

CFD Analysis of Phase Holdup Behaviour in a Gas-Liquid Bubble Column

Nur Khairunnisa Abd Halim^a, Siti Aslina Hussain^{a,*}, Mus'ab Abd. Razak^a and Mohd Amirul Syafiq Mohd Yunos^b

^a*Department of Chemical and Environmental Engineering, Faculty of Engineering, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor Darul Ehsan, Malaysia*

^b*Plant Assessment Technology, Industrial Technology Division, Malaysian Nuclear Agency, Bangi 43000 Kajang, Selangor Darul Ehsan, Malaysia*

Abstract

Experimental works on bubble column hydrodynamic are normally carried out on a laboratory scale less than 0.3 m with holes number less than 10. In this paper, we discuss several approaches to bubble column scale-up, relying on variables of parameters. Two spargers with different hole diameters (0.5 mm and 1.25 mm) and superficial gas velocities (0.0125 m/s and 0.0501 m/s) are used to determine the distribution of gas holdup and liquid flow pattern. An insignificant level of bed heights is investigated for the efficiency of hydrodynamic performance. Computational Fluid Dynamic (CFD) is used as the realistic representation of the actual reactor. The flow of the gas-liquid interface is implemented using the VOF model using the finite volume method by tracking the volume fraction of each of the fluids throughout the domain. It is observed that the initial bed heights, superficial gas velocity, and hole diameter of the sparger influence the overall gas holdup. Although the difference in sparger hole diameter affects overall gas holdup, the results are weak relative to other operating conditions. The simulation work is then compared with experimental data to improve the accuracy in analyzing the hydrodynamics of multiphase system, as well as validated the multidimensional models.

Keywords: Bubble column, CFD simulation, Gas holdup, Multiphase flow, Eulerian-Eulerian model

1. Introduction

The importance of gas-liquid bubble columns used for conducting multiphase reactions in a variety of industrial applications has been recognized for decades. This widespread application rises from the fact that bubble columns provide distinct advantages over other multiphase reactors, among which its operational simplicity, low operating and maintenance cost and have good characteristics in terms of mass and heat transfer [1-3]. Despite the apparent ease in mechanical operation, bubble columns present such complex characteristics. The flow pattern and dynamics of gas bubbles are mainly depending on the characteristics of the flow [4-5]. Three common flow regimes have been discovered and established in bubble column reactor; homogeneous flow, heterogeneous flow, and slug flow – mainly influenced by the sparging gas distribution and inlet flow of superficial gas velocity [6-8].

The bubble column's operation is often influenced by many global operating parameters. The efficiency of a bubble column is determined by column dimensions, superficial gas velocity, gas distributor design, and liquid level, according to current knowledge on bubble column dynamics flow.

* Corresponding author. Tel.: +603-97696292; fax: +603-97697120
E-mail address: aslina@upm.edu.my

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Among these parameters, sparger configuration has a notable influence on gas holdup and mixing phenomena [2, 4-5, 7-9]. It has been reported that many studies on the fundamental understanding of the effect of distributors and bubble column performance have been done by others [3, 10-11]. In contrast, Ihsana et al. [12] claimed that the differences in perforated plate diameter have no discernible impact on the overall gas holdup but other parameters did.

Several attempts have also been made to model the dynamics of gas-liquid flows in bubble columns using computer simulations. McClure et al. [15] simulated tracer injection location and successfully predicted the mixing trends at a various number of superficial velocities. Pourtousi et al. [6] has studied the significant effect of ring sparger diameter on the dynamic in a cylindrical bubble column. Even though bubble columns are widely used in many industrial processes, few studies of these devices have been conducted at high superficial velocities. Fletcher et al. [14] have analyzed the bubble column behavior conducted at high superficial velocities by comparing results using different solvers. In most previous publications of computational studies, the model is validated using data obtained with a sparger and a set of air-water systems. Based on these findings, several hydrodynamics simulations have been made for 2D and 3D geometries [3, 15-17]. Furthermore, the use of population balance is reported to elevate the holdup results compared to the use of an unchanged diameter [12, 16-18]. While some of these computational results are useful in providing general guidance for bubble column design, the actual gas distributor must be included in the simulation to account for non-uniform gas sparging and unsteady recirculatory flow patterns in the bubble column reactor [19].

Based on the brief analysis of previous studies, it appears that studying the relationship between sparger configuration and inlet gas flow rate on gas-liquid flow dynamics is essential. To identify the usual problem that occurred during the transferring of gas-liquid flows through vertical bubble columns, few methods are usually used to describe the real condition of the behavior of that multiphase system. The flow characteristics of the two-phase system and their configuration in the bubble column would be a fundamental study as well as of practical interest that needs to be considered. Many widely used industrial gas-liquid contacting devices require research into gas-liquid bubbly flows to understand their nature and operation. In many industrial chemical processes involving complex multiple reactions, engineers are concerned about selectivity to the desired product. Fluid mixing also has an effect on the reactor's efficiency in these circumstances.

