GAS-LIQUID SIMULATION OF AN AIRLIFT BUBBLE COLUMN REACTOR

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thin liquid barrier between ruptures to form a larger bubble. Breakup of bubbles is caused by collisions with turbulent eddies, approximately equal in size to the bubbles.

1.2 Problem Statement

Most industrial gas-liquid reactions are conducted in bubble columns which the gas is dispersed in a liquid. The contactors are the important part capability of bubble column to carry out slow reactions such as oxidations and chlorinations. Airlift reactor is an important device that preferentially used for bioprocess application. A few parameters like gas and liquid flow rates, geometry or type and construction of the distributors can be controlled by design and operation of these reactors. Three model of ANSYS Fluent is used to analyze the system for various hydrodynamic parameters and predict the gas-liquid performance.

1.3 Objective

The objectives of this project are:

- i. To understand the hydrodynamic behavior of a concurrent gas-liquid up-flow of an airlift bubble column reactor by CFD analysis.
- ii. To determine the relation between the gas hold up and the superficial gas velocity.

1.4 Scope

The scopes of this project are:

- The system used in this study is a concentric draft tube airlift reactor with a 0.147m column diameter and 1.818m height.
- ii. The eulerian-eulerian approach will be used for modeling the multiphase flow from air to de-aerated water in the column.
- iii. The parameter for boundary conditions were set up the inlet as velocity of gas sparger 0.75 m/s, the outlet as atmospheric pressure and wall as no slip wall.
- iv. The volume of fluid (VOF) model is used with transient time solver.
- v. The standard k- ϵ , RNG k- ϵ and k- ω model will be used to account the effect of turbulence.
- vi. Ansys Fluent software package will be used to simulate the system for various hydrodynamics parameter such as;
 - Gas hold up
 - Contact surface area
 - Gas superficial velocity
- vii. The simulated results will be comparing with those three different models.

CHAPTER 2

LITERATURE REVIEW

Review of literature is a study conducted in a project where it covers all aspects of the existing material. This chapter emphasis on the theories and previous studies related of bubble column reactor to understand their hydrodynamics behavior using computational analysis simulation. This study is referred to the facts, books, journals, theses and references the earlier results.

Airlift bubble column reactors are simple devices that have gained acceptance in gas-liquid contacting. The airlift reactor has two types classifications which are internal loop reactor and external loop reactor. An internal loop reactor is divided into two zones: riser and downcomer zone by addition of a baffle or a draught tube (Davarnejad et al., 2012). In bubble columns with internal loop, the gas may either be supplied into the draft tube region or the annular region (Miron, 2000). If efficient degassing of the down-flowing liquid is required, the draft tube region is to be preferred with a conical widening of the top part of the bubble column allowing less turbulent liquid flow in this zone (Jakobson, H. A., 2008). The external loop airlift reactor (ELALR) is composed of a riser and downcomer that are joined together with two horizontal connectors (Law et al., 2008). The airlift reactors are preferred over traditional bubble column reactors due to well directed liquid circulation, thus facilitating the cultivation of shear sensitive organisms which is widely used in the bioprocess, chemical industry and for waste water treatment (Miron et al., 2000). Due to their industrial importance and wide application area, the design and scale up of bubble column reactors, investigation of important

hydrodynamic and operational parameters characterizing their operation have gained considerable attention during the past 20 years (Kantarci et al.2005).

The principle function of airlift reactor while the gas is injected into the riser and the resulting difference between average densities in the riser and in the downcomer provides a driving force for liquid circulation. Also solid particles can be present, for example catalyst and biomass (Simcik et al., 2011). In other words, airlift reactors are distinguished by fluid circulation in a well-defined and clear cyclic pattern through channels providing a loop for recycling the liquid. The gas is injected at the bottom of the reactor then both of the gas and liquid flow upwards in the riser. The gas disengages totally or partially from the liquid. The liquid flows down from the top to the bottom of the reactor in the downcomer. The different volumes of gas retained in the riser and the downcomer create a pressure difference that forces the fluid from the bottom of the downcomer towards the riser of the liquid circulating (Veno et al., 2007). This model can be applied for a two or three-phase flow with low viscosity in a Newtonian liquid

The knowledge of the airlift hydrodynamics is needed for the design of the airlift reactor. The design and scale-up of airlift reactors are the most important factors on the flow of different phases present which is influence the geometry of the system. The distance from the reactor base to the draft tube or baffle (bottom clearance) and the distance from top of the draft tube or baffle to the top of the liquid level (top clearance) have received only minimal attention (Davarnejad et al., 2012).

