Numerical Simulation of Gas Holdup Distribution in a Standard Rushton Stirred Tank Using Discrete Particle Method*

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Abstract The discrete particle method was used to simulate the distribution of gas holdup in a gas-liquid standard Rushton stirred tank. The gas phase was treated as a large number of bubbles and their trajectories were tracked with the results of motion equations. The two-way approach was performed to couple the interphase momentum exchange. The turbulent dispersion of bubbles with a size distribution was modeled using a stochastic tracking model, and the added mass force was involved to account for the effect of bubble acceleration on the surrounding fluid. The predicted gas holdup distribution showed that this method could give reasonable prediction comparable to the reported experimental data when the effect of turbulence was took into account in modification for drag coefficient.
Keywords numerical simulation, gas holdup, stirred tank, discrete particle

1 INTRODUCTION

For multiphase flow modeling, there were mainly two approaches for the dispersed phase, namely the quasi-fluid or Eulerian[1—4] method and the discrete particle or Lagrangian[5—7] method. The former treated the dispersed phase as a continuous medium and the governing equations were similar with those of the continuous phase. The latter treated the dispersed phase as a large number of discrete particles, and the particle motion equation determining particle trajectory was established using the Newton's Second Law in a Lagrangian reference frame, with no need to the complicated continuity and momentum conservation equations for the dispersed phase. This method could incorporate more interphase forces than the former and could obtain more comprehensive information on behavior of individual particles. By tracking the motion trajectory of each particle, the discrete particle method could account for the difference of velocity of those particles with a wide range of particle size, while in the reported studies using the quasi-fluid method, all particles share the same velocity[2—4].

The discrete particle method was widely applied in gas-solid flows, but seldom applied in gas-liquid flows in past decades. The situation of surface interaction between bubbles and liquid in gas-liquid flows was more complex than that between solids and gas in gas-solid flows. Until now, available accurate and general mechanism models for gas-liquid flows are still lacking. Several studies using this method were carried out to simulate the gas-liquid flows in bubble columns with different treatments. When the added mass force and lift force being neglected, the effect of bubble wake being considered and the effective viscosity of gas being assumed equal to the eddy viscosity of liquid, the results of two-dimensional simulation showed good qualitative agreement with that by the quasi-fluid method[5]. An unsteady bubble flows with low frequency oscillation in a three-dimensional bubble column was simulated by Buwa *et al*.[6] , whose model involved the lift force and add mass force, and the bubbles was treated as rigid spheres of the same size. Gong *et al*.[7] investigated the ozone dissolution and mass transfer in a three-dimensional bubble column, established the momentum equation based on the mixture model, but omitted the bubble mass and interphase action.

In this work, the discrete particle method was introduced first time to simulate the distribution of gas holdup in stirred tanks. The turbulent dispersion of bubbles with a size distribution was modeled using a stochastic tracking model, and the added mass force being involved. The predicted results were compared with the reported experimental data.

2 MATHEMATICAL MODEL

2.1 Liquid and bubble motion equations

In the discrete particle method, the mass and momentum conservation equations for the continuous liquid phase with the assumption of an incompressible Newtonian fluid were of the similar forms with those in the quasi-fluid method:

$$\frac{\partial}{\partial t}(\alpha_l) + \nabla\cdot(\alpha_l \boldsymbol{u}_l) = 0 \tag{1}$$

$$\frac{\partial}{\partial t}(\alpha_l \rho_l \boldsymbol{u}_l) + \nabla\cdot(\alpha_l \rho_l \boldsymbol{u}_l \boldsymbol{u}_l) = -\alpha_l \nabla P + \alpha_l \rho_l \boldsymbol{g} + \boldsymbol{F}_{\mathrm{D}} + \boldsymbol{F}_{\mathrm{V}} + \alpha_l \boldsymbol{F}_{\mathrm{rol}} \tag{2}$$

where in the right side of Eq.(2), the third term being the drag force, the fourth term being the added mass force, and the last term being the added action force caused by the rotation of reference frame, which was zero in a stationary reference frame but should be