The recent development of CFD modeling and software available with low-cost and high-end computers has allowed performing 3D simulations of multiphase flow in bubble column in a short time. The proper use of CFD modeling is essential to understand such complex interactions in bubble columns and helpful in facilitating designs and scale-up tasks. To complement the simulation findings, two sparger designs with different hole diameters were employed to the identical domain model to see how distributor configuration influenced overall holdup at various heights. The simulation results were analyzed, compared, and discussed with experimental data.

2. CFD design modeler

In simulation work, a 3D model of quadrilateral-shaped bubble column shown in Figure 1 is used. The inner volume of the column is 0.2x0.2x2.0 m. Simulations are conducted using two different designs of sparger plates with liquid height set at 1.0 m and 1.2 m, respectively. The superficial gas velocity is also varied and applied for both sets of sparger models. The dimensions of column, spargers, and parameters used are compiled in Table 1. Further details about the column design are available elsewhere [20]. Commercially available CFD code, ANSYSTM CFX 2019 R3 is used to numerically model the dynamics of bubble column reactor. The code method is based on the Finite Volume Method (FVM) with the Eulerian Two-Fluid framework to simulate the multiphase flow system. Based on the two-phase flow model, a computerized model is being developed as an alternative way to describe the mixing process and the phase distribution. In the finite volume grid, the holes of the sparger are fully resolved which consists of tetrahedral cells. The simulations took into

account two different grid densities dependent on the sparger configuration (sparger A: 4033509 cells, sparger B: 3360059 cells) in otherwise similar geometries of the column.

