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CFD SIMULATION OF BUBBLE COLUMN REACTOR BY INVESTIGATING THE EFFECT OF TRAYS ON OVERALL GAS HOLDUP

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In the current research work, CFD model has been developed to estimate overall gas holdup for co-current air-water system in a Trayed Bubble Column Reactor (TBCR), operating in bubbly flow regime. The TBCR considered in this study has 19 cm inner diameter and 274 cm length. Unsteady 2d-axi symmetric, Eulerian-Eulerian multiphase model with segregated solver has been considered while turbulence effects are introduced by using generalized k-ε model with the option of each-phase turbulence model. The effect of trays has been studied on overall gas holdup while liquid superficial velocity, tray's open area and bubble diameter have been kept constant. Simulations have been performed for various values of superficial gas velocities in the range of 1-8 cm/s and constant superficial liquid velocity of 0.5 cm/sec. The overall gas holdups found by simulations, have been compared with experiments [1] and with internationally published correlations for bubble column reactors by Kato et al. [5], Chen et al. [2] and Vinaya et al. [8], which shows a fair concurrence of the CFD results. It is found that overall gas holdup significantly increases by introducing trays to the column.

Keywords: Bubble column reactors; CFD; Gas holdup; Hydrodynamics of TBCR; Effect of trays

1. Introduction

Overall gas holdup ε_g is the key parameter in the design and scaleup of BCRs. It represents the volumetric fraction of the dispersed phase in the two phase flow system. The gas holdup coupled with the knowledge of the mean bubble diameter allows the determination of the gas-liquid interfacial area, which is necessary in the prediction of gas-liquid mass transfer coefficient [6]. The average bubble size, superficial velocities, trays, tray's hole diameter and addition of surfactants are the important factors that govern the extent of the gas holdup in bubble column reactors. Important applications include oxidation, hydrogenation, halogenation, hydrohalogenation, ammonolysis, hydroformylation, Fischer–Tropsch reaction, ozonolysis, carbonylation, carboxylation, alkylation, fermentation, waste water treatment, hydrometallurgical operations, steel ladle stirring and column flotation, etc.

The introduction of trays to bubble column reactors helps to supplementary enhance the intensity of interfacial transport and to decrease the axial dispersion of the gas and liquid phases, which is desirable in a number of industrial processes. The average bubble size, superficial velocities, trays, tray's hole diameter and addition of surfactants are the important factors that govern the extent of the gas holdup in bubble column reactors.

Chen et al., 1989 [2] studied the overall gas holdup for various gas- liquid systems in both batch and co-current upward multistage units. They reported that the volumetric fraction of the dispersed phase significantly increases with each tray addition and that the variation of the surface tension of the liquid phase slightly changes the gas holdup.

Chen et al., 1986 [3] studied two types of plates in two different co-current trayed bubble columns. One of them was the Karr tray design whereas the second design was a perforated plate made out of meshed screen. They found that the Karr type yielded higher gas holdups. It was also observed that superficial liquid velocity has no significant effect on the gas phase volumetric fraction. They observed the formation of a cushion or layer of bubbles underneath the trays at low superficial

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liquid velocities. The correlations by these authors depicted the effect of the superficial velocities.

Kato et al., 1984 [5], studied the effect of tray design, stage height, superficial gas & liquid velocities and column diameter on gas holdup and reported that mean gas holdup is independent of trays and superficial velocity of liquid.

Vinaya et al., 1994 [8], developed a correlation for gas holdup of TBCR for both bubbly and churn turbulent regime, studied the effect of trays, tray's hole diameter, stage height, surface tension and gas velocity on gas holdup.

The only means to gain added knowledge and in depth understanding of the hydrodynamics in BCRs is Computational Fluid Dynamics (CFD). CFD is an efficient tool to illuminate the significance of physical effects and mechanical parameters. Wild *et al.* reported the most essential reasons for this increasing importance [7].

