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Theoretical Study on Effect of Operating Parameters on Mass Transfer in Bubbly Flow

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Abstract: A simple model of the bubble column reactor to interpret the mass transfer phenomena has been proposed in this study and its numerical simulation has been done. The important non-adjustable parameters have been explained and their dependence on various adjustable parameters has been studied to understand the bubble column operation. Mass transfer model inside BCR has been proposed in this study and its numerical simulation has been done using MATLAB software to predict the two phase mass transfer behavior in BCR. Effect of change in operating condition, column geometry and physiochemical properties of the two phases has been studied in this study. This study may helpful to further understanding of two-phase flow in bubble column and its design.

Key words: MATLAB Software, mass transfer model, BCR, Bubble diameter, flow, bubble column

INTRODUCTION

Bubble Columns Reactors (BCRs) are multiphase contactors of simple construction but complex hydrodynamics inside the reactor. It is a device in which a gas phase is bubbled through a column of liquid to promote a chemical or biochemical reactions in the presence or absences of a catalyst suspended in the liquid phase and hence are intensively used as multiphase contactors and reactors in chemical, biochemical and petrochemical industries. They provide several advantages during operation and maintenance such as high heat and mass transfer rates, compactness and low operating and maintenance costs (Deckwer, 1992). The advantages claimed for bubble columns compared to other multiphase contactors are:

- Absence of moving parts and hence low maintenance cost
- Higher effective interfacial area and volumetric mass transfer coefficients
- Less floor space requirement
- Large liquid residence times especially suited for slow reactions
- High heat and mass transfer rate

A distinct advantage of bubble columns is that the required mixing is effected by the action of rising bubbles, a process significantly more energy efficient than mechanical stirring. But the operation and performance of bubble column reactor significantly depends on the fluid dynamic characteristic of bubble column. Column parameter such as gas hold up, mass and heat transfer coefficient strictly depend on the flow regime prevailing in the column. Flow regime in BCRs are classified and maintained according to the gas superficial velocity. There are generally four types of flow regime that are generally observed in bubble column reactors: homogeneous regime (Bubbly flow), heterogeneous flow regime (Churn turbulent flow), slug flow regime and foaming regimes. Non adjustable parameter are the most important design parameter in bubble column reactor and scale up, values of these parameters are dependent on design and operating parameter cannot be changed directly, therefore they are called non-adjustable parameter. Some of these non adjustable parameters are gas hold up, bubble characteristic, mass transfer coefficient and heat transfer coefficient. Gas hold up is very important parameter in BCR design and operation. It is the fraction of volume of gas phase occupied by the gas bubble inside the bubble column reactor and is the most important factor characterizing the column parameters. Depending on the system and operating conditions several correlations (Hughmark, 1967; Akita and Yoshida, 1974; Joshi, 2001; Hikita *et al.*, 1980; Schumpe and Deckwer, 1987; Kawase *et al.*, 1992; Majumder *et al.*, 2006) have been proposed so far to evaluate the hold up. Volumetric mass transfer coefficient is the key parameter in the design of stirred and non-stirred BCRs. Overall mass transfer rate in BCR are governed by the liquid side mass transfer coefficient, the importance of gas side mass transfer coefficient is less

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significant. It mainly depends on the gas-liquid interfacial area which in turn depends on gas hold up and Sauter bubble mean diameter (Deckwer, 1992). Bubble column reactors are difficult to design because of complex fluid dynamics prevailing inside the reactor, though lot of research work have been done so far in this field, there are still lot of possibility to work on to understand the column dynamics and hence its performance. To determine the efficiency of bubble column based on mass transfer, the knowledge of extent of mass transfer is required. Literature provides information on the mass transfer coefficient for a large number of material systems. The definition of concentration difference within the reactor becomes very important when calculating mass transfer coefficient from measured absorption rates or from values characterizing the concentration of components passing through the reactor (Majumder, 2008).

This is because of concentration difference which is a function of various hydrodynamic factors. The extensive review on bubble column is reported by Kantarci *et al*. (2005). It was found that literature lacks on the simulation research on variation of concentration of solute for mass transfer rate in the complex system of bubble column device, so research is required to explore these areas.

