A CFD-PBE SOLVER FOR BUBBLE COLUMNS OPERATING AT HIGH PRESSURE

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Keywords: *OpenFOAM, high pressure, bubble column, population balance equation.*

1. Introduction

OpenFOAM (open-source field operation and manipulation) is a free source CFD (computational fluid dynamics) package written in C++, which uses classes and templates to manipulate and operate scalar, vectorial and tensorial fields [1]. Its open-source characteristics facilitate the implementation of any addition or modification in the source code, which is very suitable for the purposes of research [2]. Recently, our group has developed several solvers and carried out simulations in the framework of OpenFOAM. Cheng et al. [3] developed a CFD-PBE (population balance equation) solver for gas-liquid flows. To validate this solver, a bubble column was simulated, and the simulation results showed generally reasonable agreement with the published experimental data. The coupling of pressure and velocity is resolved with the PIMPLE algorithm, which is a combination of the PISO (Pressure-Implicit with Splitting of Operators) and the SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithms. They found the PBE could be solved outside the PIMPLE loop to save much computation time, while still preserving the temporal information on variables. On this basis, a CFD-PBE-PBE solver for the reactive crystallization in airlift loop reactors was developed then [4]. PBE describing bubble coalescence and breakage was solved by the cell average method. Primary nucleation, secondary nucleation and particle growth were considered in the PBE describing the crystallization process, and solved using the standard moment method. The solver is validated with the formation of calcium carbonate via the reaction of CO_2 gas with $Ca(OH)_2$ solution in an airlift loop crystallizer. Effects of the crystallization kinetics and operation parameters were investigated. In addition, the primary KT high-resolution finite-volume central scheme [5] for uniform grids is extended to a general form and validated for pure growth in homogeneous systems [2]. With the extended KT scheme, a solver coupling the multiphase mixture model with a micromixing model and the general discretized PBE in OpenFOAM was used for simulating the antisolvent crystallization of lovastatin from a methanol-water mixture in a confined impinging jet [2]. The shapes of crystal size distribution (CSD) at various jet velocities were consistent with experimental observations.

Gas-liquid bubble columns are encountered in many industrial processes. Most industrial bubble columns are operated at high pressure [6]. The pressure has significant influence on the hydrodynamic parameters, such as gas holdup and bubble diameter. With the increase of pressure, the gas holdup increases and the bubble diameter and bubble rising velocity decrease significantly. The simulation investigations about the ambient pressure bubble columns have been carried out by many researchers. However, the simulation about high pressure bubble columns is very limited. Based on our previous works, a CFD-PBE solver for high pressure bubble columns is developed in this work. The effects of pressure on the gas holdup, bubble diameter and bubble size distribution (BSD) are investigated.

2. Mathematical models

The gas-liquid Eulerian two-fluid model is used to simulate the flow field. Mixture k-ε equations proposed by Behzadi et al. [7] are employed to model the turbulence. The interphase momentum transfer includes drag, lift, virtual mass, wall lubrication and turbulent dispersion terms. The drag force coefficient is calculated by the model of Tomiyama et al. [8]. In order to consider the effect of bubble swarm, the drag force is modified by the model of Rampure et al. [9]. The lift coefficient model of Fank et al. [10] and a constant virtual mass coefficient C_{VM} = 0.25 are used. The turbulent dispersion force is modeled by the formula of Burns et al. [11], and the wall lubrication is by the model of Tomiyama [12]. To describe the effect of pressure, a factor of $(\rho_g/\rho_{g,atm})^{0.25}$ is employed to modify the drag force [13]:

$$\mathbf{F}_{D,g} = -\frac{3C_D}{4d_b}\rho_l\alpha_g\alpha_l\left(\frac{\rho_g}{\rho_{g,atm}}\right)^{0.25}\left|\mathbf{u}_g-\mathbf{u}_l\right|(\mathbf{u}_g-\mathbf{u}_l) \quad (1)$$