It is seen that limited work has been done for validating the experimental results of different parameters of bubble column using CFD techniques. The purpose of the present work is to fill the gap between the experimental results and CFD analysis of bubble column reactors. This will not only give the reliability of CFD codes and commercial softwares like Fluent for bubble column reactors but will also open new directions for the design and optimization of bubble column reactors and multiphase flow. Moreover, this will enable us to play with different parameters with less cost and greater advantages. Furthermore experimental work combine with CFD simulations will lead to correlate universal validity between the adjustable parameters and the physical properties.

2. Experimental Setup

The experimental setup consists of a 274 cm tall BCR with 19 cm internal diameter and co-current gas liquid flow arrangement, whose experimentations were carried out in "Sever Institute of Technology, Department of Chemical Engineering, Washington University, USA" in the year 2002 by "Javier Alvare Castro" under the supervision of Prof. Dr. M. H. Al-Dahhan [1]. The column is made of four intermediate sections plus a top and bottom section. The intermediate sections have an inside diameter of 19 cm and a total height of 52 cm each. The upper section has the same diameter as the intermediate one, but is only 33 cm tall. There is also a 33 cm tall bottom section where the gas and liquid phases enter the column and mix. The total height of the column from the base of the plenum to top of the disengagement section is 241cm. This is a five stage setup unit with a total of four trays.

3. CFD Model

In the current work, above mentioned experimental results have been simulated in the homogeneous flow regime (gas superficial velocity 1–8 cm/ sec and liquid velocity 0.5 cm/ sec) by using a commercial CFD software Fluent (Release 6.2.16). It is based on the finite volume approach to discretise the transport equations.

3.1. Grid Information

Axisymmetric simulations have been performed with 2D coordinates system assuming axial symmetry about the centerline of the column. The length of the domain is 274 cm and width is 9.5 cm, the grids used to generate the numerical results throughout this work have uniform quad-map mesh containing quadrilateral control volumes. The actual tray has been simulated in 2d domain as solid wall while the holes have been treated as interior. The further information about grid with boundary conditions is shown in figure 1.

3.2. Model information

2d-Axisymmetric, unsteady, two phase model of the BCR has been simulated using Euler-Euler multiphase model using air-water system. Air/water mixture has been introduced from bottom to the column co-currently against gravity. The column has been divided into two zones; upper and lower. Initially, it is assumed that the lower zone is filled with water (ε_g = 0), while the patched upper zone with air (ε_g = 1). The effects of gravity, liquid head and virtual mass have also been added to the model. The turbulence effects have been introduced via standard k-ε turbulence model with the option of per-phase multiphase turbulence model. All the simulations have been performed at a time step of 0.001 second. Commercial software FLUENT 6.2.13 has been used to facilitate the simulation process.

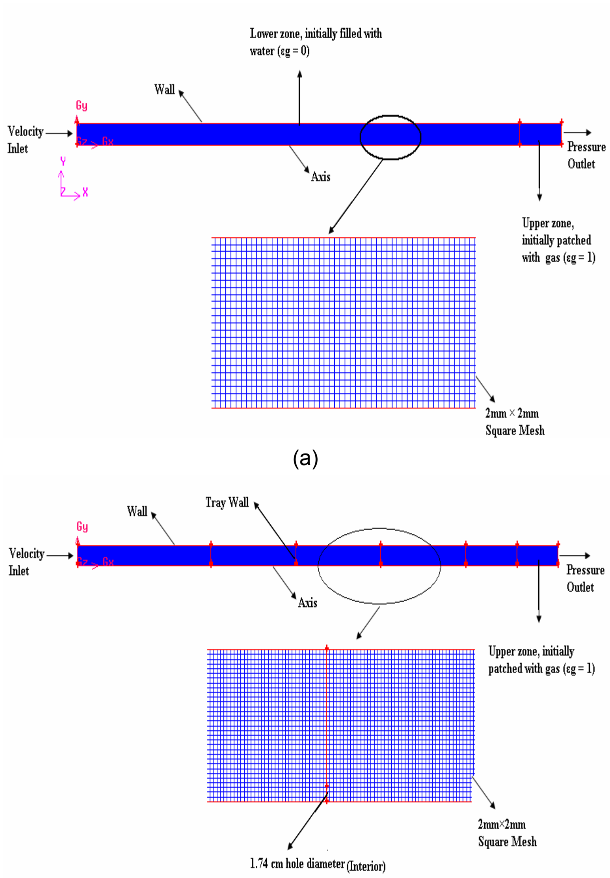


Figure 1. 2D Domain of BCR with boundary conditions and grid details; (a) Hollow BCR (b) TBCR with 1.74 cm tray's hole diameter.