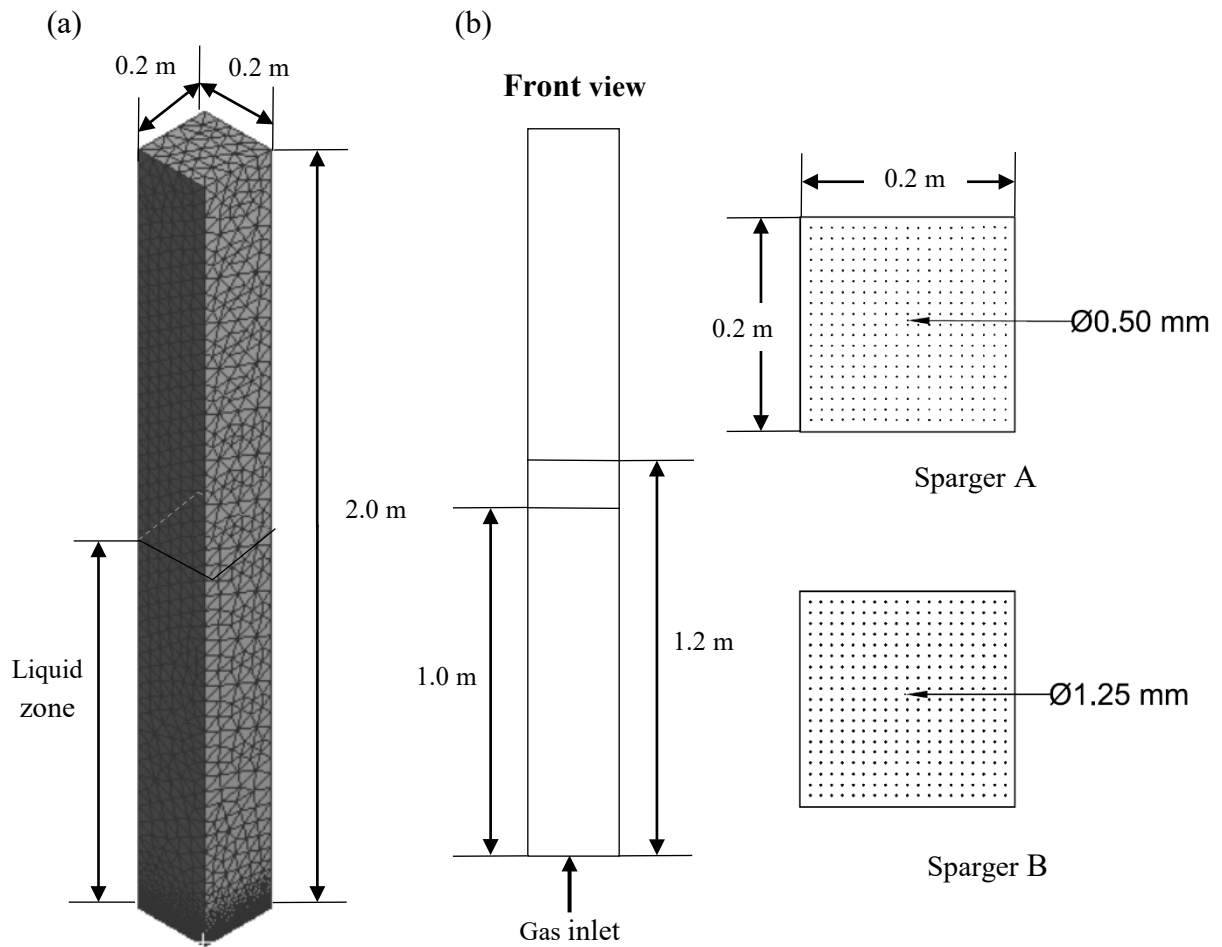


Figure 1. Geometric layout of the bubble column with boundary condition: (a) Meshing configuration, (b) Front view.

Figure 2. Sparger configurations.

Table 1. Dimensions of bubble column and parameter used.

Parameter	Dimension
Size of column	L x W x H = 0.2 m x 0.2 m x 2.0 m
Thickness of sparger	1 mm
Liquid level	1.0 m and 1.2 m
Gas flow rate	20 L/min and 80 L/min
Number of sparger holes	361 holes
Hole diameter (Sparger A)	0.5 mm
Hole diameter (Sparger B)	1.25 mm

Throughout the simulation, air and water are used and set as the dispersed phase and continuous phase respectively. To consider the free surface behavior using the Volume of Fluid (VOF) method, an air gap is formed over the water level in the column. The flow of the gas-liquid interface in the CFX VOF model is measured using the distribution of α_g , the volume fraction of gas in a computational cell where $\alpha_g = 1$ in the gas phase and $\alpha_g = 0$ in the liquid phase. As a result, the gas-liquid interface occurs in the cell where α_g is between 0 and 1. Due to its simple algorithm and low computation cost, turbulence was modeled using a standard $k-\epsilon$ equation to predict the flow pattern of liquid and gas holdup under low superficial gas velocity [21]. On the other hand, the dispersed phase zero equation model is applied for the dispersed (gas) phase. The surface tension was set at a constant value of 0.072 N/m.

The simulations were run isothermally, at atmospheric air at 25 °C with the superficial gas velocities at the inlet are set to 0.0125 m/s and 0.0501 m/s. The average static pressure is set to zero at the outlet. A single characteristics bubble size (0.004 m) for dispersed air is used in all simulations to provide drag calculations. The volume fraction of air at sparger would be high since the air inlet flows directly through sparger, thus the concept of zero contact area for the gas phase is not physically right. Therefore, a free slip boundary condition i.e., no friction between fluid and wall were set for the gas phase, while no-slip boundary condition i.e., the value of fluid velocity is zero on the walls for the liquid phase.

For interphase momentum transfer, grace correlation is used. Convergence criteria for residuals are set to 1×10^{-6} for every timestep. All simulations were performed using a high-speed Intel® Xeon® dual processor to reduce the computational time of numerical work. The CFX was processed in parallel, allowing a large number of simulations to be run at the same time with little loss in computational performance. By analyzing overall equilibrium and time history at relevant flow variables, simulations were run until a fully defined flow field was achieved.

3. Results and discussions

3.1. The impact of diameter holes sparger configuration

The CFD model is tested to see whether it can accurately forecast the operating flow regime in terms of gas holdup and bubble rise velocity. In the current work, a three-dimensional model was used for air-water phase modeling. Understanding the nature of holdup for various axial positions and examining the velocities of liquid circulation in the bubble column may help researchers better understand the flow pattern in the bubble column [3].

To analyze the effect of sparger holes, simulations are performed at the superficial gas velocity (U_g) of 0.0125 m/s and liquid height (H_L) of 1 m. Figure 3 depicts the volume rendering of a gas holdup at clip plane (0.2, 2.0, 0.1) with three distinct regions: oscillation area, disengagement zone, and near sparger. The simulations show uniformity in the oscillation region, but non-uniformities in the sparger region ($H/D = 0.5$) which is due to the hydrodynamic effect on gas injection uniformity at the distributor. However, at $H/D = 1$, where the gas holdup was nearly uniform and proceeded to the disengagement zone, these non-uniformities soon evened out.

It can be observed from Figure 3 that there is no significant effect on overall holdup between both sparger designs by a percentage difference of about 2%. The gas holdup is intertwined with the sparger holes and numbers in a complex manner. It would seem that as the diameter of the holes grows, so does the value of holdup. This complicated problem can be traced back to a variety of physical and computational phenomena. According to McClure et al., [9] the gas holdup increases linearly with increasing superficial gas velocity but may remain independent of sparger design, particularly at high superficial velocities. Figure 4 shows the distribution of gas holdup at different H/D for different sparger holes of 0.5 mm and 1.25 mm. The highest value of overall gas holdup obtained from sparger B is 0.0662 while 0.0794 for sparger A, both at $H/D = 0.5$ and $H/D = 1$ which

are near to the sparger plate. It can be seen that the graphical plot shows the non-uniform distribution of gas holdup across the width of the column. To obtain a realistic simulation of gas-liquid flow in a bubble column, non-drag forces are neglected. It is well understood that the sieve plate sparger used in numerical and experimental setup causes non-uniform gas distribution. As the gas sparged through the plate, a fraction of the total number of holes in the sparger plate is engaged at any instant, resulting in non-uniform gas distribution as well as holdup in the column [25].