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considered in a rotating reference frame. For the reference frame rotating about the z axis, the added force in the r and θ directions were

$$F_{\mathrm{rol},r} = (\rho_l - \rho_\mathrm{b})\omega^2 r + 2\omega(\rho_l u_{l\theta} - \rho_\mathrm{b} u_{\mathrm{b}\theta}) \tag{3}$$

$$F_{\mathrm{rol},\theta} = (\rho_l - \rho_\mathrm{b})\omega^2 \theta - 2\omega(\rho_l u_{lr} - \rho_\mathrm{b} u_{\mathrm{b}r}) \tag{4}$$

and $F_{\mathrm{rol},z} = 0$ in the z direction, where α_l denoted the void fraction of liquid, α_b the local gas holdup, satisfying Eq.(5):

$$\alpha_l + \alpha_\mathrm{b} = 1 \tag{5}$$

The local gas holdup was given by

$$\alpha_\mathrm{b} = Q_\mathrm{b}\Delta\tau / (\rho_\mathrm{b} / \Delta V) \tag{6}$$

where Q_b being the total net mass flow rate of bubbles, $\Delta\tau$ the bubble residence time in a computational cell, and ΔV the volume of cell.

According to the Newton's Second Law, the equation of motion for an individual bubble through the force balance could be written in a Lagrangian reference frame as follows:

$$\rho_\mathrm{b}\frac{\mathrm{d}\boldsymbol{u}_\mathrm{b}}{\mathrm{d}t} = \frac{3\rho_l}{4d_\mathrm{b}} C_\mathrm{D} |\boldsymbol{u}_l - \boldsymbol{u}_\mathrm{b}| (\boldsymbol{u}_l - \boldsymbol{u}_\mathrm{b}) + C_\mathrm{V}\rho_l\left(\frac{\mathrm{D}\boldsymbol{u}_l}{\mathrm{D}t} - \frac{\mathrm{d}\boldsymbol{u}_\mathrm{b}}{\mathrm{d}t}\right) + g(\rho_\mathrm{b} - \rho_l) + \nabla P - \boldsymbol{F}_\mathrm{rol} \tag{7}$$

where in the right side from the left to right presenting for the drag force, added mass force, buoyancy and gravity, added rotation action force, respectively.

2.2 Interphase force coefficients

Although the added mass force were neglected in recent works[2—4] when simulating the gas-liquid flows in stirred tanks, the numerical modeling performed by Sun[8] indicated that this force has the same order of magnitude as the drag force in the region of discharge flow. So in our simulation this force was considered. For the coefficient C_V, a constant value or different correlations were used[9], but in the case of gas holdup low than 10%, the values calculated by those correlations approached to 0.5—0.69. In this work, since the predicted gas holdup in most positions of stirred tank ranged down to 10%, a constant value of C_V had been set to 0.5 for simplification.

At present, it was difficult to use the experiment approach to obtain the accurate drag coefficient for bubbles in turbulent flow, and the exact mechanisms of turbulence on the slip velocity were still unknown[4]. So when the gas-liquid flows were modeled in gas-liquid stirred tanks, the correlations used in calculating drag coefficient, in general, were those developed from the simple cases, such as bubbles or particles in stagnant liquids or their modifications. Wang and Mao[1] used a constant for the drag coefficient, and Sun *et al.*[10] adopted a correlation for varying acceleration flow field and neglected the effect of turbulence on the drag coefficient. According to the finding obtained by Magelli *et al.*[11], if the particle diameter was larger than 10 times of Kolmogoroff length scale λ, the dissipating eddies would be able to interact with particles, leading to significant changes in particle drag and settling velocity. The experimental results performed by Brucato *et al.*[12] also confirmed that turbulence had an obvious influence on the settling velocity of particle, smaller than that in the still liquid. They correlated the particle size with the scale λ and made a modification for the drag coefficient as follows:

$$\frac{C_\mathrm{D} - C_\mathrm{D0}}{C_\mathrm{D0}} = K\left(\frac{d_\mathrm{b}}{\lambda}\right)^3 \tag{8}$$

A value about 8.76×10^{-4} of K was given according to the plot of experimental data obtained by Brucato *et al.*[12]. Both Lane *et al.*[2] and Khopkar *et al.*[13] adopted Eq.(8) to simulate the gas-liquid stirred tanks, but the latter took a smaller coefficient K as 6.5×10^{-6}.