4. Results of CFD Simulations

4.1. Grid and time independence

Several simulations have been carried out to check the grid independence on the basis of gas hold up. As a result of these simulations, square grids of 2mm×2mm and 3mm×3mm have been found to give same results throughout the domain, as shown in Figure 2. Finally a grid of 2mm×2mm has been chosen for simulations.

After selecting the best grid for simulation, time independence has also been checked on the same grid and gas holdup is plotted against time (sec.). It has been found that gas holdup upto four decimal points is time independent after 10 sec whereas upto seven decimal points, the time independence is obtained after 40 sec. So for better and reliable results, time duration of 40 sec and time step of 0.001 sec have been selected. The time independence results are shown in Figs. 3 and 4.

4.2. Validation of constant d_{32} assumption

All the simulations are based on the assumption of a constant bubble size in homogenous bubbly flow regime (1–8 cm/s) throughout the column. In Figure 5, a straight trend line for CFD results proves that this assumption is valid within the simulated regime.

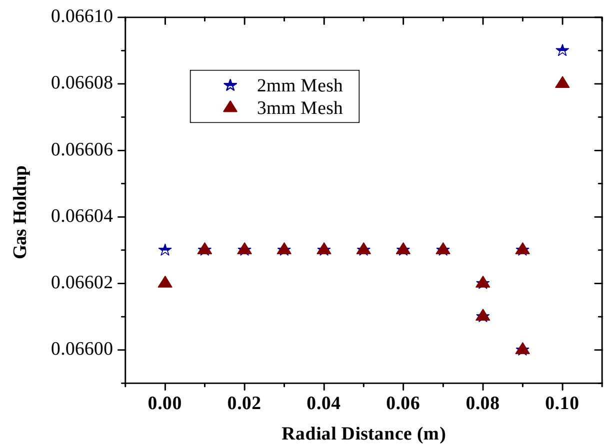


Figure 2. Grid independence of 2mm and 3mm square grid.

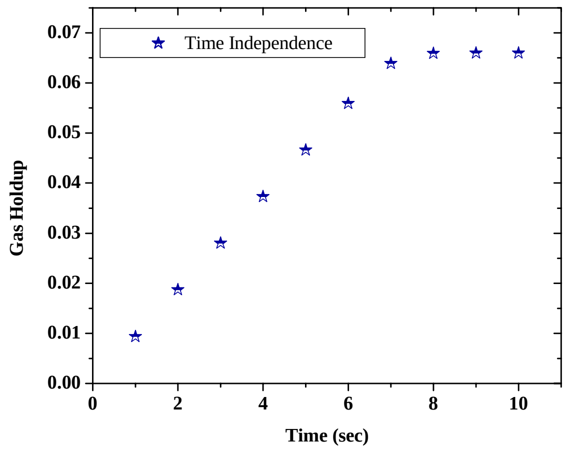


Figure 3. Time independence after 2 decimal places.

4.3. Comparison of CFD results

The results of CFD has been justified by the following means

1. Experimentation carried out in "Sever Institute of Technology, Department of Chemical Engineering, Washington University, USA" in the year 2002 by "Javier Alvare Castro" under the supervision of Prof.Al-Dahhan [1].