The two important hydrodynamic parameters of airlift reactors are gas holdup and liquid velocity. There are play important roles in design and simulation modes. The liquid velocity affects the mixing and rate of mass transfer while the gas holdup is an index of gas means residence time. This index affects the gas liquid mass transfer efficiency and liquid velocity (Jafari Nasr et al., 2004).

Many investigators studied extensively on the effects of the aeration rate on gas holdup and liquid velocity of two-phase airlift reactors. It was found that the gas holdup and liquid velocity increases while the aeration rate increased. The factors causes such as reactor type, external or internal loop, internal geometry, downcomer to riser cross sectional area ratio, range of superficial gas velocity, type and location of the gas sparger. Airlift Bubble column reactors have advantages of ease of operation, low operating and maintenance costs as it requires no moving parts, and compactness. Also, they have the characteristics of high catalyst durability and excellent heat and mass transfer characteristics (Vial et al., 2001). Furthermore, airlift bubble column reactors can be adapted to specific configurations according to practical requirements. Besides that an airlift bubble column presents several advantages such as high gas dispersion efficiency, rapid mixing, simplicity of construction and low probability for the loss of sterility (Veno et al., 2007).

The process especially occur involving reactions such as oxidation, chlorination, alkylation, polymerization and hydrogenation. For example of bubble column reactor application in chemical process that famous Fischer–Tropsch process which is the indirect coal liquefaction process to produce transportation fuels, methanol synthesis, and manufacture of other synthetic fuels which are environmentally much more advantageous over petroleum-derived fuels. Table 2.1 is shows the application area in bioprocess to produce industrially valuable product (Kantarci et al., 2005).

Bioproduct	Biocatalyst
Thienamycin	Streptomyces cattleya
Glucoamylase	Aureobasidium pullulans
Acetic acid	Acetobacter aceti
Monoclonal antibody	Hybridoma cells
Plant secondary metabolites	Hyoscyamus muticus
Taxol	Taxus cuspidate
Organic acids (acetic, butyric)	Eubacterium limosum
Low oxygen tolerance	Arabidopsis thaliana
Ethanol	Saccharomyces cerevisiae

Table 2.1: Biochemical applications of an airlift bubble column reactors (Kantarci et al., 2005)

Generally the design and scale-up of bubble column reactors depend on the quantification of three main phenomena. That is heat and mass transfer characteristics; mixing characteristics and chemical kinetics of the reacting system. Thus, the reported studies emphasize the requirement of improved understanding of the multiphase fluid dynamics and its influence on phase holdups, mixing and transport properties (Kantarci et al., 2005). Scale-up problems basically stem from the scale-dependency of the fluid dynamic phenomena and heat and mass transfer properties. Scale-up methods used in biotechnology and chemical industry range from know-how based methods that are in turn based on empirical guidelines, scale-up rules and dimensional analysis to know why based approaches that should begin with regime analysis. The regime analysis is then followed by setting-up appropriate models that may be simplified to deal with the complex hydrodynamics.

There are three basic flow regimes in bubble columns, homogeneous, heterogeneous and slug flow. The bubble size distribution is relatively narrow and the bubbles rise uniformly through the column. This is known as homogeneous flow. Homogeneous bubbly flow may occur in small scale apparatus with superficial gas velocities below 5 (cm/s). This state is not maintained when the gas passes more rapidly through the column. Coalescence and bubble breakage lead to a wider bubble size distribution. Large bubbles are formed and these may rise more rapidly than the smaller bubbles. This type of flow is referred to as heterogeneous and is quite common as a result of the high gas rates frequently adopted in industry. For water and dilute aqueous solutions heterogeneous churn-turbulent flow may occur in columns with diameters larger than about 20 (cm) and when the superficial gas velocity exceeds about 7 (cm/s). The slug flow regime is the superficial gas velocity increasing further will lead to the formation of very large bubbles stabilized by the reactor walls (Jakobson, H. A., 2008). Figure 2.1 illustrates the differences between the possible regimes.