Bakker and Van den Akker[14] used a correct form of bubble relative Reynolds number using a different method, and added a viscosity caused by turbulence to the molecular viscosity term:

$$Re = \frac{\rho_l d_\mathrm{b} |\boldsymbol{u}_l - \boldsymbol{u}_\mathrm{b}|}{\mu} \tag{9}$$

$$\mu = \mu_\mathrm{L} + C\mu_{\mathrm{T},l} = \mu_\mathrm{L} + C_1\rho_l\frac{k^2}{\varepsilon} \tag{10}$$

where Kerdouss *et al.*[15] proposed a value 0.3 for C and 0.02 for C_1 by Bakker and Van den Akker[14]. Laakkonen *et al.*[4] assumed that the turbulent kinetic energy equal to $0.5\times u'^2$. The turbulent fluctuation velocity u' was related to the bubble size and the dissipation rate of turbulent energy, namely:

$$k = 0.5\times u'^2 = \varepsilon^{2/3} d_\mathrm{b}^{2/3} \tag{11}$$

So Eq.(11) was modified as follows:

$$\mu = \mu_\mathrm{L} + C_1\rho_l\varepsilon^{1/3} d_\mathrm{b}^{4/3} \qquad (C_1 = 0.02) \tag{12}$$

3 SIMULATION METHOD

The simulated conditions for a standard Rushton stirred tank with a six bladed impeller were the same as those in experiments by Wang[16] ($Q=2.222\times10^{-4}$ $\mathrm{m^3\cdot s^{-1}}$, $T=0.38$m, $C=T/3$, $\omega=30.8\mathrm{rad\cdot s^{-1}}$). To reduce the computational costs, the simulation was carried out in a half of the geometry of stirred tank with non-uniform hexahedral grids of 63, 27 and 96 cells in the axial, radial and azimuthal directions, respectively. All walls were treated as non-slip boundaries using the standard wall functions, and the liquid surface was treated as a zero gradient boundary. Bubbles were introduced at the ring sparger with $N_\mathrm{in}=10$ nozzles and escaped at the liquid surface. The bubble size was divided into $N_\mathrm{group}=24$ groups from 0.25 to 6mm and the mean diameter being 3.35mm.

In order to couple the interphase momentum exchange, the two-way approach was performed by alternately solving the steady liquid phase flow field and bubble trajectories of each injected bubble until the convergence criteria of 10^{-4} for both phases were satisfied. In order to obtain an appropriate statistical representation of the bubble trajectories, several numbers of tracked bubble in each size group was performed during each iteration for each injection. The total number of tracked bubbles was as follows:

$$N_{\text{tracked bubble}} = N_{\text{trajectory}} \times N_{\text{group}} \times N_{\text{in}} \qquad (13)$$

The multiple frames of reference method[17] were used to simulate the interaction between the baffles and impeller. To avoid the trouble caused by the transition of reference frames, the trajectories and positions of bubbles were tracked based on the absolute velocity instead of the relative velocity. The standard $k-\varepsilon$ turbulent model was used to model the continuous phase, and the momentum exchange between liquid and bubbles was calculated using the two-way coupling approach[6].

The stochastic tracking model was adopted to simulate the turbulent dispersion of bubbles in the liquid phase flow field[6]. This model could account for the interaction between the particles and turbulent eddies and the continual processes of birth and death of eddies, and could describe reasonably the random motion of bubbles. In this model, the integral time scale which represented the time spent in turbulent motion along the particle track was assumed to equal the fluid Lagrangian integral time, for the $k-\varepsilon$ model the integral time scale approximately equaled to $0.15k/\varepsilon$. The concepts of eddy lifetime and eddy crossing time were introduced to determine the interaction time of particles with a succession of discrete stylized turbulent eddies during the eddy lifetime, and the fluid fluctuation velocity given by a Gaussian distributed random function kept as a constant when particles crossed the current turbulent eddy.

