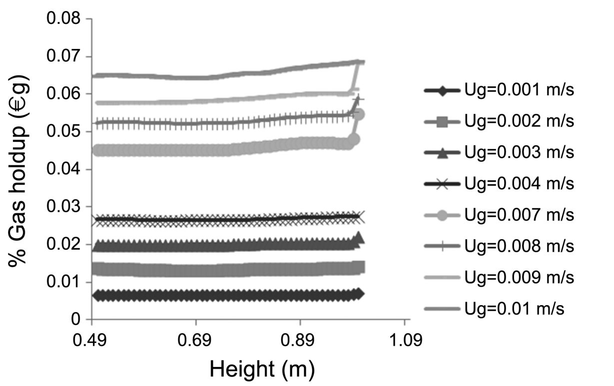

Figure 4. Gas Holdup Distribution along Column Height, values measured from a height of 0.5 m from gas distributer (For lower gas velocities).

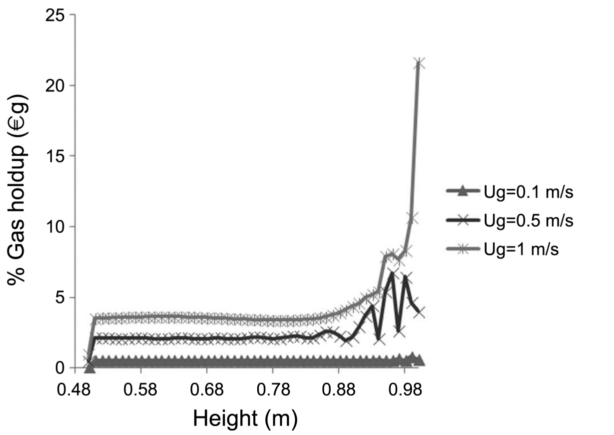

Figure 5. Gas Holdup Distribution along Column Height, values measured from a height of 0.5 m from gas distributer (For higher gas velocities).

heights in the column is shown in Figure 4 and Figure 5. For low gas velocities (Ug = 0.001 m/s to 0.01 m/s), (Figure 4) gas holdup remains constant with increasing height. For higher gas velocities (Ug = 0.1 m/s to 1 m/s), (Figure 5), upto 0.8 m (initial part of graph) height the gas holdup remains constant but with further increase in height gas holdup starts increasing with increase in gas velocity.

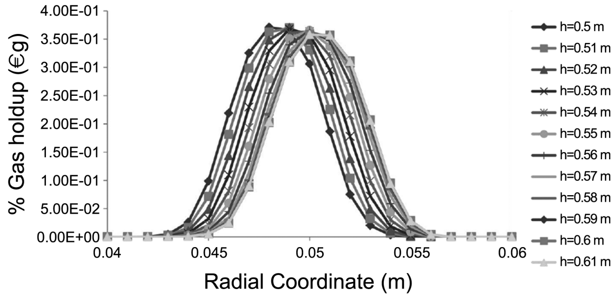

Figure 6. Radial distribution of gas holdup at varying heights.

Predicting Wavy Nature. Figure 6 shows the radial distribution of gas holdup at different heights. It is useful in predicting the wavy flow nature of gas. The peaks of the each curve are not situated along a straight line but these peaks of each curve are displaced in radial direction. This indicates the movement of the central core of gas. So it is clear that the gas follows a certain wavy flow pattern. Similar results are also reported by Joshi *et al.* (2002).

Conclusions

A CFD model is developed to describe the hydrodynamics of air-water bubble column reactor. The studies for overall gas holdup and its distribution along the radial and axial direction are discussed. Cross sectional area averaged gas holdup increases with increase in gas velocity. From the radial distribution of gas holdup it is observed that the gas bubble tend to concentrate more and more in the central core of the column. For low gas velocities the gas holdup remains constant with increase in height. With increase in height the radial distribution of gas holdup follows a shift in peaks which indicates the movement of central core of the gas along a wavy path.

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