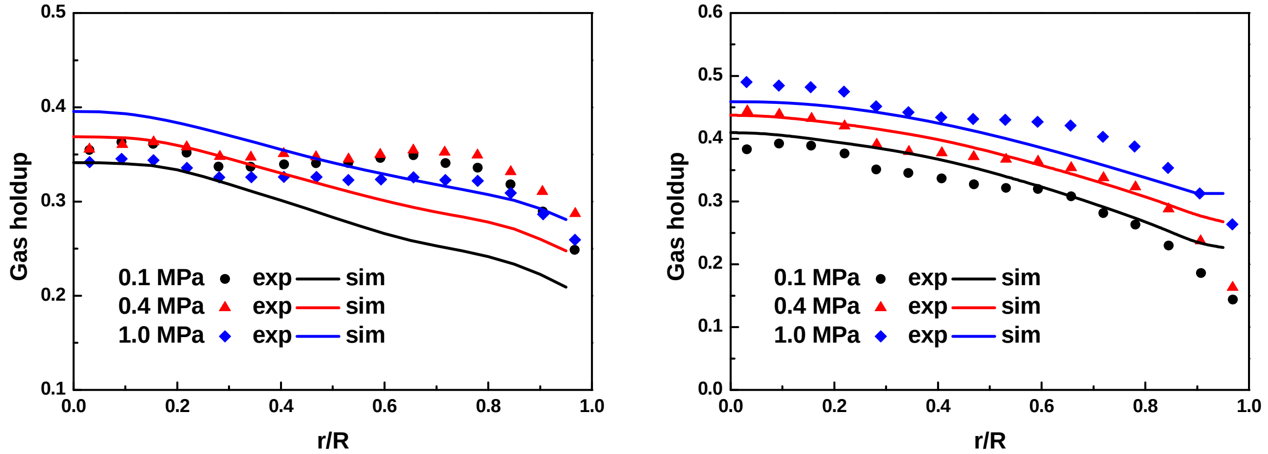
It is found that the bubble diameter is decreased with the increase of pressure. The higher pressure enhances the breakup of large bubbles [14-16]. In order to describe the influence of the pressure on the bubble breakage rate, a factor B is used to modify the bubble breakage rate according to Yang et al. [6] as shown below:

$$B = \begin{cases} \rho_g^{70d-2800d^2} & d < 0.018 \\ \rho_g^{0.35} & d \geq 0.018 \end{cases} \tag{2}$$

The PBE is solved using the cell average method, which is an extension of the widely used fixed pivot method and has been proved more accurate in predicting the BSD. The bubble aggregation model of Prince and Blanch [17] and breakage model of Lehr et al. [18] are employed.

3. Results

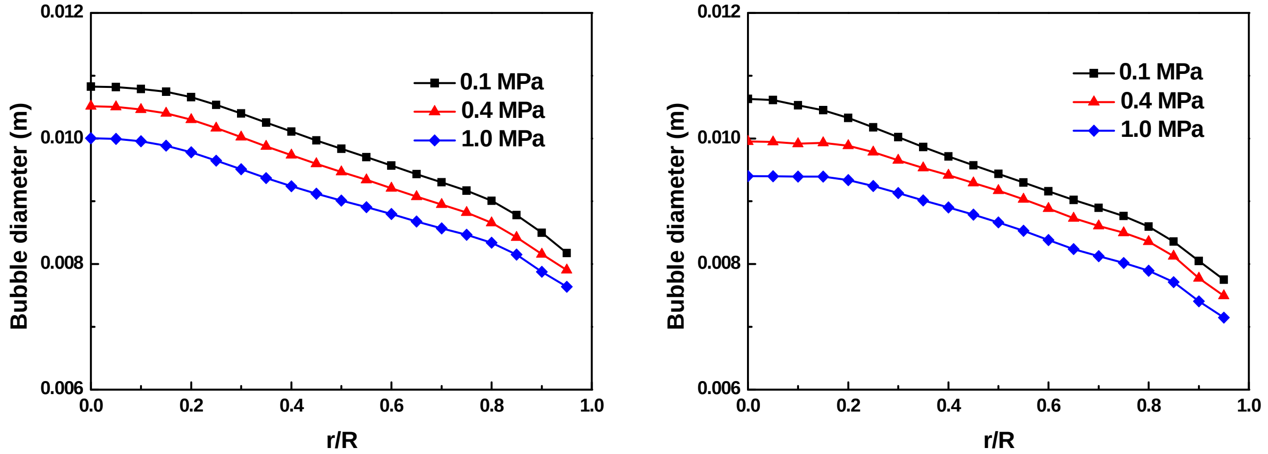
Figure 1 shows the comparison of the simulated radial profiles of gas holdup with the published experimental results [19] at different pressures. It can be seen that, the simulated gas holdup increases with the increasing pressure. At the superficial gas velocity of 0.08 m/s, the variation of gas holdup with the pressure in the experiment is not very obvious. When the superficial gas velocity increased to 0.14 m/s, the distinction between the gas holdup measurements is significant, and the simulated results are in good agreement with the experimental data.