4 RESULTS AND DISCUSSION

Figure 1 showed the comparison of the averaged gas holdup predicted using different amount of tracked bubbles. It was clear that when the amount of calculated bubbles was very small, the predicted gas holdup distribution exhibited a considerable sharp profile, but with the increase of amount, it tended to be smooth gradually. From Figs.1(a) and 1(b), it could be seen that the gas holdup based on the cases of both 120000 bubbles and 300000 bubbles approached fairly, which suggested that the predicted results didn't change obviously any more when the amount of bubbles was enough to represent the statistical characteristic on behavior of bubbles in the whole flow field. In this paper, all other simulations were carried out based on the amount of 120000 bubbles

The effect of bubble contamination on the gas holdup was tested. For dilute bubble flow, Tomiyama *et al.*[18] proposed a drag law as follows:

$$C_{\mathrm{D0}} = \max\left\{\min\left[\frac{A}{Re}\left(1+0.15Re^{0.687}\right), \frac{B}{Re}\right], \frac{8}{3}\frac{Eo}{Eo+4}\right\} \qquad (14)$$

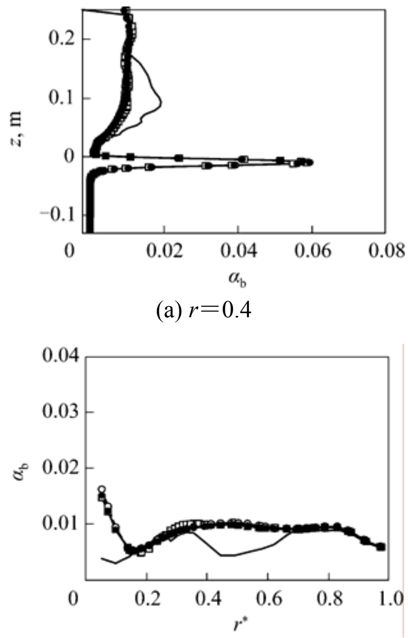


Figure 1 Effect of the amount of bubbles
—— 2400 bubbles; □ 120000 bubbles; ○ 300000 bubbles; ● 1200000 bubbles

where for a pure system: A=16, B=48; for a slightly contaminated system: A=24, B=72; for a fully contaminated system: A=48, B=0.

Figure 2 showed the effect of bubble contamination on the averaged gas holdup calculated by Eq.(14). It could be seen that when some bubble surfaces were slightly contaminated, the predicted results were slightly higher than that in a pure system in some

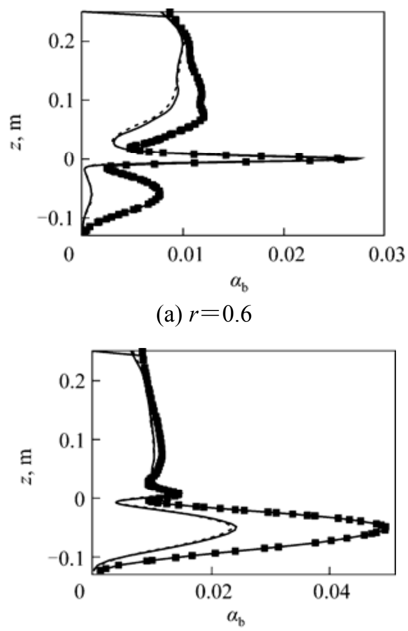


Figure 2 Effect of bubble contamination
- - - - cleanly; —— slightly; —■— fully

positions of stirred tank, but for the fully contaminated system, the simulated results were obviously higher than that in the former two cases, in particular, being over-predicted about 50% in the lower circulation region.