Figure 5 shows the effect of sparger holes diameter through radial gas holdup profile at five different heights viewed from the top of the column. The inlet air seems not simultaneously flow through all holes in sparger A at a height of 0.02 m, near to the sparger which may be caused by dead zones compared to sparger B. As the height above the sparger plate increases to 0.1 m and 0.2 m, the small bubbles (3-6 mm) [22] coalesce forming larger bubbles (10-80 mm) [22] and concentrated at few locations. This is because the potential for the bubbles to coalesce to form bigger bubbles is higher as the bubbles move farther from the sparger plate. Bubbles with a size greater than the critical diameter (4.43 mm) have a negative lift force coefficient which forces the movement of bubbles towards a certain point of location of the column.

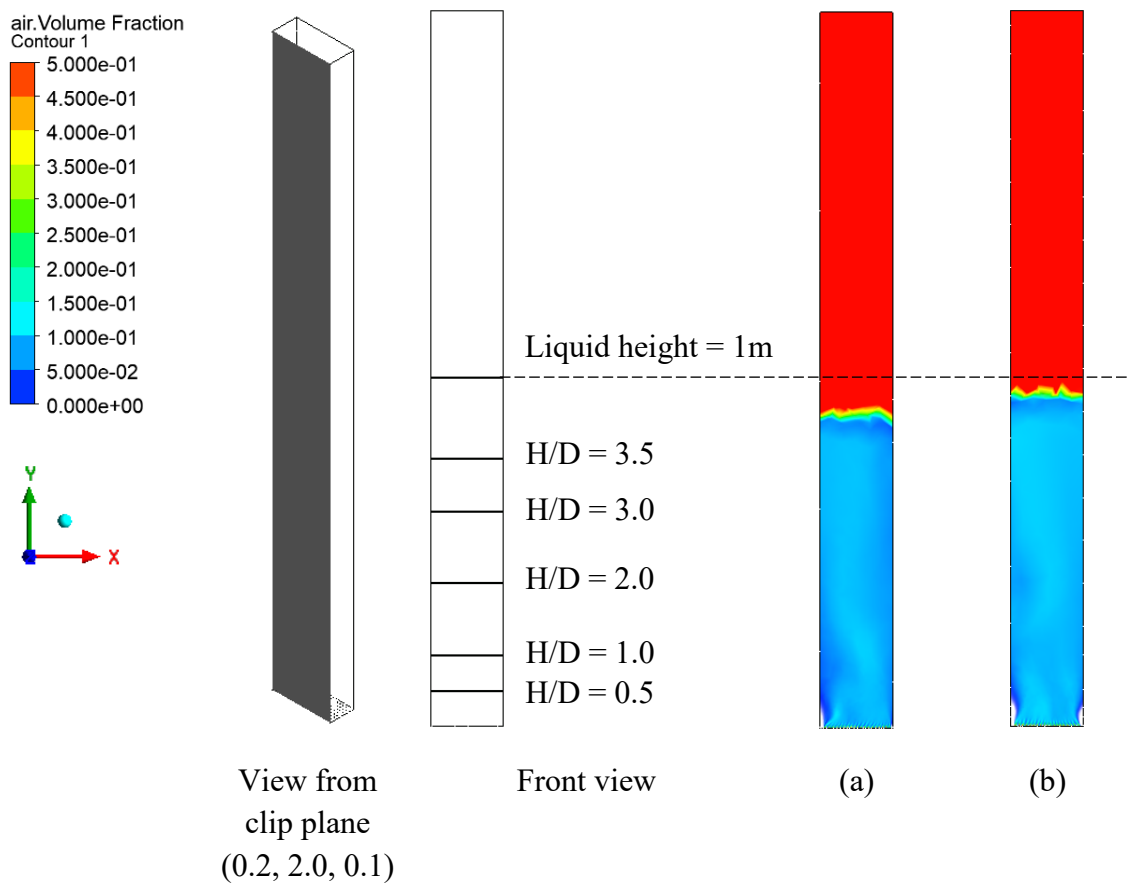


Figure 3. Overall holdup in sparger with holes diameter (a) 0.5 mm of sparger A and (b) 1.25 mm of sparger B.