Figure 2.1: The flow regime in bubble column (Jakobson, H. A., 2008)

Gas hold up is one of the most important parameters characterizing the hydrodynamics of bubble columns. It can be defined as the percentage by volume of the gas in the two or three phase mixture in the column. Gas hold up depends mainly on the superficial gas velocity. Other important parameter that has a strong influence on the hydrodynamic behavior is bubble size distribution. The large gas bubbles rise quickly through the column than small bubbles. Therefore the gas residence time decrease and cause to reduce the total gas hold up (Mohstari et al, 2009). The relation between superficial gas velocity and gas sparger type with gas hold-up are important designing parameters to predicting the hydrodynamic behavior of bubble column reactors.

Full scale experimentation of airlift reactors is expensive and more cost. The effective approach is by using validated computational fluid dynamics (CFD) models (Law et al., 2008). Computational fluid dynamics is a powerful numerical tool that is widely used to simulate many processes in industry. It is uses numerical methods and algorithms to solve and analyze problems that involve fluid flows. CFD is becoming more and more popular for the design and scale-up of reactors with low cost and high reliability especially for reactors operating under high pressure and high temperature (Huang et al., 2010). In this study, the simulation of two phase flow in airlift bubble column reactors produce using computational fluid dynamics developed by FLUENT Inc.

It is found that CFD simulation for bubble columns is strongly dependent on the closure models involving drag, lift and virtual mass forces and bubble induced turbulence models. Even the grid resolution and discretization schemes for convection term may affect the simulation. There is still no general consensus on model formulation. This may be due to the fact that the terms reflecting gas-liquid interaction occurring at different scales are difficult, if not impossible, to be extracted or generalized from experimental measurements or microscale and direct numerical simulations (Yang et al., 2009).

The main part of this study is to analyze the hydrodynamics parameters of bubble column reactors which are predicted through computational fluid dynamics simulation. Various approaches have been suggested for solving the same fundamental flow problem modeling the hydrodynamic behavior of bubble columns. This problem may be solved at various levels of sophistication. It also can choose to treat either the dispersed and continuous phases as interpenetrating pseudo-continua (Euler-Euler approach) or the dispersed phase as discrete entities (Euler-Lagrange approach). The simulation may be done in fully transient and dynamic mode or only for the unsteady-state time-averaged results. An appropriate mesh and a robust numerical solver are crucial to get accurate solutions. Finally it is highly imperative to validate the simulation results against experimental work (Irani, M., & Khodagholi, M. A., 2011).

There are several unique advantages of CFD over experimental-based approaches to fluid systems design such as substantial reduction of lead times and costs of new designs, ability to study where controlled experiments are difficult or impossible to perform, ability to study systems under hazardous conditions at and beyond their normal performance limits, and practically unlimited level of detail of results. The variable cost of an experiment, in terms of facility hire and or man-hour costs is proportional to the number of data points and the number of configurations tested. In contrast CFD codes can produce extremely large volumes of results at virtually no added expense and it is very cheap to perform parametric studies for instance to optimize equipment performance (Al-Masry, W. A., 2006).

2.1 Fluid dynamics and flow regimes

The fluid dynamics characterization of bubble column reactors has a significant effect on the operation and performance of bubble column. These also depend on the regimes prevailing in the column. The flow regimes in bubble columns are classified and maintained according to the superficial gas velocity employed in the column. They are three types of flow regimes are commonly observed in bubble column which are the homogenous (bubbly flow) regime, the heterogeneous (churn-turbulence) regime and slug flow regime (Zehner, P., & Kraume. M., 2005). The relationship between superficial gas velocity and reactor diameter is illustrated by the flow map of Figure 2.2. The broad transition regions are due to the effects of the gas distributor, the gas-liquid system and the liquid rate.



Figure 2.2: Flow Regimes Map in Bubble Colum (Zehner, P., & Kraume. M., 2005)

Rising gas bubbles entrain liquid in their wakes. This upward flow of liquid is much greater than the net liquid flow rate. Because of continuity, the liquid is predominantly moving downward (Jakobson, H. A., 2008). Figure 2.3 is shown the mean liquid axial velocity profiles of a force balance over an annular.



