CFD Investigation of Bubbly Flow through a Bubble Column with Cross-Flow and Rectangular Geometry

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Abstract:
In this study, a 2D CFD Simulation is presented to investigate the hydrodynamics of a rectangular bubble column reactor for bubble enhanced CO_2 absorption process. Understanding the complexity of fluid dynamics of two-phase flow in a rectangular bubble column contactor will provide important insights on how to enhance CO_2 absorption efficiency of the PCC process. CFD simulation was used to investigate key hydrodynamic parameters to gain useful insight on the best column geometry for a bubble enhanced absorption process for PCC using chemical solvents. These insights could be useful in column design, process optimization and cost reduction of the PCC process.

Keywords: Bubble Column, CFD Modelling, Multiphase flow, Cross flow, Liquid-Holdup

1. Introduction

Bubble column reactors have been widely used as multiphase contactors or reactors in chemical, biochemical, petrochemical and metallurgical industries. Bubble columns are used particularly in processes involving chemical reactions such as absorption, oxidation, alkylation, chlorination, polymerization, hydrogenation [1] and in biochemical processes such as fermentation [2] and biological wastewater treatment such as bioremediation [3]. The wide application of bubble column could be explained based on its advantages compared to other categories of multiphase contactors e.g. packed bed. Some of the advantages of bubble column reactors include; simple to construct, low operating and maintenance cost, high heat and mass transfer rate, larger surface area, longer retention time and compactness and absence of any moving parts [1,4].

In multiphase reactors, the continuous phase is either liquid or gas while the disperse phase can be bubbles, droplets, particles or combinations of them. Size and velocity distribution of the disperse phase has been identified as its governing features. Other key parameters that significantly affect the performance of a bubble column reactor include column diameter, column height, bubble diffuser design (sparger design), column internal design, and geometry [4].

Flow dynamics in bubble column reactors are very complex; therefore, development of detailed fluid dynamic model is important to understand these complex interactions, which is beneficial for the reliable and efficient design of these reactors. The complex hydrodynamics of bubble columns has inhibited the development of design procedures from first principle [5], Figures 1 and 2 summarizes the advantages and challenges of bubble column reactors design and applications.

Typically, two basic ways to simulate flow dynamics of two-phase gas-liquid systems are the two fluid approach (Euler-Euler) in which both the liquid phase and the gas-phase motion are considered as homogeneous or inter-penetrating continua. In the second approach (Euler-Lagrange), the volume averaged Navier-Stokes equations are used to describe the motion of the liquid and computes the motion of the dispersed gas-phase elements (e.g bubbles) in a Lagrangian way by individually tracking them on their way through the liquid body. Two fluids Euler-Euler model is basic macroscopic model for two-phase fluid flow. The derivation of the model equations for the two-phase bubbly flow starts with the assumption that both phases can be described as continua, governed by the partial differential equations of continuum mechanism. The phases are separated by an interface, which is assumed to be a surface [6,7].

Co-current and counter current bubbly flow reactors are the most commonly designed and applied in both industries and in research and development. In this paper, we study a design of bubbly flow reactors with cross flow and internals design because of it offers a significant practical interest.

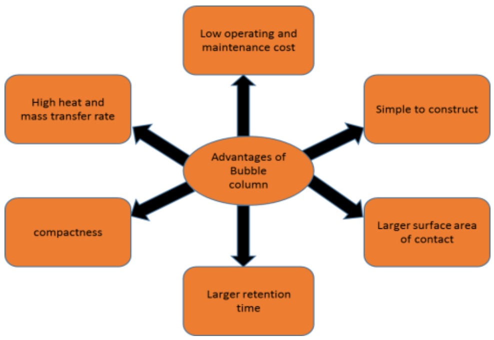

Figure 1. Advantages of bubble column

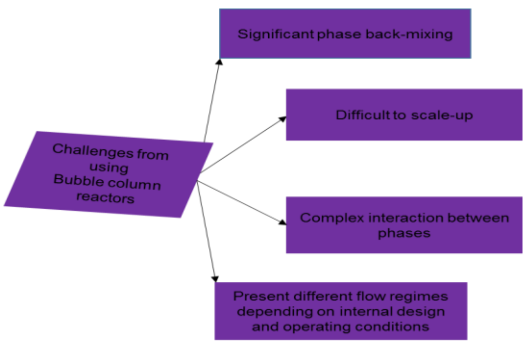

Figure 1. Challenges of bubble column

2. Computational Model Governing Equations

The two-phase laminar bubbly flow interface is suitable for macroscopic modelling of flow comprising of liquids and gas bubble mixture. The bubbly flow interface solve for average volume fraction occupied by each phase instead of tracking each bubble precisely and clearly. In this interface, each phase has its own velocity field (COMSOL 5.2 user guide).