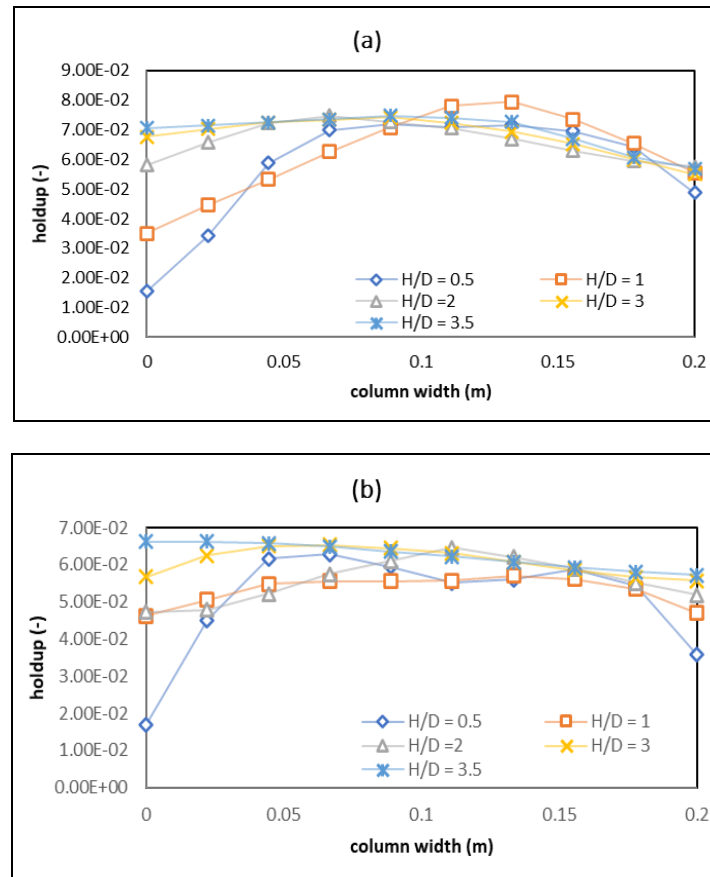


Figure 4. The radial distribution of gas holdup at different heights for different diameters of sparger holes (a) 0.5 mm of sparger A and (b) 1.25 mm of sparger B.

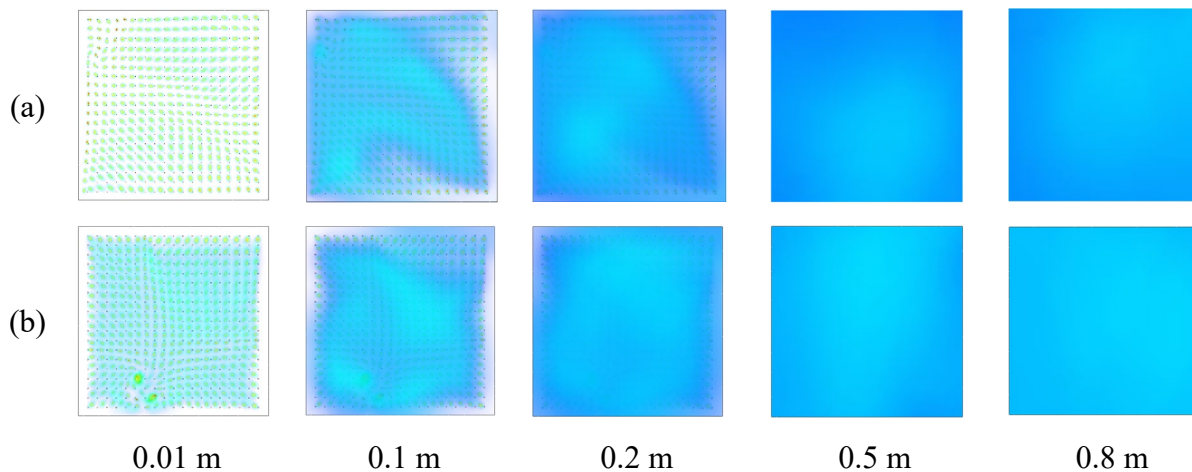


Figure 5. The radial profile of gas holdup under the different diameters of sparger holes (a) 0.5 mm of sparger A and (b) 1.25 mm of sparger B.

3.2. The impact of superficial gas velocity on the overall gas holdup

To investigate the impact of varying values of superficial gas velocity, computations were carried out using a larger hole diameter of sparger, 1.25 mm. Figure 6 shows the liquid velocity vectors for sparger B at 0.0125 m/s and 0.0501 m/s of superficial gas velocity, respectively. The relative axisymmetric flow pattern vanishes at elevated superficial gas velocity (>0.05 m/s). As a result, when extrapolating process variables like the superficial gas velocity, the pattern of bubble column flow should be handled with care before drawing any descriptive conclusions.