Figure 2.3.: Liquid Flow Profile in Bubble Column (Jakobson, H. A., 2008)

2.2 Gas holdup

Gas holdup is one of the most important operating parameters because it not only governs phase fraction and gas phase residence time but is also crucial for mass transfer between liquid and gas. Gas holdup depends chiefly on gas flow but also to great extent on the gas-liquid system involved. It is basically defined as the volume fraction of gas phase occupied by the gas bubbles. The equation of the dispersion:

$$\varepsilon_G = \frac{V_G}{V_G + V_L} \tag{2.1}$$

The relationship between gas holdup and gas velocity generally described by the proportionality of $\varepsilon_G \sim u_G^n$. In the homogenous regime, n is close to unity. When large bubbles are present, the exponent decreases. Figure 2.4 is shown the higher contribution of large bubbles to the total gas hold up, the smaller is exponent *n*. In the fully

developed heterogeneous flow regime, n finally takes on values between 0.4 and 0.7, depending on gas-liquid system (Zehner, P., & Kraume, M., 2005).



Figure 2.4: Gas holdup and fraction of large bubbles (Zehner, P., & Kraume. M., 2005)

2.2.1 Gas sparger

Gas sparger type is an important parameter that can alter bubble characteristics which in turn affects gas holdup values and thus many other parameters characterizing bubble columns. The sparger used definitely determines the bubble sizes observed in the column. Small orifice diameter plates enable the formation of smaller sized bubbles. Some common gas sparger types that are used in literature studies are perforated plate, porous plate, membrane, ring type distributors and arm spargers (Kantarci et al. 2004).

In homogenous flow regime, bubbles of almost uniform size and shape rise in the form of a swarm distributed uniformly over the column cross section. As shown in Figure 2.5 used the reactors diameter and height is 0.44 meter and 5 meter with perforated plate gas distributor 3mm. The large bubbles have a rise velocity that is four or more times larger than small ones. Thus most of the transport in the heterogeneous

flow regime is accomplished by large bubbles. In this regime, the quantity of the gas transported by small bubbles remain constant whereas the quantity transported by large bubbles increases linearly with gas velocity. This relationship applies to coalescing and coalescence-hindered gas-liquid systems (Zehner, P., & Kraume. M., 2005).



Figure 2.5: Velocities of Rising Bubbles for the System Water-Air. (Zehner, P., & Kraume. M., 2005)

2.3 Interfacial area

The area of the gas-liquid interface is very important process parameters especially at high reaction rates. For example, when the bubble column employed as an absorber, the interface area become a crucial factor in equipment sizing. Like gas hold up, interface area depends on the geometry, operating conditions and gas-liquid system. Gas holdup and interface area per unit volume are related as

$$a = \frac{A}{V_R} = \frac{6\varepsilon_G}{d_{bs}} \tag{2.2}$$

where V_R is the volume of the reaction mixture and d_{bs} is the main bubble diameter Figure 2.6 shows the interfacial area increases with increasing gas flow rate. A diameter of porous plate is 0.102 meter refer to a. Although the perforated plate has three different diameters are 0.29 meter, 0.14 meter and 0.1 meter refer to b, c and d respectively. An exception occurs when a porous plate sparger is used, like gas holdup, interfacial area decreases on transition to the heterogeneous flow regime and then approaches the same values observed with perforated plates. The growth in interfacial area with increasing gas velocity is always greater in the homogeneous than in the heterogeneous flow regime. The reason lies in the formation of large bubbles in the heterogeneous regime, the interfacial area of large bubbles per unit volume is markedly lower than that of smaller ones.



Figure 2.6: Specific interfacial area as a function of superficial gas velocity (Zehner, P., & Kraume. M., 2005)

2.4 Mass transfer

In gas-liquid reactors, mass transfer from the gas to liquid phase is the most important goal of the process. The mass transfer between the gas and the liquid phase in a bubble column can be describe in by the volumetric mass –transfer coefficient, $k_L a$ which is the liquid-phase mass transfer for coefficient k_L multiplied by the specific interfacial area. Gas-phase resistance can usually be neglected, so k_L a gives an adequate description. In

industrial units $(d_t > 1m)$, estimates can be based on the assumption of complete mixing in both liquid and gas phase.