The cause yielding this difference might be the surface tension gradient caused by the surface contamination, which resulted in a tangential stress *viz*. so-called Marangoni stress[19]. It had the important effect of decreasing mobility of bubble surface, so the bubbles would experience a higher drag and slower rise than in a pure system. Thus it could be seen that if bubble surfaces were indeed contaminated, the effect of contamination should be taken into account for the simulation of gas holdup in gas-liquid stirred tank. The effect of turbulence correction for drag coefficient was investigated using several versions of drag coefficient (shown in Table 1), including the effect of bubble contamination.

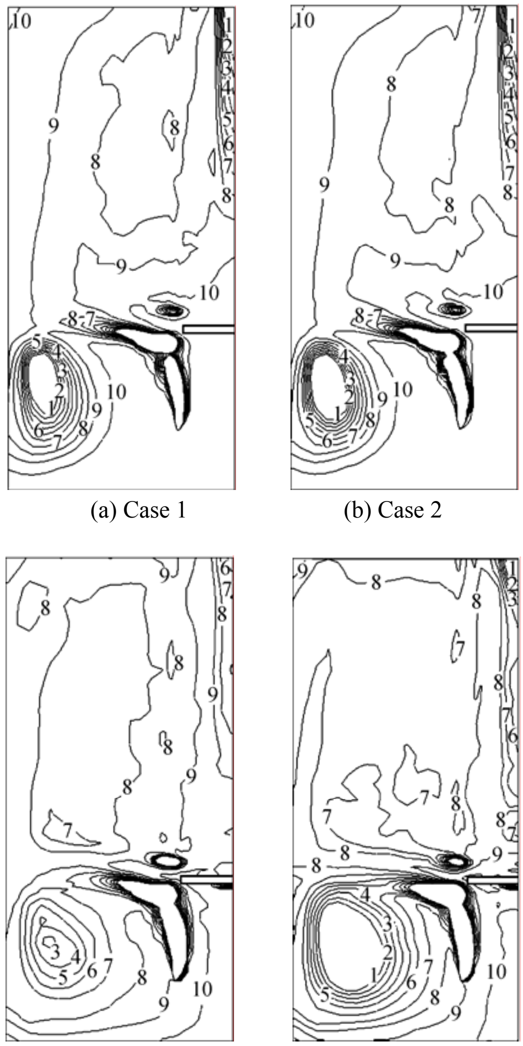
Table 1 Several versions of drag coefficient

Case	Coefficient closure
1	Eq.(14)
2	Eqs.(8) and (14), $K=6.5\times10^{-6}$
3	Eqs.(9), (10) and (14), $C=0.3$
4	Eqs.(9), (12) and (14)

The local and averaged distributions of gas holdup were shown in Figs.3 and 4, respectively. It could be seen that the predicted results were sensitive to the modification for drag coefficient. Both cases 1 and 2 gave a similar pattern of gas holdup distribution, but case 2 gave slightly higher values of gas holdup in lower circulation region.

The method using a modified Reynolds number to calculate the drag coefficient obtained obvious different patterns. Comparing the predicted results between different cases, case 4 was found to give the highest value of gas holdup, which quite approached the reported experimental data in lower circulation region of tank. Cases 2, 3 and 4 took into account the effect of turbulence on the slip velocity caused by the balance of drag and other interphase forces[2], so the modification for drag coefficient reduced the rise velocity of bubbles and resulted in higher values of gas holdup.

From Figs.3 and 4(a), it could be seen that more bubbles arrived at the region close to the shaft than that near the center axis under the impeller, where the trend of gas holdup distribution corresponding well to the experiment[16]. Comparing the patterns in different radial sections, the distribution of gas holdup was fairly evenly in the upper circulation region above the impeller, which suggested the bubbles were fully dispersed. But in the lower circulation region, with the gradual closing to the center of the large circulation eddy, the gas volume fraction increased. The main reason for the results might be that the motion of turbulent eddies dominated the dispersion of bubbles in



(a) Case 1 (b) Case 2

(c) Case 3 (d) Case 4

Figure 3 Comparison of local gas holdup contours predicted by different turbulence corrections for drag coefficient with slight bubble contamination

contour value, %: 1—3.5; 2—3.1; 3—2.7; 4—2.4; 5—2.1; 6—1.6; 7—1.2; 8—0.9; 9—0.5; 10—0.1

this region, where most bubbles of small size might remain comparatively coincident with the liquid, so that the bubbles would not become uniformly distributed, but showed a tendency to concentrate in the region close the center of large eddy.