In the present research, the main objective is to study the mass transfer characteristic of solute present in gas phase to liquid phase. Mass transfer study is limited to the bubbly flow regime (mass transfer in slug flow regime and churn turbulent flow regime are out of the limit of present research). Bubbly flow regime prevails at low gas superficial velocity in the column in which the bubbles are assumed to be of uniform size. Aim of the this research is to study the effect of changes in various parameters such as geometrical parameters of the reactor, operating condition and physiochemical properties of gas-liquid phase on mass transfer characteristic inside BCRs.

MATERIALS AND METHODS

In this study, the mass transfer phenomena were analyzed only in the homogeneous flow regime of bubble column (Fig. 1). The various factors influencing the regime transition point in gas-liquid bubble columns are examined. Increasing gas density delays regime transition. This phenomenon is described in a qualitative way by the correlations of Reilly *et al*. (1986) and Wilkinson *et al*. (1992) of which the Reilly correlation is found to be more accurate. However, both correlations are unable to account for the influence of the addition of small quantities of surface tension reducing agents. The upper boundary of this flow regime was determined by the formulas of Reilly. In this study, the mass transfer efficiency of bubble column reactor is analyzed with different operating variables in carbon dioxide-water system. The operating conditions are considered as minimum to maximum of the existing data in the literature published as column diameter: $0.01 \le d_c \le 0.63$ m, $0 \le h \le 6.0$ m, $0.1 \le d_h \le 10$ mm, $0 \le u_g \le 0.89$ m s^{-1} and $0 \le u_l \le 0.044$.

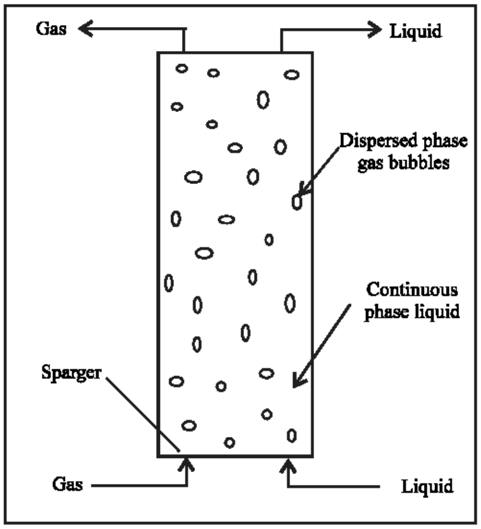

Fig. 1: Schematic diagram of bubble column

Model: Consider a bubble column operating with a gas and a liquid mixture where the gas is flowing homogeneously and concurrently in the flow of continuous liquid without reaction as a dispersed phase of bubble. A schematic diagram of the bubble column has been shown in Fig. 1. It is assumed that the gas leaving the reactor is in equilibrium with the liquid phase. Let's take the liquid flow rate to Q m^3 s^{-1} and the interfacial area between liquid and gas phase is a m^2 per unit volume of the reactor, as the gas-liquid mixture flows up the column the liquid phase undergoes a concentration change of dc mol m^{-3} in the differential height dh along the column height:

$$Q\frac{dC}{dt} = A_c K_l a(C^* - C) \tag{1}$$

Last term in Eq. 1 shows the driving force for the mass transfer between gas and liquid phase. A_c is column cross section area. K_la is the volumetric mass transfer coefficient. It is dependent on physiochemical properties of gas and liquid phases. The overall mass transfer rate per unit volume of the dispersion in a bubble column is governed by the liquid-side mass transfer coefficient, k_la where the gas side resistance is considered negligible. In a bubble column reactor the interfacial area influences the variation in $k_l a$ (Deckwer, 1992). For spherical bubbles, the specific gas-liquid interfacial area is related to the gas holdup and the Sauter mean bubble diameter. The specific interfacial area is expressed as:

$$a = \frac{6\varepsilon_g}{d_s} \tag{2}$$

Depending upon the choice of gas-liquid combination lots of correlation have been proposed to predict volumetric mass transfer coefficient. Hikita *et al*., 1980 developed a correlation for mass transfer coefficient in bubble column which is given as:

$$K_l a = \left(\frac{14.9g}{u_g}\right)\left(\frac{u_g \mu_l}{\sigma_l}\right)^{1.76}\left(\frac{\mu_l{}^4 g}{\sigma_l \rho_l{}^3}\right)^{-0.246} \left(\frac{\mu_g}{\mu_l}\right)^{0.243}\left(\frac{\mu_l}{\rho_l D_l}\right)^{-0.604} \tag{3}$$