2. Kato et al. correlation (1984) [5].

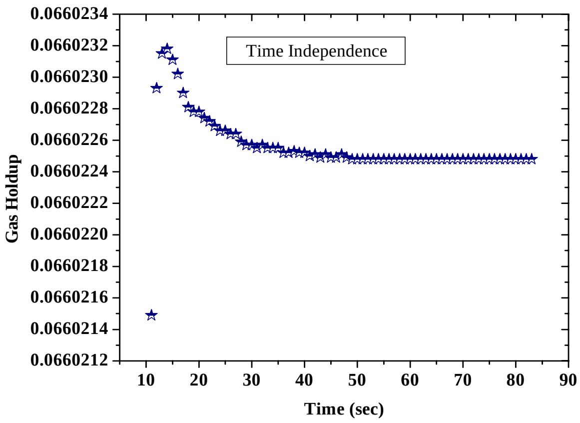


Figure 4. Time independence after 7 decimal places.

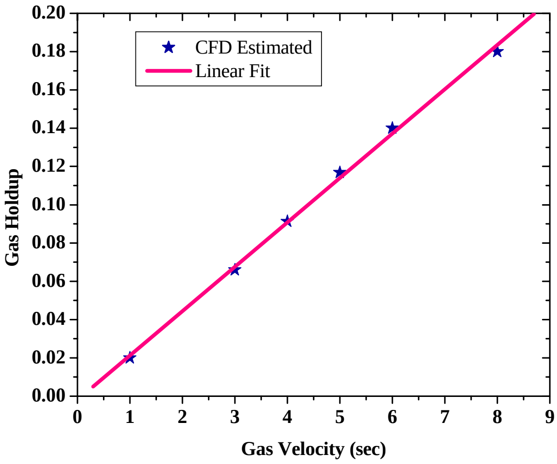


Figure 5. Representation of bubbly flow regime.

$$\varepsilon_g = \frac{V_g}{30 + 3.3 V_g^{0.8}} \quad (1)$$

Chen et al. Correlation (1986) [2]

$$\varepsilon_g = 0.448 V_g^{0.81} V_l^{-0.055} \quad (2)$$

Vinaya et al Correlation (1994) [8]

$$\varepsilon_g = 2.4 \left[\frac{V_g^2}{g d_0}\right]^{0.54} \left[\frac{d_0}{H_s}\right]^{0.26} \mathrm{O.A}^{-0.22} \left[\frac{\sigma}{\sigma_w}\right]^{-0.3} \quad (3)$$

Simulated results of gas holdup in bubbly flow regime for cocurrent trayed bubble column reactor have been generated. Air-water system has been simulated. Figures 6-7 show the comparison of CFD results obtained by simulations with internationally published correlations of Kato et al. [5], Chen et al. [2], Vinaya et al [8] and with the experimental results of Alvare [1]. The CFD simulated results show a very good agreement with the experimental results of Alvare [1]. Other correlations also confirm the accuracy of CFD results.

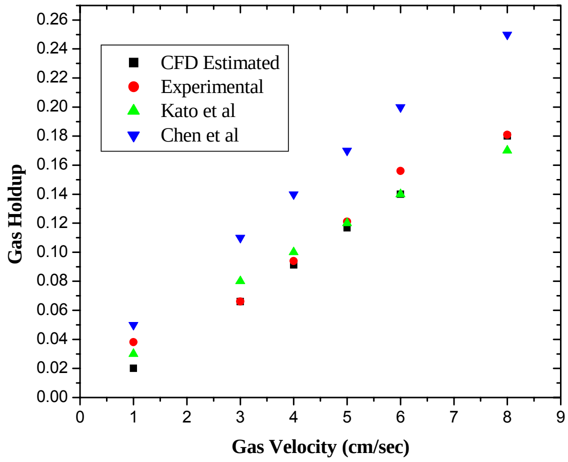


Figure 6. Comparison of CFD and international correlations for hollow column.