Figures 5(a) and 5(b) gave the predicted local gas holdup distribution and it could be seen that bubbles concentrated in the region of fluid trailing eddy behind the impeller blade [see Fig. 5(a)]. It could be attributed to the formation of low pressure in this region, which leads to the suction of bubbles and the formation of gas cavities. Since the radial discharge flow of liquid phase was strong before the impeller blade, the suction of bubbles was relatively weak and most bubbles could be discharged following the fluid when rising into this region and dispersed into the circulation flow regions. Thus the concentration region disappeared in the section before the impeller blade [see Fig.5(b)].

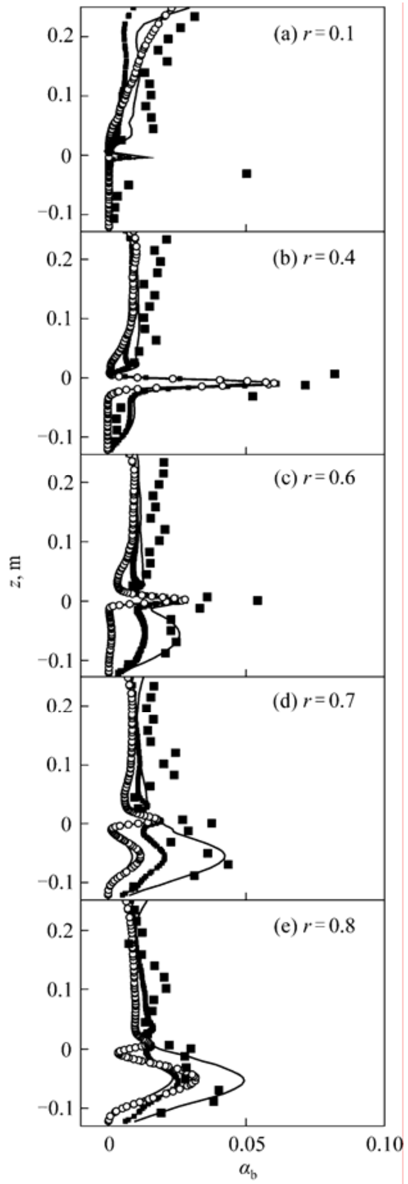
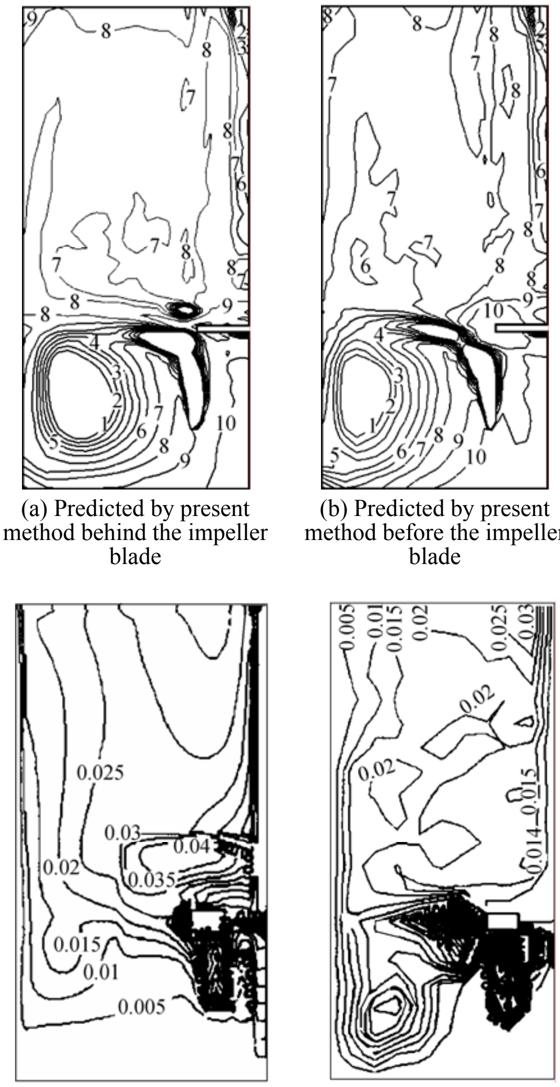