The saturation interface concentration in liquid phase C* is a function of column height. As per Henry's law the saturation interface concentration in liquid phase can be written as (Majumder, 2008):

$$C^* = \frac{yp_t[1+\alpha(1-h_{r)}]}{H} \tag{4}$$

Where h_r is the normalized height as defined by h/h_m. The total internal column pressure at any height h can be written as (Majumder, 2008):

$$P_t = P_{atm} + \rho_l gh + \frac{4\sigma_l}{d_b} \tag{5}$$

The ratio between the hydrostatic pressure (at the gas distributor) and the total internal column pressure P_t denoted by α can be written as (Majumder, 2008):

$$\alpha = \frac{\rho_l g(1-\varepsilon_g)h_m}{p_{atm} + \rho_l gh + \frac{4\sigma_l}{d_b}} \tag{6}$$

Along with geometrical condition of the column gas holdup mainly depends on superficial velocity of gas and physical properties of gas and liquid phase inside the column. Gas holdup for the present simulation has been calculated from the correlation developed by Hikita *et al.* (1980):

$$\varepsilon_g = 296 u_g{}^{0.44} \sigma_l{}^{-0.16} \rho_l{}^{-0.98} \rho_g{}^{0.19} + 0.009 \tag{7}$$

Researches on bubble size distributions and factors affecting bubble sizes such as gas density, liquid viscosity, surface tension and operating conditions (pressure, temperature) are widely reported in literature (Schafer *et al*., 2002). Many literature correlations are proposed to predict the sizes of bubbles and most important one (Bahavaraju *et al*., 1978) has been used in this study is:

$$d_b = 3.23 d_0 \left(\frac{4\rho_l Q}{\pi \mu_l d_0}\right)^{-0.1}\left(\frac{Q^2}{d_0^5 g}\right)^{0.21} \tag{8}$$

RESULTS AND DISCUSSION

In this study different mass transfer phenomena in bubble column has been explained. The mass transfer phenomena in bubbly flow regime depnd on the different dynamic variables like gas and liquid velocities, geometric variables like column diameter, gas distributor, column height and the different physical properties of gas and liquid. For the simulation, different variables considered has been mentioned in earlier.

Variation of liquid phase concentration with dimensions of column and gas distributor: After simulation it is observed that carbon dioxide concentration in liquid phase is increasing as liquid-gas mixture move up the column co currently as shown in Fig. 2. This nature seems to be correct because as the gas and liquid move up the column solute particles from gas phase are tranferred to the liquid phase. That is why the liquid phase concentration of carbon dioxide increases with increase in column height. Mass transfer variations along the column obtained from the model are in agreement with those obtained by Majumder (2008).

At a particuler height of the column, liquid phase concentration is heigher for column having larger diameter. Verma and Rai (2003) reported that the mass transfer coefficient was independent of initial bed height which may give the different profile of concentration variation of gas in the bed. When column diameter is very small slug formation may take place inside column which may hinder the mass transfer operation. This is because of decreasing overall gas holdup. The variation of liquid phase concentration with the column diameter has been shown in Fig. 3. Krishna and van Baten (2003) carried out CFD simulations and showed that mass transfer coefficient decrease with column diameter but Vandu and Krishna (2004) reported counter result that the

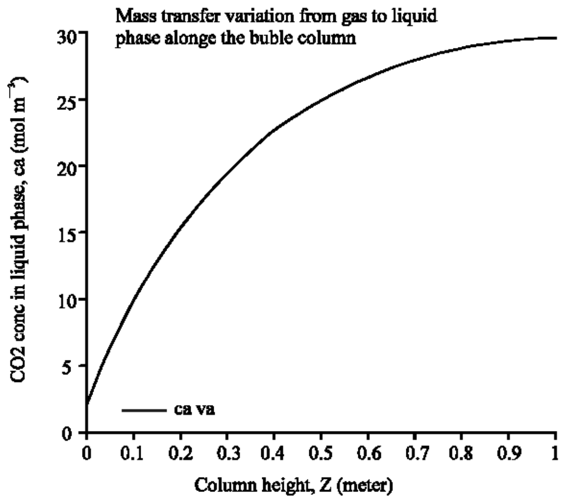

Fig. 2: Variation of concentration of solute in the liquid at height h = 1.0 m of the column