2.1 Two phase laminar bubbly flow equation

Two phase laminar bubbly flow physics interface was used to simulate the gas-liquid flow in the packed bed.

$$\phi_l\,\rho_l\,\frac{\partial u_l}{\partial t} + \phi_l\rho_l u_l * \nabla u_l = -\nabla p + \nabla * \left[\phi_l\,(\mu_l + \mu_\tau)(\nabla u_l + \nabla u_l^{\tau} - \frac{2}{3}(\nabla * u_l)I)\right] + \phi_l\rho_l g + F$$

Where:

u_k *is the velocity vector for the* k^{th}*phase* (m/s)

P is the pressure (Pa)

ϕ_k is the phase volume fraction k^{th} *phase* (m^3/m^3), ρ_k is the density of the k^{th} *phase* (kg/m^3),

g is the gravity vector (m/s^2),

F is any additional volume force (N/m^3),

μ_k *is the dynamic viscosity of the* k^{th} phase

The continuity equation for the bubbly flow interface is given as:

$$\frac{\partial}{\partial x}\left(\rho_l\phi_l + \rho_g\phi_g\right) + \nabla.\left(\rho_l\phi_l u_l + \rho_g\phi_g u_g\right) = 0$$

Gas phase transport equation is given by:

$$\frac{\partial y}{\partial x} + \nabla.\left(\phi_g\rho_g u_g\right) = -m_{gl}$$

Where m_{gl} is the mass transfer rate from the gas to the liquid ($kg/(m^3.s)$), for low gas volume fractions ($\phi_g \sim 0.01$) you can replace momentum equation and the continuity equation with:

$$\phi_l\rho_l\frac{\partial u_l}{\partial x} + \phi_l\rho_l u_l.\nabla u_l =$$

$$-\nabla_P + \nabla.\left[\phi_l(u_l + \mu_T)\left(\nabla u_l + \nabla u_l^T\right)\right] + \phi_l\rho_l g + F$$

$$\rho_l\nabla.u_l = 0$$

In COMSOL Multiphysics, the bubbly flow interface use equation (3.4) and (3.5) by default to switch to equation (3.1) and (3.2), the low gas concentration check box under the physical model section has to be cleared by clicking it. The physics interface solves for ul, p and $pho_{geff} = \rho_g\phi_g$.

3. Numerical Methodology

The finite element method was used to discretize the governing equations. The geometry of the simulation model is schematically presented in Figure 3. The geometry consists of 2D rectangle height 250mm, width 300 mm. Physics controlled uniform grid was used. Time dependent study was used for the simulation until steady state was achieved. The other boundary conditions of all simulations are presented in Table 1. The composition of liquid and gas phase media is presented in Table (2).

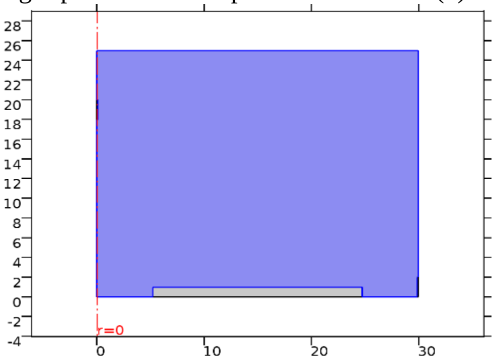

Fig. 3 Schematic diagram of 2D rectangular geometry of bubble column reactor.

Boundary	**Materials**	**Type**	**Value**
Liquid inlet	30 wt % MEA	Volumetric flow rate	0.1-0.2 L/min
Gas inlet	Flue Gas	Volumetric flow rate	1-15 L/min
Liquid outlet		0 Pa	
Gas outlet		0 Pa	

Table 1. Other boundary conditions for all simulations

		Flue gas		Liquid Solvent	
Flux	L/min	1-20		0.1 – 0.2	
Mass content	%	air	87.1	H_2O	80
		CO_2	11.4	MEA	30
		H_2O	1.5	additives	0

Table 2. Liquid and Gas media composition

3.1 Model boundary conditions

In gas-liquid (two-phase) flow simulation, at first the reactor is full of liquid. The bottom of the column contains a rectangular shape bubble diffuser with the following dimensions; width 20mm, length 195 mm, with extremely fine pore size that produces bubbles of 100-500 microns. Gas inlet velocity boundary conditions is assigned to the bubble diffuser. A pressure boundary conditions is applied to the top of the column with an average static pressure 0 Pa. No-slip boundary conditions where velocities increased from zero at the walls to free stream velocity away from the wall surface were applied to the walls of the column.

