Numerical simulation of side-entry bubbling reactor

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Abstract. In this paper, the numerical simulation of bubbling reactor was carried out under the condition of the amplification design of chlorine dissolving bubbling reactor in the epoxy propane chlorohydrin production process. The gas hold-up and flow field distribution in a side-entry bubbling reactor were studied. The simulation results show that the side-entry bubbling reactor can intensify the fluid disturbance near the wall so that the gas substance can contact with the liquid fully and the reaction time can also be increased. Hence, the mass transfer between the gas-liquid two phases was enhanced.

1. Introduction

The liquid-gas reactive process is a characteristic process of the chemical industry. Many types of reactors are used to carry out reactions. The bubbling reactors as the widely used devices have been studied for several decades, such as Shah et al. [1], Doraiswamy and Sharma [2], and Decker [3].

The principal advantages of bubbling reactor are the absence of moving parts, leading to easier maintenance, high interfacial areas and transport rates between the gas and liquid phases, good heat transfer characteristics, and large liquid hold-up, which is favourable for slow liquid-phase reactions[4]. However, the hydro mechanical behaviour of gas-liquid flow in bubbling reactor is very complex and the experimental study is very difficult because of the existence of a large number of bubbles. In recent years, with the development of computational fluid dynamics and the improvement of physical models, numerical simulation has gradually become an important means of bubbling reactor research. Remade and Taya Lia [5] investigated the influence of two different ring sparer’s on the hydrodynamics of bubble reactors using standard $k-\varepsilon$ model. Becker [6] who assumes that the viscosity of the turbulence is about 100 times that of the molecular viscosity has adopted two fluid model for numerical simulation. The simulation results were close to the experimental results. However, the turbulence model were not used to calculate the turbulent viscosity and the result depended on the mesh size. Tomiyama [7] have used VOF model to test the rising behaviour of single bubble under different flow conditions. The study of D. Pledger [8] shown that the standard $k-\varepsilon$ model can predict the main characteristics of the low frequency velocity pulsation and describe the instantaneous large scale turbulence structure.

A new type bubbling reactor, the side-entry bubbling reactor, were simulated in this paper. The internal flow field and gas hold-up distribution of the reactor are studied.
2. **Numerical Calculation**

2.1. **Geometrical configuration**

The structure of the side-entry bubbling reactor is shown in Fig. 1.

![Side-entry bubbling reactor](image)

**Figure 1.** Side-entry bubbling reactor.

The diameter of the reactor is 80 mm, the height is 100 mm, and the diameter of the side-entry hole is 1.5 mm. The holes spacing is 10 mm, and the number of holes is 108. The positions of the holes on the layers are arranged crosswise.

2.2. **Mathematical model**

2.2.1. **Governing equation.** In the bubbling reactor, the gas was set as dispersed phase and the liquid was set as continuous phase. In this study, the gas phase is assumed to be incompressible and the mass transfer and heat transfer are not considered. The governing equations are shown as follows:

Continuity equation:

\[
\frac{\partial \alpha_i}{\partial t} + \nabla \cdot (\alpha_i \mathbf{U}_i) = 0
\]

Momentum conservation equation:

\[
\frac{\partial \alpha_i \rho_i \mathbf{U}_i}{\partial t} + \nabla \cdot (\alpha_i \rho_i \mathbf{U}_i \mathbf{U}_i) = -\alpha_i \nabla p + \nabla \cdot (\alpha_i \mathbf{r}_i) + \mathbf{F}_e + \alpha_i \rho_i g
\]

The turbulence in liquid phase is calculated by \( k - \varepsilon \) turbulence model. The equations of \( k \) and \( \varepsilon \) are given respectively:

\[
\frac{\partial (\rho k)}{\partial t} + \frac{\partial (\rho k u_j)}{\partial x_j} = \frac{\partial}{\partial x_i} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] + G_k + G_k - \rho \varepsilon - Y_M
\]

\[
\frac{\partial (\rho \varepsilon)}{\partial t} + \frac{\partial (\rho \varepsilon u_j)}{\partial x_j} = \frac{\partial}{\partial x_i} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_i} \right] + \rho C_{1k} \varepsilon - \rho C_{2k} \frac{\varepsilon^2}{k + \sqrt{\varepsilon}} + C_{1e} \frac{\varepsilon}{k} C_{3e} G_b
\]
\[
C_1 = \max \left[ 0.43, \frac{\eta}{\eta + 5} \right], \quad \eta = \frac{k}{\varepsilon}, \quad S = \sqrt{2S_{ij}S_{ij}}
\]  