Figure 4 Effect of the turbulence correction for drag coefficient on the averaged gas holdup distribution with slight bubble contamination
■ Exp. data[16]; —— case 1; ○ case 2; ▪ case 3; —— case 4



(a) Predicted by present method behind the impeller blade (b) Predicted by present method before the impeller blade

(c) Predicted by Wang[16] (d) Experimental data[16]

Figure 5 Comparison of the gas holdup contours predicted by different methods and the experimental pattern
(Q=2.222×10^{-4}m^3·s^{-1}, T=0.38m, ω=30.8rad·s^{-1})
contour value, %: 1—3.5; 2—3.1; 3—2.7; 4—2.4; 5—2.1; 6—1.6; 7—1.2; 8—0.9; 9—0.5; 10—0.1

Wang[16] had given the predicted gas holdup contours using the quasi-fluid method and corresponding experimental data [see Figs.5(c) and (d), respectively]. The comparisons of the simulated results and measured data showed the quasi-fluid approach fairly under-predicted the gas holdup in the region below the impeller, while the simulated results using the discrete particle method showed a more reasonable approach to experimental data. But it should be also noticed that the simulation performed by Wang[16] didn't involve the added mass force and the modification for drag coefficient.

5 CONCLUSIONS

In this work, the discrete particle method was used to simulate the distribution of gas holdup in a standard Rushton stirred tank. The numerical results showed that: (1) The predicted results were not obviously changed when the amount of tracked bubbles exceeded an appropriate amount; (2) the contamination should be considered when some bubbles were contaminated; (3) the predicted results were sensitive to the turbulence modification for drag coefficient, a reasonable and good approach of the predicted results and the reported experimental data could be obtained using the case 4.

The numerical results also indicated this method would become a useful and promising tool to simulate the gas-liquid stirred tank. Further study is necessary on the mechanisms of bubble-eddy interaction by means of combining experimental method. It should involve the effect of bubble sizes on the interaction. The present work would provide a basis for such a work.

NOMENCLATURE

C	clearance of impeller center plane to tank bottom, m
C_{D0} , C_D	initial, corrected drag coefficient
C_V	added mass force coefficient
d_b	bubble diameter, mm
Eo	Evotos number [$Eo = g(\rho_l - \rho_\delta)d_b^2/\sigma_l$]
k	turbulent kinetic energy, $m^2 \cdot s^{-2}$
Q	gas volume flow rate, $m^3 \cdot s^{-1}$
Q_b	bubble mass flow rate, $kg \cdot s^{-1}$
Re	relative Reynolds number
r	radial coordinate, m
r^*	dimensionless radius
T	diameter of stirred tank, m
$\boldsymbol{u}$	velocity vector, $m \cdot s^{-1}$
u	velocity, $m \cdot s^{-1}$
z	axial coordinate, m
α	void fraction of phase
ε	dissipate rate of turbulent energy, $m^2 \cdot s^{-3}$
θ	azimuthal coordinate, m
μ, μ_L	effective, molecular viscosity, Pa·s
$\mu_{T,l}$	turbulent viscosity of liquid phase
λ	Komogrov length scale, m
ρ	density, $kg \cdot m^{-3}$
ω	angular speed, $rad \cdot s^{-1}$

Subscripts

b	gas phase
l	liquid phase
r, θ, z	radial, azimuthal and axial direction

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