(a) (b)

Figure 1: Comparison of simulated radial profiles of gas holdup with the reported experimental data [19] at different superficial gas velocities: (a) *V*g = 0.08 m/s; (b) *V*g = 0.14 m/s.

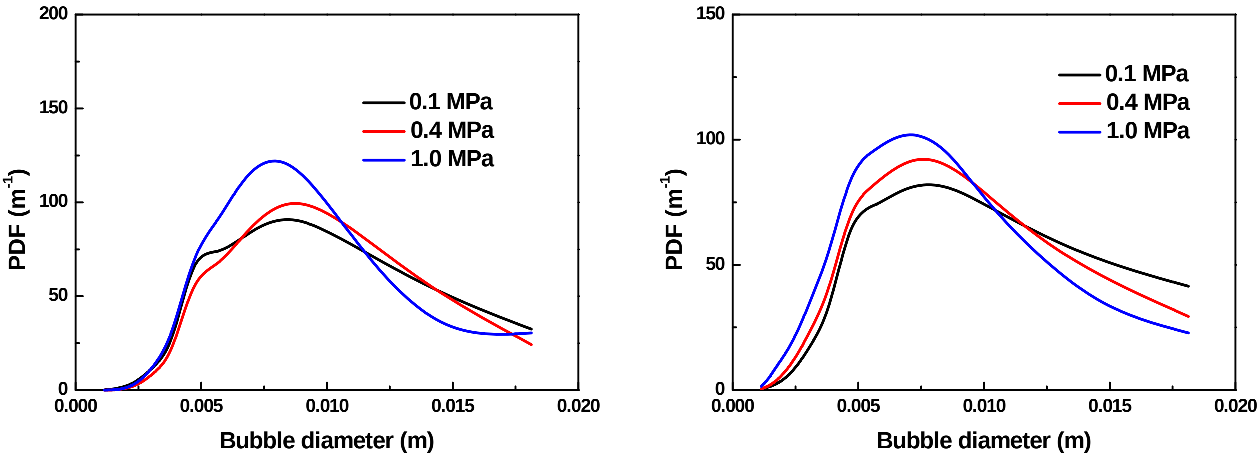
Figure 2 shows the variation of the radial profiles of the bubble mean diameter with the pressure at the superficial gas velocities of 0.08 and 0.14 m/s. It is obvious that, at the constant superficial gas velocity, the bubble diameter decreases when the pressure is changed from 0.1 to 1.0 MPa. A decrease of bubble diameter from the center of the reactor to the wall is captured by the simulation, which is consistent with the experimental observations.



(a) (b)

Figure 2: The effect of pressure on the radial profiles of bubble mean diameter at different superficial gas velocities: (a) *V*g = 0.08 m/s; (b) *V*g = 0.14 m/s.

Figure 3 is the variation of the bubble size distribution with the pressure at different superficial gas velocities. From the simulation results, one can found that the bubble size distribution becomes narrower when the pressure increases. Meanwhile, the number of large bubbles decreases obviously with the increase of pressure, implying that the bubble breakage rate increases.



(a) (b)

Figure 3: Effect of pressure on the bubble size distribution at different superficial gas velocities: (a) Vg = 0.08 m/s; (b) Vg = 0.14 m/s.

4. Conclusion

A CFD-PBE solver for high pressure gas-liquid bubble column is developed in the framework of OpenFOAM in this work. The predicted bubble diameter is larger in the center and smaller in the wall region, indicating that large bubbles are tend to gathering in the center region. With the increase of pressure, the bubble diameter decreases and the BSD is narrower, and the number of large bubbles decreases and that of small bubbles increases. These results show the feasibility of this solver in simulating the high pressure bubble columns.

Acknowledgements

Financial supports from National Key Research and Development Program (2016YFB0301702), National Natural Science Foundation of China (21776284, 21476236), and Key Research Program of Frontier Sciences, CAS (Grant No. QYZDJ-SSW-JSC030) and the Instrument Developing Project of the Chinese Academy of Sciences (YZ201641) are gratefully acknowledged.

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