(5)

The parameters are shown as follows: 
\[C_{1e} = 1.44, \quad C_2 = 1.9, \quad C_\mu = 0.09, \quad \sigma_e = 1.3, \quad \sigma_k = 1.0.\]

2.2.2. Grid and operating conditions. In order to simulate more exactly, the bubbling reactor was divided into the whole layers and the column part with the dividing function of the Gambit software. The grids of the whole layers were fined and those of the column part were meshed automatically by the software. The final grid structure is shown in Fig. 2 and the total number of grids is 2779641.

**Figure 2.** Grid partition.

Boundary conditions including the velocity inlet of gas-liquid phase, the pressure outlet and the non-slip wall boundary were chosen. The convective term of the volume fraction equation uses the Quick format. The second-order upwind scheme was adopted by the convection term of the other equations. The pressure-velocity coupling were adopt the phase-coupled simple method and the rest uses the default value.

3. Results and Discussions

In this study, the steady state numerical simulation is carried out on atmospheric pressure operation using air-water system. The air enters from the side wall of the reactor at a speed of 120 m/s and the water enters the bottom of the reactor at a speed of 2.89 m/s.

3.1. Gas hold-up distribution at different heights

Fig. 3 shows the distribution of gas hold-up at different heights in the reactor. From the picture, we can see that the gas hold-up decreases gradually from the wall to the reactor centre at the first hole layer (Z=30mm). With the increase of the height of the liquid phase, the gas hold-up increased gradually in the reactor at the second hole layer (Z=40mm) and the third hole layer (Z=50mm). At the height of Z=60mm, Z=70mm and Z=80mm, the gas hold-up fraction near the wall of the reactor decreases significantly and the distribution of gas hold-up in the reactor increases significantly.
3.2. Gas hold-up cloud and liquid vector
The gas hold-up cloud of Fig. 4 (A) shows that the gas hold-up decreases from the wall to the center of the reactor. As shown in Fig. 4 (B), the liquid velocity in the center of the reactor is upwards along the Z axis. Due to the entry of high velocity gas, the liquid phase is highly disturbed and vortex appears near the wall, which is conducive to the full contact of gas and liquid phases, thus increasing the mass transfer efficiency.

3.3. Vector graph of gas phase velocity at different heights
Fig. 5 analyzes the vector graph of gas phase velocity at different heights. It can be seen from the diagram that the gas phase in the X axis is higher at the orifice, the level of the turbulence is violent and the vortex is obvious. With the increase of the liquid layer height, the vortex moves to the reactor center, and the gas phase velocity decreases, and the turbulence level decreases.
4. Conclusions
In this paper, the flow velocity and gas phase distribution in the side-entry bubbling reactor are numerically studied. The flow velocity and gas hold-up distribution at different height of the Z axis and the velocity field of the liquid phase in the central axis of the reactor is analyzed.

By analyzing the distribution of gas hold-up at the different height of the side-entry bubbling reactor, the following conclusion is drawn: on the cross section of the whole layer, the gas hold-up decreases from the wall to the center of the device. However, with the increase of the height of the pore layer, the gas hold-up at the center of the reactor increases gradually, which is due to the full development of the lower pore layer gas phase and the disturbing behavior caused by the higher pore layer. For the columnar part above the pore layer, the higher gas hold-up area moves toward the reactor center.

In addition, through the analysis of the flow field behavior in the center direction of the reactor and the velocity distribution at different heights, the results show that, for the region near the pore layer, the liquid phase disturbance at the different height sections is relatively violent and the disturbance vortex appears at the different height section, so that the gas-liquid phase can be fully contacted which is beneficial to the mass transfer of gas-liquid phase. The velocity vector diagram of axial center can also clearly reflect this flow behavior.

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