Like gas holdup and interfacial area, k_L also depends on the gas flow rate, type of sparger, and gas-liquid system. The mass transfer coefficient and gas rate proportional to one another:

$$k_L \sim u_G^n \tag{2.3}$$

where n can be between 0.7 and 0.92.

Mass transfer coefficient two to threefold higher can be achieved in the homogeneous flow regime if a porous plate is used as sparger instead of a perforated plate as shown in Figure 2.7. In the heterogeneous regime, the effect of the sparger is negligible.



Figure 2.7: Mass transfer coefficient in bubble column (Zehner, P., & Kraume. M., 2005)

2.5 Heat transfer

Thermal control in bubble columns is of importance since in many chemical and biochemical processes, chemical reactions are usually accompanied by heat supply (endothermic) or removal (exothermic) operation. In many cases, heat must be removed when operating bubble column. The heat transfer rate in gas–liquid bubble columns is reported to be generally 100 times greater than in single phase flow. The turbulent flow generated by rising bubbles increases heat transfer even at low gas rate as shown in Figure 2.8. It is used the bubble column in diameter 0.196 meter, the height is 6.20 meter and the liquid volume is 1.2 cm/s. The increase in heat transfer coefficient, α with gas throughput is markedly grater in the homogeneous than in the heterogeneous regime.



Figure 2.8: Heat transfer coefficient at reactor wall (Zehner, P., & Kraume. M., 2005)

Measurements of heat transfer coefficients in general a heat source and measurements of surface and bed temperatures (Katarci et al. 2004). To estimate the local instantaneous heat transfer coefficient, h (W/m² °C) for a heated object-to-bed system for instance, the temperature difference between the probe surface and the bulk, ΔT (°C) and the corresponding heat transfer flux, Q (W/m²) should be measured. The following relation can then be applied:

$$h = \frac{Q}{\Delta T} \tag{2.4}$$

The basic parameters affecting the heat transfer are mainly the superficial gas velocity, particle size and concentration, liquid viscosity, particle density, axial/radial location of the heat transfer probe and column dimensions.

2.6 Computational Fluid Dynamic

Computational methods for multiphase flows have been developed during the past decades (Ranganathan, P. & Sivaraman, S., 2011). In general, there are two major approaches, that is the Eulerian-Eulerian model and the Eulerian-Lagrangian model. The Eulerian-Eulerian model treats both phases as continuous phases which are interpenetrating. The Eulerian-Lagrangian model considers the liquid phase as a continuous phase, while it treats the other phases as a dispersed phase in form of discrete elements. For example those elements are particles or bubbles. In addition, direct numerical simulations that are capable of predicting the interface as well as the flow field of the two phases are also frequently used in two-phase flow modelling. Direct numerical simulation can be used to obtain closures for forces acting on discrete elements such as the drag, lift and virtual mass (Bai, W., 2010).

2.7 Study of gas hold-up and bubble behavior in gas-liquid bubble column

Moshtari et al. (2009) in their research about experimental study of gas hold-up and bubble behavior in gas –liquid bubble column. The experimental consists of a cylindrical glass column with 15cm inner diameter and 2.8 m height. The column is equipped with two spargers in bottom with a perforated plate and a porous plate respectively. Both plates are 0.1 % porosity. The designing of perforated plate is based on Weber number which sparger consist 19 holes with 1 mm diameter.

Figure 2.9 shows the effect of superficial gas velocity on gas hold up in air-water system. The homogeneous regime occurs at low gas flow and turns into the heterogeneous regime at high gas flow. At low superficial gas velocity, the bubble size is small and uniform and bubble travel upwards in a helical path without any major collision or coalescence. With increasing the superficial gas velocity the bubbles are coalescenced therefore at high superficial gas velocity (more than about 9 cm/s) all the bubbles will be large. The large bubbles have higher rise velocity than small bubbles, therefore residence time of large bubbles decrease and cause to decrease rate of increasing gas hold up. The transition from homogeneous to heterogeneous regime is observed at a superficial gas velocity between 0.9 to 0.11 m/s.