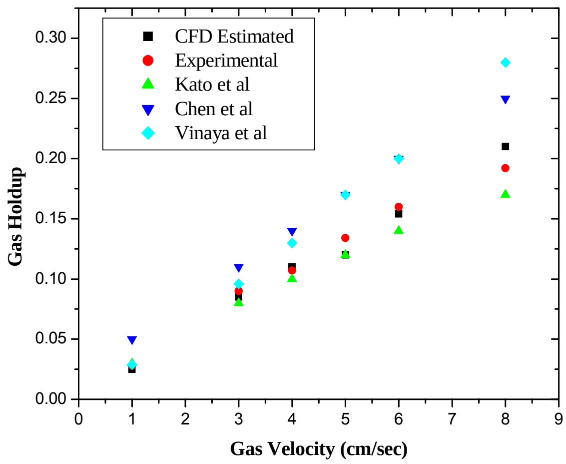


Figure 7. Comparison of CFD and international correlations for TBCR with tray's hole diameter of 1.74 cm.

4.4. Effect of trays on gas holdup

Effect of trays has been studied on over all gas holdup of BCR by simulating the column in CFD. In first set of simulations, the effect of superficial gas velocity has been investigated and it is found that over all gas holdup increases almost linearly by increasing superficial gas velocity in bubbly flow regime of BCR.

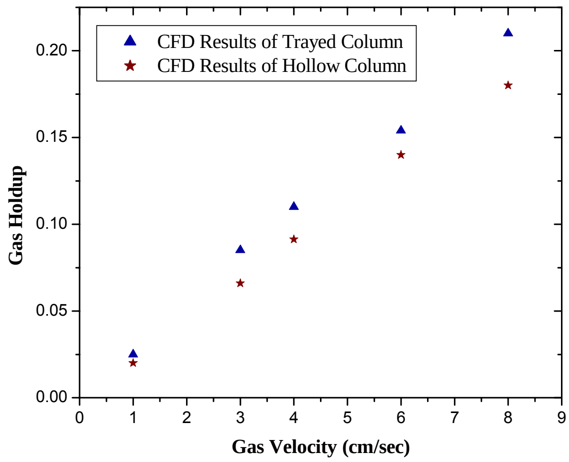
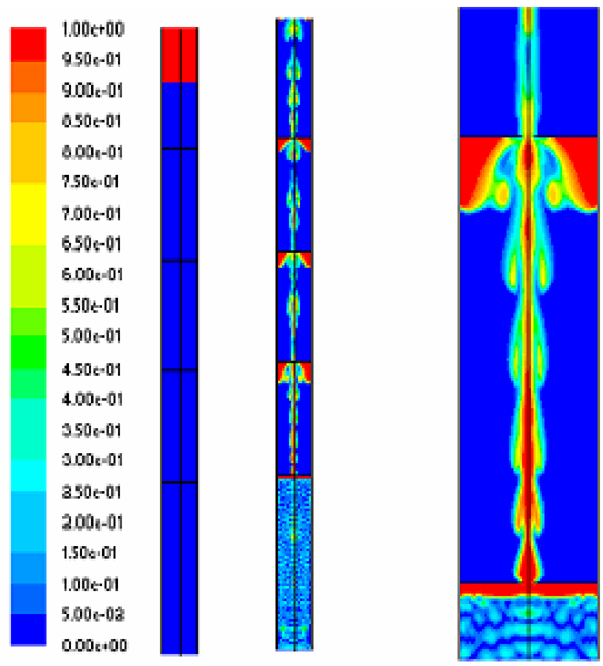


Figure 8. Results of CFD simulations showing the effect of trays on gas holdup.



(a) (b) (c)

Figure 9. Gas Holdup contours; (a) Column during initialization (b) Full column (c) One stage.

In the second set of simulations, the effect of staging the column, by the introduction of sieve trays has been studied. When trays of constant hole diameter (1.74 cm) and constant open area (10 %) have been introduced then overall gas holdup increases by an amount of 17 % as compared to hollow BCR. This increase in overall gas holdup is due to the following reasons.