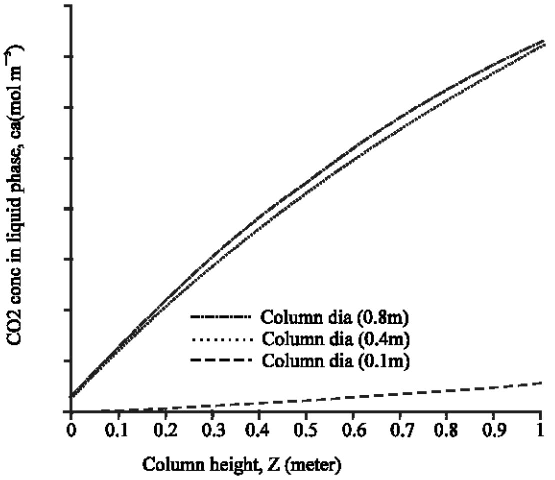

Fig. 3: Variation of liquid phase concentration with column height

mass transfer coefficient slightly increase with column diameter in case of slurry bubble column. As the gas holdup increases with gas sparger, the variation of the concentration may change with the sparger diameter. Higher values of mass transfer coefficient exhibited with perforated plate distributor.

Variation of liquid phase concentration with superficial gas velocity: The superficial gas velocity has significance effect on the mass transfer phenomena. As the superficial gas velocity increases, the mass transfer from gas to liquid increases. The effect of superficial gas velocity on the liquid phase concentration is shown in Fig. 4. With increase in superficial gas velocity the mass transfer rate are found to be increased. As the superficial gas velocity increases the gas holdup increases which results in increase of gas transfer from gaseous phase to liquid phase. Also the interfacial area between gas and liquid increases with increase in gas holdup. This may also the increase the mass transfer from gas to liquid. The mass transfer increased with increasing gas velocity in the same trend as the gas holdup increased with superficial gas velocity (Krishna and van Baten, 2003). Verma and Rai (2003) reported that the mass transfer increases monotonically with the gas velocity. Behkish *et al.* (2002) investigated the volumetric mass transfer coefficient and bubble size distribution for four different gas phases and in two different organic liquid mixtures and reported that mass transfer increases with gas velocity in slurry system. As increase in gas velocity, the volumetric mass transfer coefficient increases as the specific interfacial area increases (Fig. 5). Volumetric mass transfer coefficient (k_la) is found to be increasing with gas superficial velocity which is in agreement with results obtained by Alvarez (2000). Increase in gas velocity enhences the momentum exchange between phases. The momentum exchange increases the breakup efficiency of the bubble. More breakup results the finer bubble and increase in interfacial area. Hence, the mass transfer increases with the increase in gas velocity. The monotonic increase in the solute concentration in the liquid phase resulted due to the enhencement of mass transfer from gas phase to the liquid phase.

Variation of liquid phase concentration with surface tension of liquid: From the simulation result, it was found that mass transfer between gas and liquid phase will be higher for a liquid having lower surface tension. With increase in surface tension bigger bubble will be form and this will eventually lead to decrease in overall gas holdup which inturn is responsible for mass transfer between phases.

Simulation of the model shows that overall gas holdup is increasing with increase in superficial velocity. At high superficial velocity smaller bubble will be form in bubble flow regime. Smaller bubble will produce high gas holdup and large gas liquid interfacial area. Variation of gas holdup with liquid surface tension and the superficial gas velocity is shown in Fig. 6. Decrease in gas holdup will lead to decrease in interfacial area between gas and liquid phases.