Figure 7 shows the average values of overall gas holdup for various values of superficial gas velocity. Due to increased eddy turbulence in the liquid phase, the gas holdup increases as the superficial gas velocity increases, as shown in the graphical plot. The gas holdup values for sparger B, on the other hand, are lower than those for sparger A, implying that gas holdup is unrelated to sparger layout, especially at high superficial velocity. At low superficial gas velocity, a smaller hole diameter suggests the opposite. We can safely conclude that the gas holdup is proportional to the superficial gas velocity based on these results, which is consistent with previous past findings by Wagh et al., [23].

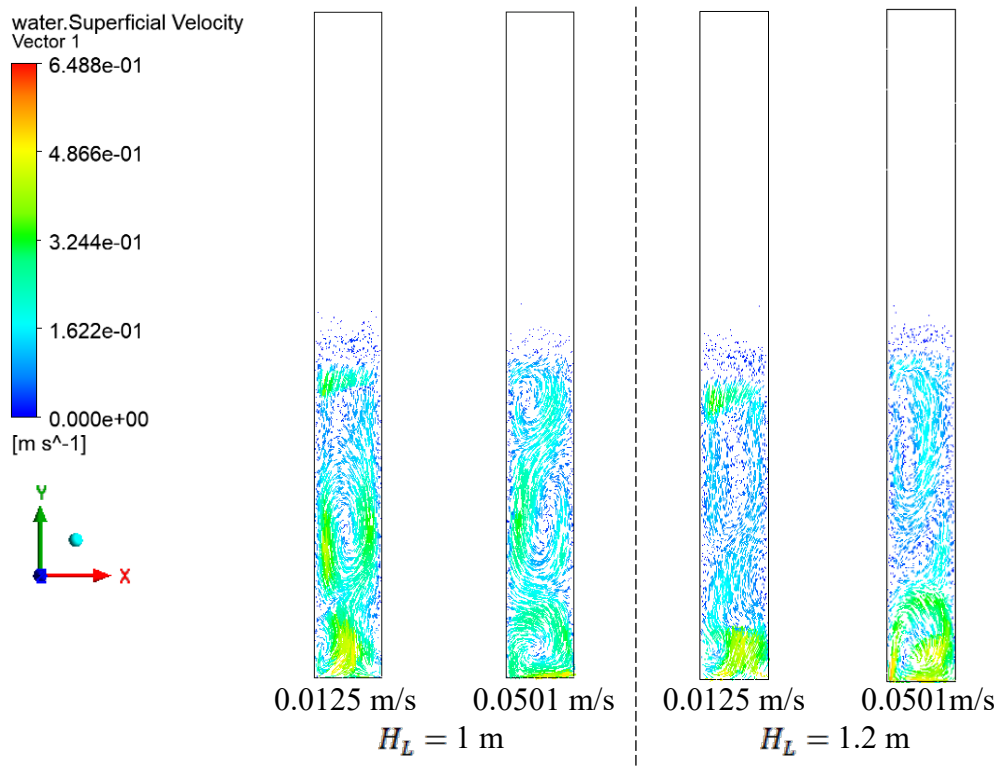


Figure 6. Liquid velocity vectors for sparger B at a superficial gas velocity of 0.0125 m/s and 0.0501 m/s.

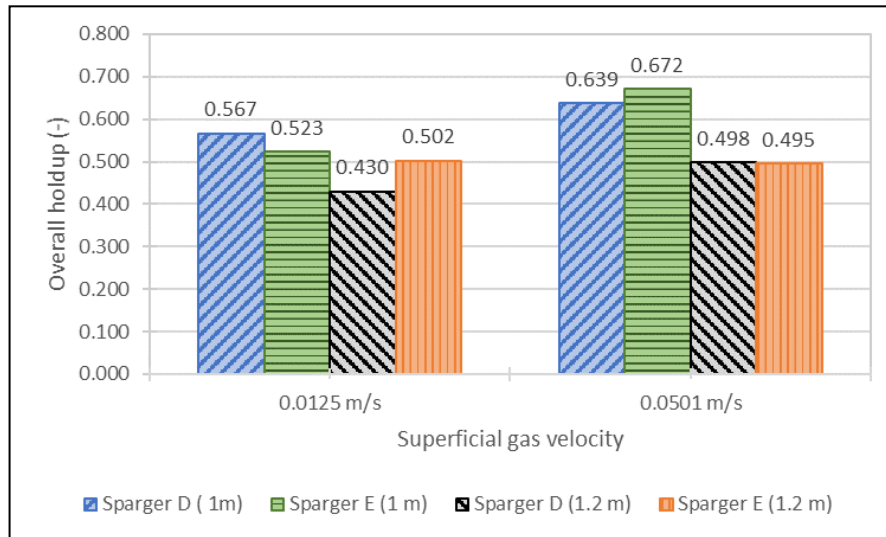


Figure 7. Average gas holdup distribution at various sparger configurations.