4. RESULTS AND DISCUSSION

A rectangular bubble column of with the following dimensions; width 250 mm and length 300 mm has been simulated in COMSOL multiphysics® version 5.2, the results of the simulation has been presented graphically. Time dependent solver was employed for the simulation. It was observed from the simulation results that the column profiles changes with time initially, but after some time, it approaches quasi steady state in which no significant changes occur.

4.1 Velocity Magnitude

In multiphase flow e.g. gas-liquid systems in a bubble column reactor, the velocities of liquid and gas phases changes with time and distance in the column. Figure 4 presents the vector of liquid phase velocity magnitude obtained after attaining quasi-steady state. The velocity profile indicates that there is an intensive liquid circulation (vortex) developing in the column due to cross-flow and presence of some no flow region, which is upward in the central region above the gas diffuser and downward towards the near wall as presented on Figures 4 and 5. The velocity profile has also shown that there are regions of accelerated flow above the gas distributor and regions of low and negative flow towards the wall. The arrows indicate the gas flow pattern and direction in the column. The arrows also shows that some gas are driven by liquid through the liquid outlet. Dead zones (No flow zones) were also observed in Figure 4 due to the shape of the column and the bubble diffuser.

To correct these two problems of gas driven through the liquid outlet and presence of no flow region, liquid deflector and adjustable gas separator were incorporated to the design to increase the gas residence time and to eliminate dead zones in the column. Figure 6 presents a proposed column design with internals.

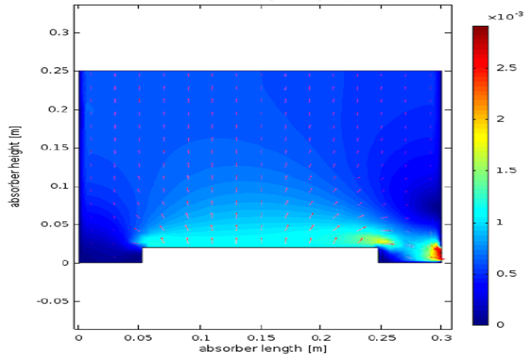

Fig. 4 Surface plot: velocity maganititude, liquid phase and arrows is gas velocity pattern and direction of gas flows.

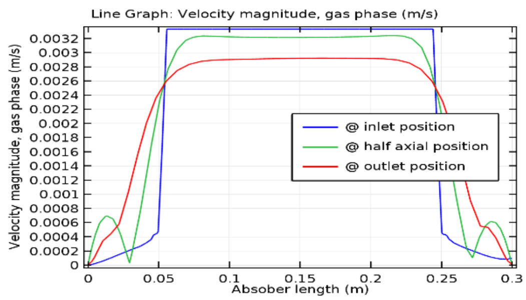

Fig. 5. Line graph: Gas velocity maginitute and different locations in the column.

Figure 5 presents a line graph for gas velocity profile at three different locations along the height. The line velocity profiles indicates that the pattern of gas velocity is not similar throughout the column, the velocity is higher in the area above the gas distributor and tends to reduce towards the column walls and also along the height of the column as the gas pass through the liquid in the column.

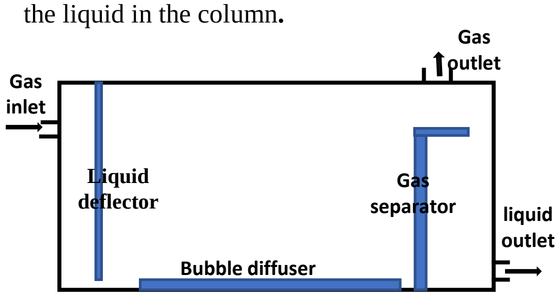

Fig. 6 Proposed bubble column design with internals

4.2 Gas Volume Fraction

2D surface plot of gas volume fraction for gas and liquid volumetric flowrate of 5 and 0.1 l/min until the system reached steady state was reached. The gas volume fraction is identical all over the column except at the dead zones as shown in Figure 7. Gas volume fraction is the measure of the mean average weighted area of gas volume fraction at acceptable number of points in the column.

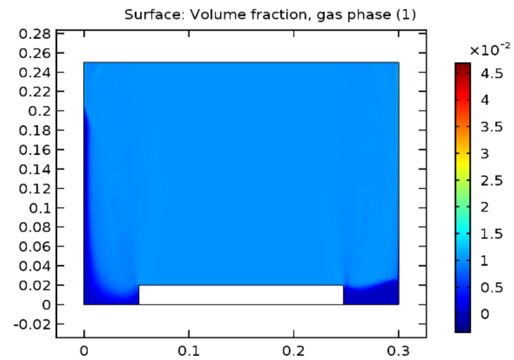

Fig. 7 2D Surface plot of Volume Fraction Gas

CFD simulation was used to obtain the gas volume fraction values at sufficient points in the bubble column. The gas volume fraction was obtained to be between 0 to 0.045 as presented on Figure 7. Figure 4 shows that the gas bubbles are being washed away as the liquid flow across the bubble column. In conventional co-current and counter-current flow geometry, the gas holdup decreases with increase in liquid velocity because the gas bubbles are being washed away by the liquid.