Due to high surface tension gas holdup will increase in, therefore the mass transfer between gas and liquid phase will decrease. This variation is shown in Fig. 7. Muller and Davidson (1995) performed experiments with viscous media. They reported that surface active agents

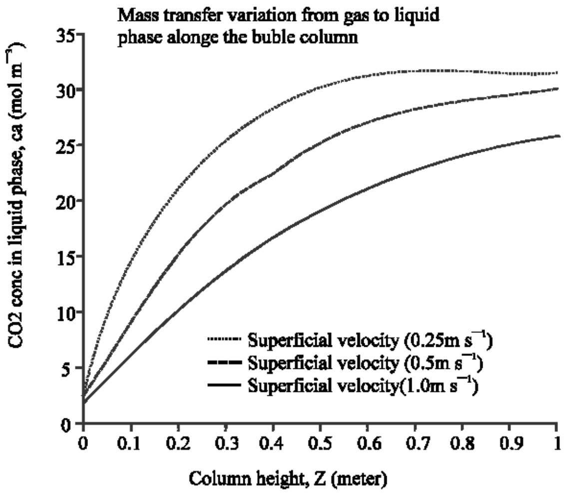

Fig. 4: Variation of liquid phase concentration with column height for different gas velocity

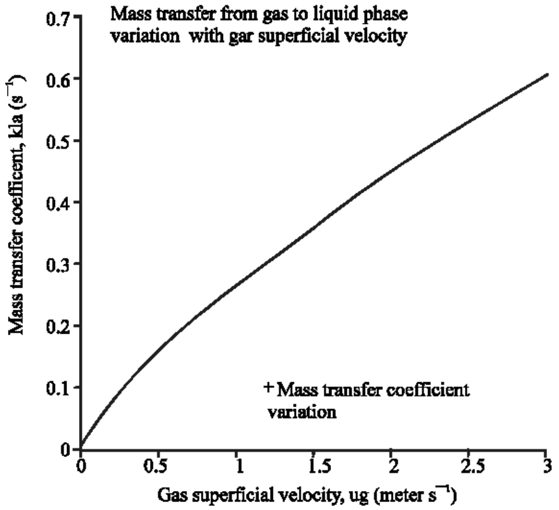

Fig. 5: Variation of mass transfer coefficient with gas superficial velocity

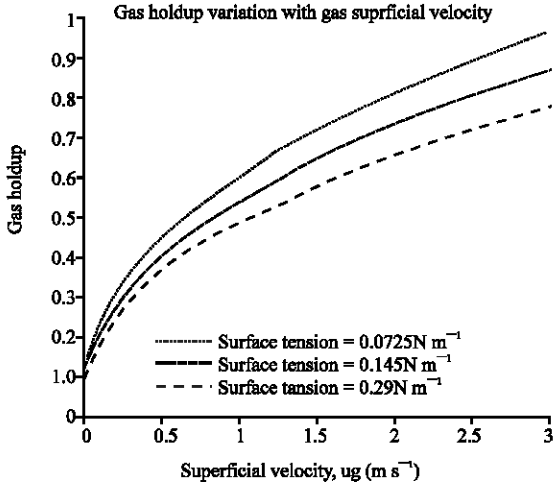

Fig. 6: Variation of gas holdup with superficial velocity for different surface tension

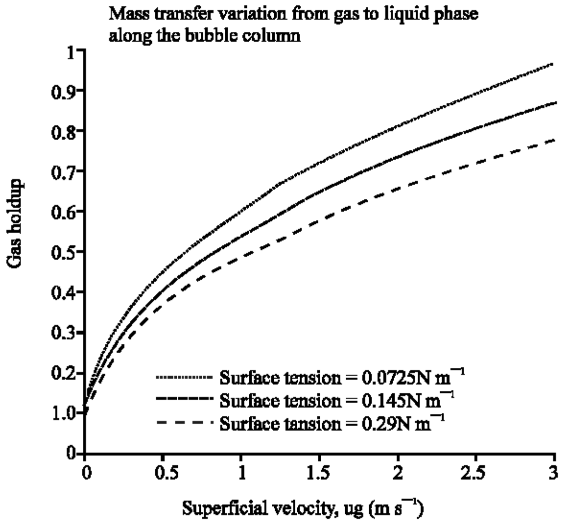

Fig. 7: Variation of liquid concentration with surface tensiona

have immense effect on the mass transfer which is controlled by mass transfer coefficient. Results obtained from simulation of bubble column shows that liquid side mass transfer coefficient is higher for liquid with lower surface tension.

