Sensitivity study of Bubble diameter for prediction of flow pattern in homogeneous bubble column regime

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Abstract. Determining the bubble diameter size in a bubble column reactor plays an important role to accurately predict flow pattern in a bubble column reactor. This paper employs the Eulerian-Eulerian method to numerically investigate the sensitivity study of bubble diameter size in a cylindrical bubble column reactor. Existing experimental results in the literature are used to validate the implementation of the proposed numerical method. In our simulation various bubble diameter size (i.e., 3-5.5mm) are used to find an appropriate bubble size inside the bubble column when the regime is homogeneous (superficial gas velocity = 0.005m/s). The result shows that bubble diameter 4mm is a reasonable size for flow pattern prediction inside the column.

1. Introduction

Bubble column reactors are used as multiphase contactors and reactors in chemical, petrochemical, biochemical and metallurgical industries such as fermentation and biological wastewater treatment [1-4]. The bubble column reactors are often cylindrical vessels equipped with a gas distributor at the bottom. The gas distributor spargers fluids bubbles into vessel containing either a liquid phase or a liquid–solid suspension. Bubble column reactors have many advantages over other types of reactors such as high heat and mass transfer coefficients, low maintenance and operating costs and high durability of the catalyst or other packing material [4-6].

To date, the numerical approaches have been used in many studies to predict the bubble column reactors because of the difficulties that are still found in designing and scaling-up the bubble columns [7, 8]. Computational fluid dynamics (CFD) has improved our partial knowledge of the complex hydrodynamic processes occurring inside the bubble column [9].

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Inside the bubble column, an interaction exists between the dispersed gas and the liquid that affects the interphase forces (e.g. drag force, lift force, etc.), turbulence and bubble diameter in the column. Therefore, a proper solution for the bubble columns is dependent on the correct modeling of interphase forces, turbulence models and appropriate bubble diameter inside the column [7, 10]. Several models for interphase forces and turbulence have been reported in the literature, [7, 10, 11]. For instance the drag force, lift force, turbulent dispersion and added mass model have been studied by [7, 10]. In addition, various turbulence models (e.g. standard $k-\varepsilon$ model, Reynolds Stress Model (RSM), Large Eddy Simulation (LES)) have been used to predict flow pattern inside the bubble column [8, 10, 12, 13]. Since many investigations studied interface forces and turbulence models on prediction of bubble column, this study specifically focuses on effect of bubble diameter size on prediction of flow pattern using Eulerian–Eulerian framework in a homogeneous flow regime.

2. Methodologies

2.1 Governing equations

The two-phase model based on the Eulerian–Eulerian approach is used to simulate dispersed gas-liquid flows in bubble columns. Each fluid (or phase) is treated as a continuum in the domain under consideration in this approach. The phases share this domain and interpenetrate as they move within it. The Eulerian modelling framework is described as follows:

Continuity equation:
\[
\frac{\partial}{\partial t}(\rho_k \varepsilon_k) + \nabla \cdot (\rho_k \varepsilon_k \mathbf{u}_k) = 0
\]  

Momentum transfer equation:
\[
\frac{\partial}{\partial t}(\rho_k \varepsilon_k \mathbf{u}_k) + \nabla \cdot (\rho_k \varepsilon_k \mathbf{u}_k \mathbf{u}_k) = -\nabla p + \varepsilon_k \rho_k g + M_{L,k}
\]  

The terms on the right hand side of Eq. (2) represents the stress, the pressure gradient, the gravity and the ensemble-averaged momentum exchange between the phases due to interface forces. The pressure is shared by both of the phases. The stress term of phase $k$ is described as follows:
\[
\tau_k = -\mu_{\text{eff},k}\left(\nabla \mathbf{u}_k + (\nabla \mathbf{u}_k)^T - \frac{2}{3}\nabla (\nabla \cdot \mathbf{u}_k)\right)
\]

where $\mu_{\text{eff},k}$ is the effective viscosity. The effective viscosity of the liquid phase is composed of three contributions: the molecular viscosity, the turbulent viscosity and an extra term due to bubble induced turbulence as given below:
\[
\mu_{\text{eff},L} = \mu_L + \mu_{T,L} + \mu_{BLL}
\]

The model proposed by Sato and Sekoguchi [14] was used to take account the turbulence due to the movement of bubbles, which can be written as
\[
\mu_{BLL} = \rho_L C_{\text{BL}} d_B \varepsilon_G |u_G - u_L|
\]

with the model constant of $C_{\text{BL}}$ is set to 0.6 as recommended in ref [14]. The calculation of the effective gas viscosity is based on the effective liquid viscosity [23] which is:
\[
\mu_{\text{eff},G} = \frac{\rho_G \mu_{\text{eff},L}}{\rho_L}
\]

The total interfacial force acting between the two phases are based on the interphase drag force and turbulent dispersion force, which can be written as follows:
\[
M_{LL} = -M_{LG} = M_{DL,L} + M_{TD,L}
\]

The interphase momentum transfer between the gas and liquid due to the drag force is given by:
\[
M_{TD,L} = -\varepsilon_k \rho_k \frac{C_D}{d_g} |u_G - u_L|(u_G - u_L)
\]

In our numerical study a constant drag coefficient of 0.44 is used which is suggested in references [12, 15]. The turbulent dispersion force derived by Lopez de Bertodano [16] is used, which is
\[
M_{TD,L} = -M_{TD,L} = -C_{TD} \rho_L k \nabla \varepsilon_L
\]
where \( k \) and \( C_{TD} \) are the liquid turbulent kinetic energy per unit of mass and turbulent dispersion coefficient respectively. In our simulations, values of 0.3 is used for the turbulent dispersion coefficient as suggested in References [10, 16]. Turbulence has been modelled using a ‘standard’ \( k-\varepsilon \) model.