Figure 2.10 shows shows the effect of sparger type on gas hold up. Porous plate with smaller pore diameters generates smaller gas bubbles when compared to perforated plate. The gas hold up in this system equipped with porous plate at high superficial gas velocity is approximately 40% higher than system equipped with perforated plate. The initial bubble size is depended on the sparger type.



Figure 2.9: Effect of superficial gas velocity on gas hold up in air-water system (Moshtari et al., 2009)



Figure 2.10: Graph superficial Gas Velocity versus Gas Hold Up (Moshtari et al., 2009)

2.8 Gas-Liquid Simulation of an airlift bubble column reactor

Blazej et al. (2003) in their research of simulation two-phase flow for an experimental airlift reactor using Fluent software. The experimental using 32 litre concentric drafttube airlift reactor with dimension of the column are 1.818 m liquid height and 0.147 meter diameter. The gas sparger containing 25 holes with 0.5 mm in diameter. The data from simulation is compared with the experimental data obtained by tracking of a magnetic particle and analysis of the pressure drop to determine the gas hold-up. Comparison between vertical velocity and gas holdup were made for a serious of experiments where the superficial gas velocity in the riser was adjusted between 0.01 and 0.075 m/s. In this case of gas phase holdup and liquid phase velocities in the riser appropriate trends are followed and values are modeled to good accuracy as shown in Figure 2.11 and Figure 2.12, but the downcomer flow characterization is poor due to effects caused by the choice of the bubble size, volume fraction equation and mesh resolution used. Figure 2.13 and Figure 2.14 are represent the downcomer flow characterization. Therefore to accurately model the motion of gas and liquid phases in airlift reactors, the use of complex multiple gas/discrete phase model equation must be implemented, where each discrete phase presents a single bubble size for the same gas phase composition.



Figure 2.11: Liquid phase velocity (m/s) as influenced by the superficial gas velocity in the riser (m/s) (Blazej et al., 2003)



Figure 2.12: Gas phase holdup (%) as influenced by the superficial gas velocity in the riser (m/s) (Blazej et al., 2003)





Figure 2.13: Liquid phase velocity (m/s) as influenced by the superficial gas velocity in the downcomer (m/s) (Blazej et al., 2003)

Figure 2.14: Gas phase holdup (%) as influenced by the superficial gas velocity in the downcomer (m/s) (Blazej et al., 2003)

2.9 Study of geometrical effects with internal loop on gas hold up and flow pattern

Salehani et al. (2011) worked on the hydrodynamics of two configurations of internal airlift reactor with a riser diameter of 4 cm and 5 cm which was operating with an airwater system. The gas phased sparged into the column by four different spargers with different number of holes in 1 mm diameter. The number of holes in the sparger is as the same trend. The first one has the most number of the holes and the fourth one has the less number as shown in Figure 2.15. The bubble distribution in the column in the first sparger is more uniform so that, the mixing gives an effect on mass and heat transfer coefficients especially on gas hold up. Figure 2.16 shows the effect of different sparger on gas hold up.



Figure 2.15: Shape and Structure of Different Sparger Type (Salehani et al. 2011)



Figure 2.16: Gas Hold Up versus Superficial Gas Velocity of Different Sparger (Salehani et al. 2011)

2.10 CFD Simulation of scale influence on the hydrodynamics of an internal loop airlift reactor

According to Davarnejad et al. (2012) two phase air-water flow in internal loop airlift reactor with three various scale (10.5, 32 and 200 l) was simulated using Computational Fluid Dynamic. The gas hold up is important parameter in this study because it determines the amount of the gas phase retained in the system at any time. The gas hold up in the riser for the three reactors increased by increasing the superficial gas velocity. Figure 2.17 shows the gas hold up in the riser between experimental data and CFD simulation. From that figure, when the superficial gas velocity is equal to 0.015 m/s and up to this value, the gas hold up increases with lower rate of three various scale reactors. Figure 2.18 shows the distribution of volume fraction in the reactor by volume of 10.5 l

with aeration of 0.03 m/s.



Figure 2.17: Gas hold up versus superficial gas velocity between experimental data and CFD result (Davarnejad et al. 2012)

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