Liquid having lower surface tension will provide lower resistance to surface stretching, hence liquid with lower surface tension will provide high interfacial are between gas and liquid phase. The variation of liquid side mass transfer coefficient with surface tension is shown in the graph in Fig. 8. According to their observation the mass transfer increase in the presence of surfactants due to creation of small bubbles and reduced bubble coalescence due to surfactants.

Variation of liquid phase concentration with fluid viscosity: From the simulation it was found that mass transfer chracteristic will be higher for the liquid having lower viscosity, due to increase in liquid viscosity larger bubbles will be form which inturn result in decrease in overall gas holdup. Presence of more larger bubble will decrease the overall gas holdup and hence mass transfer rate will decrease with increase in liquid viscosity. Variation of mass transfer between gas and liquid phase is shown in Fig. 9. Behkish *et al.* (2002) and Verma

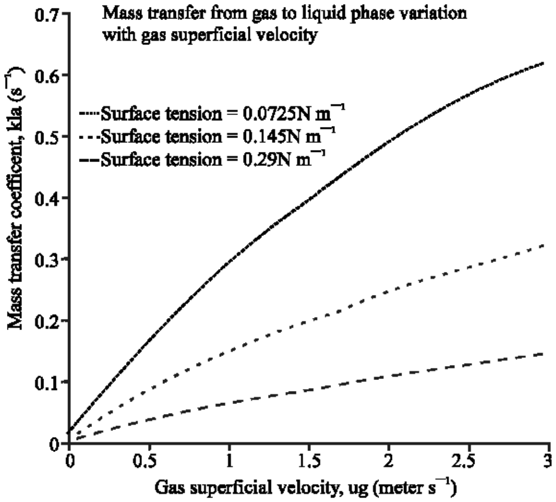

Fig. 8: Variation volumetric mass transfer coefficient of the liquid phase with surface tension

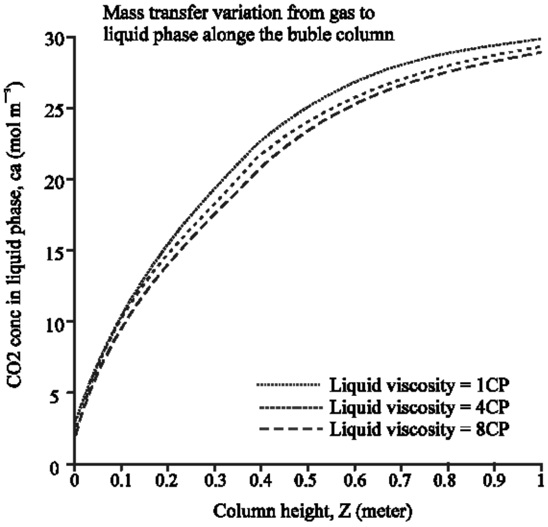

Fig. 9: Variation of liquid concentration with viscosity

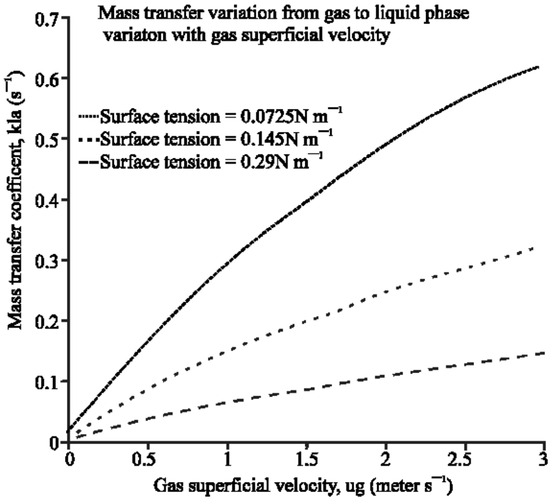

Fig. 10: Variation volumetric mass transfer coefficient of the liquid phase with liquid viscosity