3.3. The impact of liquid height on the overall gas holdup

There are two initial liquid height sets for both sparger models which are 1.0 m and 1.2 m. Observations on the impact of the initial liquid heights are made on both spargers at two values of superficial gas velocities. Figure 8 shows the value of overall gas holdup increases as the initial liquid height increases. In the simulation, the gross fluid level shifts obtained at the superficial gas velocities of 0.0125 m/s and 0.0501 m/s are 3 cm and 6 cm respectively. Based on Figure 8. The contour shows that the overall gas holdup of both spargers affected by the liquid level, 1 m and 1.2 m respectively. The graphical plots show that the value of overall gas holdup is influenced more by the liquid level rather than sparger configuration and superficial gas velocity. This might be because the ratio between the initial height of the liquid is more significant as the initial liquid level increases [12]. Khan [24] has stated that the gas holdup changes considerably if the initial liquid level and column ratio are between 2 and 20. In other words, if the column diameter is increasing, the gas holdup will also have an insignificant effect, even though the ratio liquid level to the column is less than 2.

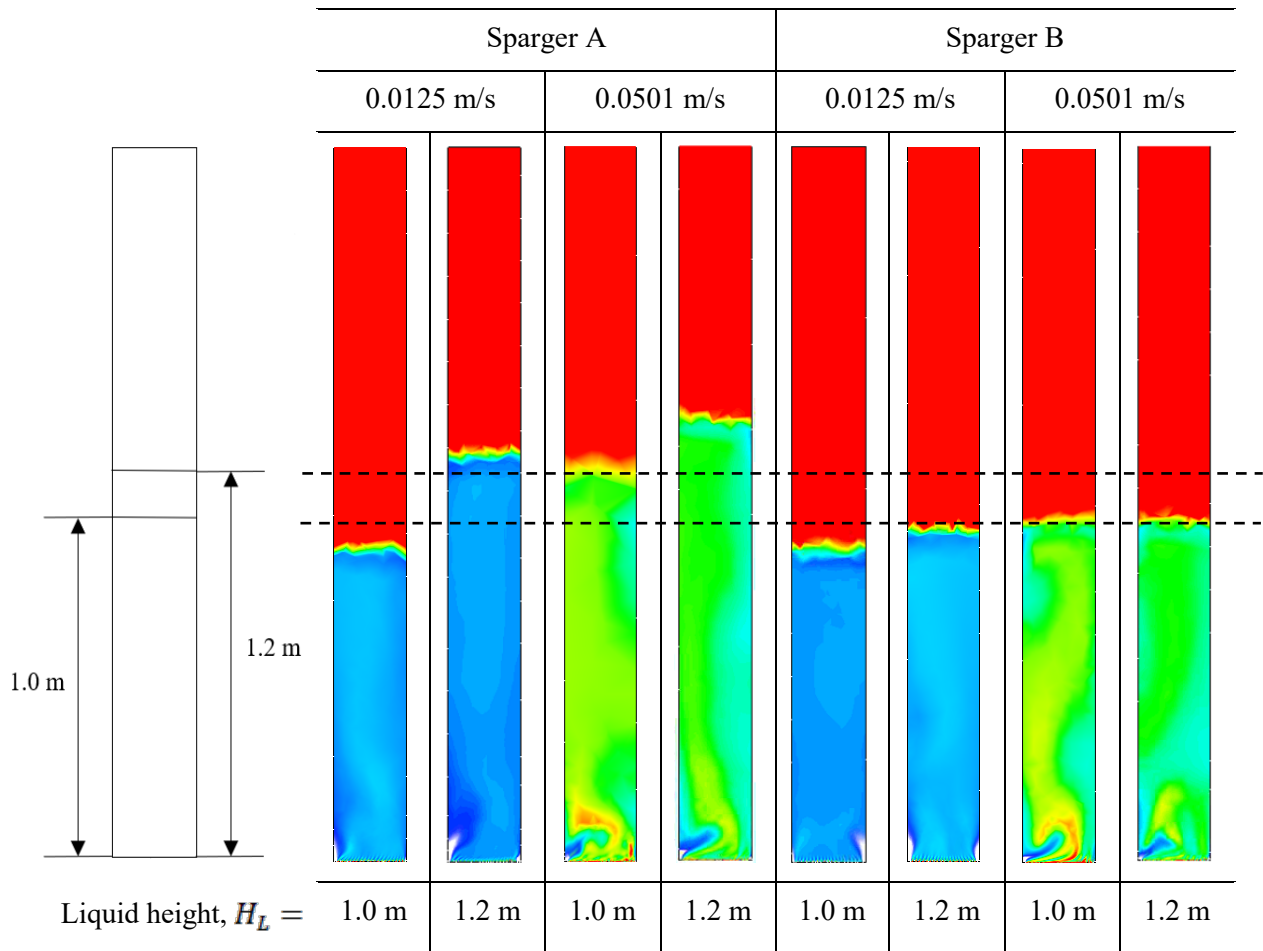


Figure 8. Effect of the overall holdup on different initial liquid heights.