4.3 Gas Holdup Studies in Cross-flow Bubble Column without Internals

Relationship between total gas holdup and superficial velocity in horizontal bubble column without internals is presented in Figure 8. It is obvious from Figure 8 that the gas holdup increases sharply at low superficial velocity between 0.004-0.0011 [m/s], this regime correspond to homogeneous regime. The gas holdup then starts decreasing with increase in gas superficial velocity, initially it drops sharply then gradually until the superficial velocity reaches 0.0022[m/s], thus the transition regime can be found between 0.0011- 0.0022[m/s] from the slope changes of gas holdup. The rapid increase of bubble holdup with increase in superficial velocity in the homogeneous regime is because coalescence rarely happen in the homogenous bubbly flow. In the heterogeneous regime, the increase in gas superficial velocity has insignificant effect on the gas holdup.

Liquid properties such as viscosity, density and flowrate has an impact on bubble formation and or coalescence tendencies hence is an important factor affecting liquid holdup. It was observed that gas holdup decreases slightly with increase in liquid flowrates in this geometry. Like in co-current and counter-current geometry configuration, this could be due to liquid washing the gas bubbles away quickly as the liquid velocity increases.

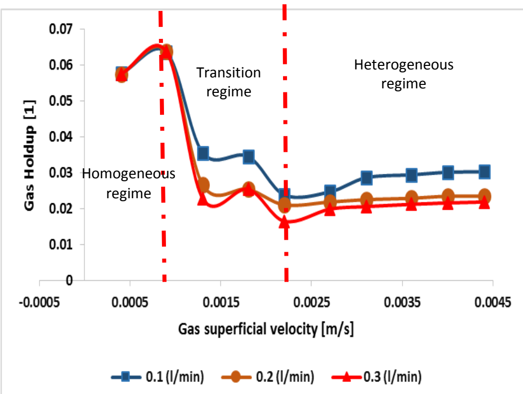

Fig. 8 Gas holdup as a function of superficial velocity calculated at different liquid flowrates in horizontal bubble column without internals

4.4 Gas Holdup Studies in Cross-flow Bubble Column with Internals (liquid deflector & gas separator).

Several studies show that gas holdup depends largely on gas superficial velocity. Gas holdup has been found to increase with increase in superficial velocity. Another factor that affect gas holdup is column geometry, internal design, bubble diffuser diameter and column diameter. Unlike in our first case of geometry without internals, gas hold up was found to increase with increase in gas superficial velocity. Another important finding in this column design is increase in gas holdup with increase in liquid flowrate. This could be due to formation of vortex and increase in residence time due to the introduction of gas separator and liquid deflector in the column. From Figure 9, it was observed that increase in superficial velocity has little or no effect on gas holdup then increase continually with increase in both gas superficial velocity and liquid flowrate.

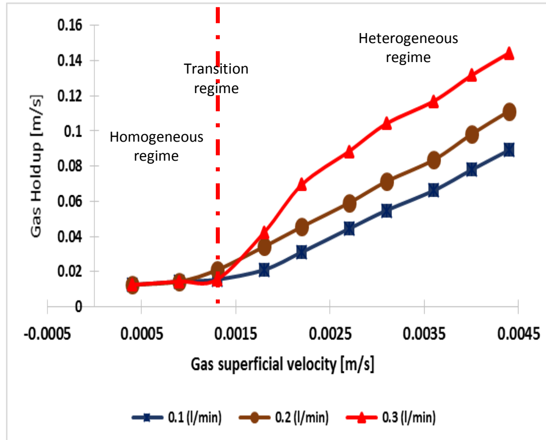

Fig. 9 Gas holdup as a function of superficial velocity calculated at different liquid flowrates in horizontal bubble column without internals

5. CONCLUSIONS

CFD simulation of hydrodynamics of a cross-flow rectangular bubble column (height 0.25m and length 0.30m) has been performed using COMSOL Multiphysics by employing the laminar bubbly flow model interface. The hydrodynamic parameters investigated are gas holdup and velocity profiles under different design and operating conditions such as column internals design and liquid and gas flow rates. The results of this work indicate that hydrodynamics in bubble column varies significantly with internal design and column configuration, hence the need for hydrodynamics studies after every change in column internal design is required. For column design without internals, the gas holdup was found to decrease initially with increase in gas superficial velocity and became unchanged at higher gas superficial velocity. The gas holdup also decreases with increase in liquid velocity. For column design with internals, the gas holdup was found to increase with both increase in gas and liquid superficial velocities.

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