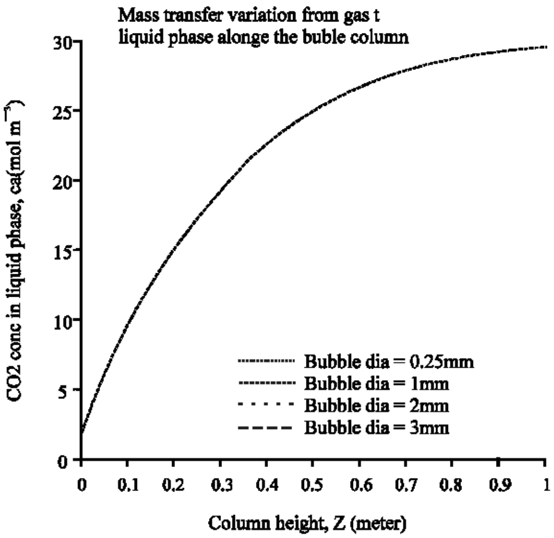

Fig. 11: Variation of liquid concentration with bubble diameter

and Rai (2003) studied the mass transfer phenomena with viscous media. They showed that the mass transfer decrease with increasing liquid viscosity. They barbed out that higher viscosity led to increase of the volume fraction of the large bubbles which leads to much lower gas–liquid interfacial areas. Ozturk *et al.* (1987) investigated mass transfer coefficient in various organic liquids and observed that mass transfer increases with increasing gas density.Variation of liquid side mass transfer coefficient with liquid viscosity is shown in Fig. 10. It was found that liquid phase mass transfer coefficient is higher for liquid having low value of viscosity. This phenomenon can be explained by the fact that liquid with low viscosity will provide lower resistance to mass transfer from gas to liquid phase. Mass transfer coefficient decreases with liquid surface tension. It may be due to the effect of resisting the stretching of interface and reducing disturbances in the bulk phase.

Variation of liquid phase concentration with bubble diameter: Results from simulation shows that slight change in bubble diametr will not affect the mass transfer between gas and liquid phase. The variation of mass transfer with bubble diameter is shown in Fig. 11. Though if the increase in bubble diameter is large mass transfer between gas and liquid phase will change drasticaly. Presence of larger bubble will lead to decrease in overall gas holdup. The mass transfer between gas and liquid will decrease with decrease in overall gas holdup. Most investigations performed are limited to the determination of the mass transfer which is effected by volumetric mass transfer coefficient (Kantarci *et al*., 2005). The volumetric mass transfer coefficient is the product of the liquid mass transfer coefficient k_l and interfacial area a. This parameter is global and not sufficient to provide an understanding of the mass transfer mechanisms. The separation of the parameters k_l and a should be considered for better comprehension of the gas-liquid mass transfer mechanisms (Kantarci *et al*., 2005). It is required to identify which parameter (k_l or a) controls the mass transfer. The gas-liquid mass transfer mechanism based on either of the parameter may influences the concentration of the solute of gas in the liquid phase in bubbly flow.

CONCLUSION

Modeling and simulation of the bubble column reactor has been done in this study, variation of mass transfer with column height is done using a MATLAB function, it is found to be of somewhat exponential nature. The liquid phase concentration is increasing almost exponentially as gas-liquid mixture moves counter currently up the column. Dependence of liquid phase concentration on various operating, geometrical and physiochemical properties of gas-liquid phase has been shown graphically and results obtained from simulations are compared with the results present in literature. Volumetric mass transfer coefficient is found to be dependent on gas superficial velocity, this variation has been shown graphically through a MATLAB code, finally dependence of k_la on operating and physiochemical properties of gas-liquid properties have been shown graphically using MATLAB m files.

Nomenclature:

a = Specific interfacial area (m^{-1})
d_b = Bubble diameter (m)
d_c = Column diameter (m)
d_o = Orifice diameter (m)
d_s = Sauter mean diameter (m)
D_l = Diffusion coefficient (m2 s^{-1})
C = Molar concentration (mol m^{-3})
C^* = Interface concentration (mol m^{-3})
g = Gravitational acceleration (m^2 s^{-1})
H = Henry's law of constant
L_m = Height of entire column (m)
K_la = A Volumetric mass transfer coeff. (1 s^{-1})
P_t = Total pressure (N m^{-2})
Q = Heat flux (J m^{-2}.s)
y = Mol fraction of gas
P_l = Density of liquid (kg m^{-3})
P_g = Density of gas (kg m^{-3})
a = Parameter defined in Eq. (6)
ε_g = Fractional gas holdup (-)
μ_l = Viscosity of liquid (kg m^{-1}.s)
σ = Surface tension (N m^{-1})

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