3.4. Model validation

As previously stated, an accurate description of the flow pattern in a bubble column is critical for determining the column's operating regime. An experimental setup consists of a transparent bubble column with the same dimensions, equipped with a sparger plate at the bottom. The gas was blown from the bottom of the column and the pressure at the top of the column was atmospheric. The superficial gas velocity was set at 20 L/min and 80 L/min employing the appropriate combination of volumetric flow rates. By measuring the differential in height of water in the bubble column before and after gas injection, the gas holdup can be determined. More information on the experimental setup can be found elsewhere [20].

The numerical results of overall gas holdup for sparger A and B are shown in Figure 9, along with experimental data. Based on the figure, the CFD model predicts a new trend that is practically similar to experimental results. The comparison of experimental data with numerical predictions reveals the CFD codes calculates satisfactorily the gas holdup at both superficial gas velocity. By having an error of overall gas holdup of 9.34 % and 5.18 % for sparger A at $U_g = 0.0125$ m/s and 0.0501 m/s, respectively, while 7.65 % and 6.24 % for sparger B at $U_g = 0.0125$ m/s and 0.0501 m/s, respectively, the simulation could be said to agree with what experimentally observed, however implementation on bubble size distribution may support more on the validation.

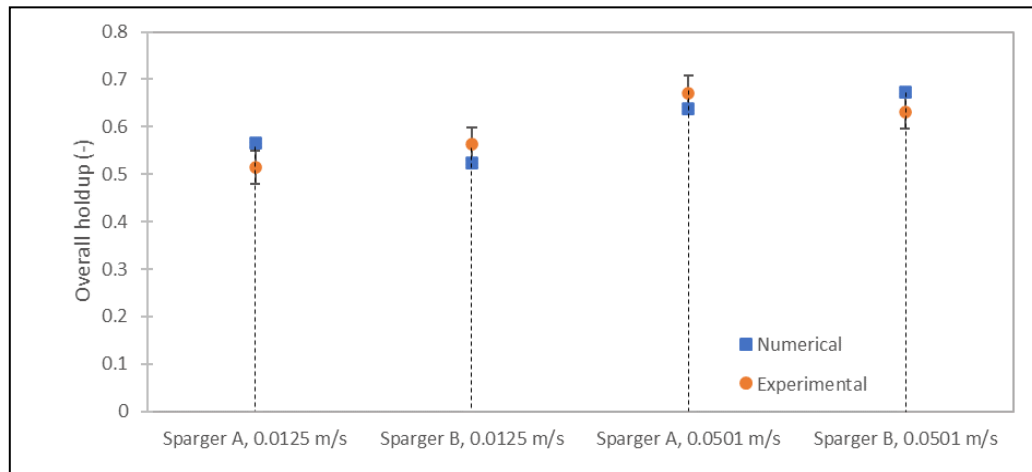


Figure 9. Comparison of experimental and numerical data on overall gas holdup for sparger A and B at preliminary liquid height, H_L = of 1 m and U_g = 0.0125 m/s and 0.0501 m/s.

4. Conclusion

A CFD model is constructed to illustrate the hydrodynamics behavior of an air-water bubbly column reactor. Two spargers of the same number of holes of 361 but different diameters of sparger holes (0.5 mm and 1.25 mm) were run at a set of initial liquid heights, $H_L = 1.0$ m and 1.2 m and superficial gas velocities, $U_g = 0.0125$ m/s and 0.0501 m/s. A column with sparger A and B containing 4033509 cells and 3360059 cells, respectively was used for CFX. The VOF is calculated by the distribution of gas volume fraction, where $\alpha_g = 1$ for gas and $\alpha_g = 0$ for liquid. From the results displayed, the spargers, initial liquid height, and inlet velocity are highly significant at the lower region of the column near to sparger as they tend to influence more on gas holdup and liquid flow structure. The highest inlet velocity is acquired through the centerline area of the bubble column but vertical velocity profiles and holdup values tend to become constant as the bed height increases. The overall gas holdup depended significantly on the liquid height rather than the diameter of air sparging holes. This demonstrated the importance of accurately modeling dispersed gas and liquid phase direct interactions in two-phase flow. The experimental results were subsequently applied for the development and validation of the model used. The comparison of data of overall gas holdup in experimental is in good agreement with data from numerical work. Therefore, it is shown that the computational cost is low enough even when using high grid density to obtain results that are in good compliance with the experiments and in a reasonable amount of time for chemical engineering applications.

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