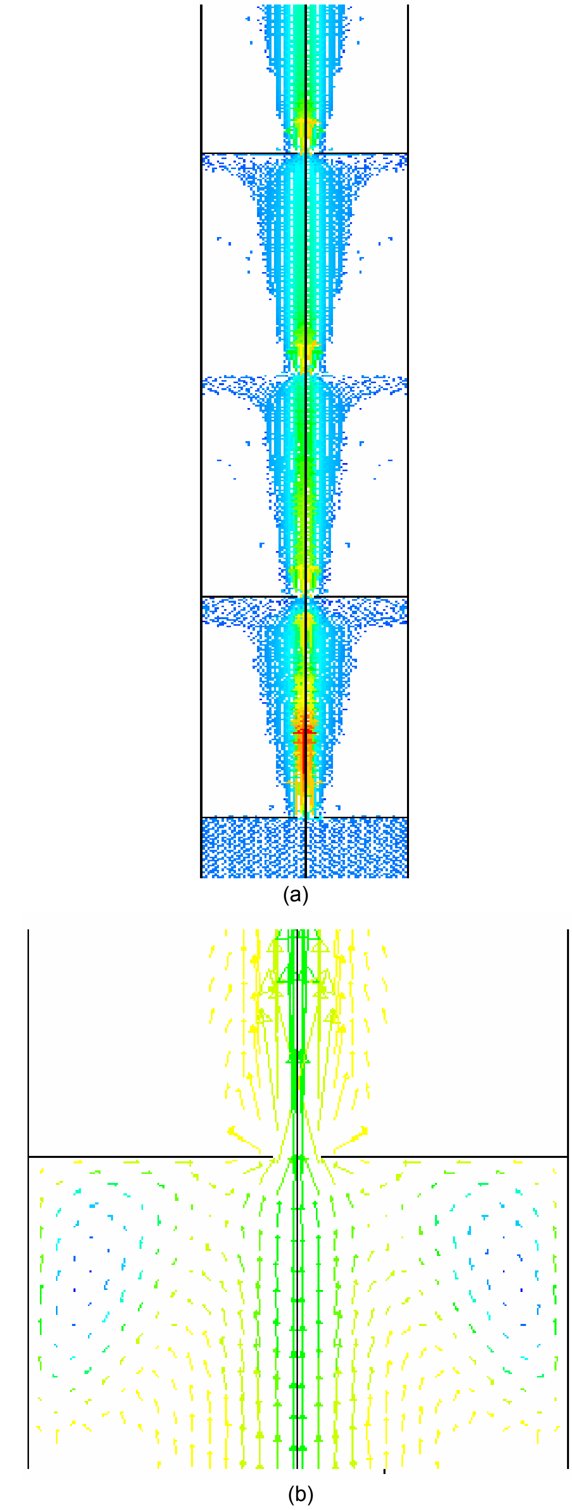


Figure 10. Representation of gas phase recirculation beneath trays (a) Full column (b) Single stage.

5. Conclusions

In this study, CFD simulations of co-current TBCR have been carried out. A 2d axisymmetric domain is selected to investigate the effect of trays and superficial gas velocity on overall and staged gas holdup. The CFD estimated results show good agreement with experimental results conducted by Alvare (2002) [1] and with some internationally published correlations [2, 5, 8] for air-water system, It has been found that gas holdup is very sensitive to some design parameters of the column and physical properties of liquid system. It increases significantly by the addition of trays and increasing superficial velocity of gas. It has been concluded that design parameters of the column and physical properties of liquid phase greatly influence the overall gas holdup in bubble column reactor.

Notations

d_{32} = Sauter mean bubble diameter

d_0 = Tray's hole diameter

g = Acceleration due to gravity

k = Kinetic energy

V_g, V_l = Gas and liquid superficial velocity

ρ_l = Density of liquid phase

ρ_g = Density of gaseous phase

μ_l = Viscosity of liquid phase

μ_l = Viscosity of gaseous phase

σ = Surface tension

σ_w = Surface tension of water

ε_g = Gas holdup

ε = Dissipation rate

Hs = Stage height

O.A = Open area

TBCR= Trayed bubble column reactor

BCR = Bubble column reactor

CFD = Computational fluid dynamics

2d = Two dimensional

Acknowledgement

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