2.2 Geometrical structure and Simulation cases
A three-dimensional (3D) domain of a bubble column with a height and diameter of 2.6 m and 0.288 m, respectively is used. Air bubbles are sparged in the quiescent water in the column using a ring sparger. The gas has a superficial velocity of 0.005 m/s at the ambient condition.

2.3 Grid
A structured grid based on hexahedral grid as shown in Figure 1 is used throughout the domain. The type of grid adopted herein is almost identical to that used in Boutet et al. [17]. The axial length of the domain is divided into 60 grid elements. The grid namely Grid 1, typically has about 40500 elements.

![Grid intensity of the computational model consisting of 40500 structural elements.](image)

2.4 Boundary conditions and numerical methods
The gas velocity from each nozzle of the ring spargers is calculated based on a superficial gas velocity of 0.005 m/s. The top surface of the bubble column is treated as the ‘degassing’ boundary condition. On the side walls, a no-slip boundary condition is used for the liquid phase and a free-slip condition for the gas phase. Simulations were carried out using the commercial CFD software package of ANSYS-CFX 13. The time step of 0.1s is used in our simulations and the sensitivity of a much lower time step, i.e., 0.01s are investigated.

3. Results and discussion
In industrial bubble column, bubble usually sparges trough the sparger. As bubbles travel to the top surface of the column, they merges and break into number of small bubbles. These interaction results in bubbles with different diameters inside the bubble column. In homogeneous regime, bubbles have almost same diameter and velocity and the rate of interaction between bubbles are small. Therefore, we can select one bubble diameter instead of range of bubble size and this way requires less computational time in comparison with other methods (e.g., population balance model). We specify only one bubble diameter for one case study and the sensitivity of the use of different diameters of gas bubble in predictions of axial liquid velocity and gas hold-up in the bubble column have been also investigated. The radial distribution of the time-averaged axial liquid velocity and the gas hold-up at column height 1.6 m is shown in Figure. 2 and Figure. 3, respectively based on bubble diameters of 4 mm to 5.5mm. Figure. 4 shows the planar averaged gas hold-up at various column heights. Such results from the experimental investigation of Pfleger and Becker [12], which both used a bubble diameter of 4mm, are included in the Figures for a comparison. The use of a bubble diameter of 4.5mm, an increase about 0.5 mm from that of bubble with 4mm diameter, only results in small
differences in the radial of the axial liquid velocity (Figure 2), the gas hold-up (Figure 3) and the averaged gas hold-up (Figure 4) in the column. However, this is not the case for the bubble diameter of 5 mm (or 5.5 mm) with an increase of 1mm (or 1.5mm) from that of bubble with 4mm size. The differences are significant. For example, the radial profile of the axial liquid is asymmetric with more positive velocity at right side of the column. Consequently, the radial profile of the gas rises asymmetrically in the column (Figure.3) and has a two-peak profile at the central region of the column.

Figure 2. Comparison between the average of axial liquid velocity from various bubble diameter sizes and that from experimental and numerical from Pfleger and Becker [10] at height 1.6m.

Figure 3. Comparison between the average of gas hold-up from various bubble diameter sizes and that from experimental and numerical from Pfleger and Becker [10] at height 1.6m.
The amount of gas for case of bubble diameter 5 and 5.5mm at different heights of bubble column is lesser than smaller bubble (i.e., 4 and 4.5mm). For example, at 2m height the planner average gas hold-up for 4 and 5mm are 0.0156 and 0.0138 respectively (see Figure 5). The increase of gas hold-up may attribute to the fact that, as bubble size decreases, bubble interfacial area increases. This finding is consistent with previous studies [18].

Figure 4. Local averaged gas hold-up for various bubble diameters at different column heights.

Figure 5 shows that the amount of gas tends to move to the center specially near the sparger region. As bubbles travel to the surface, the fraction of the gas decreases. It is interesting to say that merging bubble near the sparger may be more than other parts of the bubble column and this is a good reason that near this region bigger bubble have a good agreement with Pfleger' experimental study.

Figure 5. Contour plot for air fraction inside the bubble column.
4. Conclusions
In this investigation we studied various bubble diameter sizes to show the appropriate prediction of the flow pattern inside the bubble column. In view of all bubble diameter sizes, the bubble diameter 4mm is in reasonable agreement with the experimental data for the overall and local gas hold-up. In addition, the results show that the bubble diameters near the sparger region are 5mm and 5.5mm.

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