Experimental determination and numerical simulation of mixing time in a gas–liquid stirred tank

Qinghua Zhang*, Yumei Yonga, Zai-Sha Maoa, Chao Yanga,b,*, Chengjun Zhaoa

aKey Laboratory of Green Process and Engineering, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, China
bJiangsu Marine Resources Development Research Institute, Lianyungang 222005, China
cShijiazhuang Chemical Fiber Corporation, Hebei 050032, China

ARTICLE INFO

Article history:
Received 24 July 2008
Received in revised form 16 March 2009
Accepted 19 March 2009
Available online 31 March 2009

Keywords:
Mixing
Stirred tank
Multiphase flow
Computational fluid dynamics
Simulation
Turbulence

ABSTRACT

In this work, mixing experiments and numerical simulations of flow and macro-mixing were carried out in a 0.24 m i.d. gas–liquid stirred tank agitated by a Rushton turbine. The conductivity technique was used to measure the mixing time. A two-phase CFD (computational fluid dynamics) model was developed to calculate the flow field, $k$ and $e$ distributions and holdup. Comparison between the predictions and the reported experimental data [Lu, W.M., Ju, S.J., 1987. Local gas holdup, mean liquid velocity and turbulence power of gas–liquid two-phase system, only a few studies on CFD predic-
tions have been reported, including mixing time in gas–liquid reactors such as bubble columns (Rampure et al., 2007; Ekambaram and Joshi, 2003; Joshi, 2001; Thakre et al., 1999) and loop reactors (Roy et al., 2006). However, no study on mixing time with CFD is found and coloration–decoloration methods (Cabaret et al., 2007; Delaplace et al., 2004; Melton et al., 2002). Of all the above-mentioned techniques, the conductivity technique is mostly used to determine mixing time.

In addition to experimental studies on mixing time, some researchers also got correlations of mixing time from experimental data (Lu et al., 1997; Fox and Gex, 1956). Although these correlations were proved useful, they are not expected to be valid beyond the range of variables investigated in the original experiments and may often produce erroneous results when applied to other systems. So a universal method should be developed to predict mixing time in a chemical reactor.

1. Introduction

Gas–liquid reactors are widely used in process industries for wastewater treatment, aerobic fermentation and gas–liquid reaction. To obtain high-quality products and high efficiency processes, mixing must satisfy not only the needs of mass and heat transport but also the required homogeneity in the vessel in the shortest time. Thus, mixing plays an important role in these systems.

Mixing time is a key parameter for the scale-up and design of agitated reactors. It can be compared with mass transfer time or reaction time in order to evaluate the controlling mechanism of a process. Over the past years, many researchers studied mixing time and a lot of measurement methods appeared, such as conductivity (Bouaffi and Roustan, 2001; Lu et al., 1997; Raghu Rao and Joshi, 1988), pH (Guillard and Tragardh, 2003; Merchuk et al., 1998), thermal (Espinosa-Solares et al., 2002; Rewatkar and Joshi, 1991), electrical resistance tomography (Holden et al., 1998), fluorescent spectroscopy with image analysis (Mann et al., 1995) and coloration–decoloration methods (Cabaret et al., 2007; Delaplace et al., 2004; Melton et al., 2002). Of all the above-mentioned techniques, the conductivity technique is mostly used to determine mixing time.

For the complexity of gas–liquid two-phase system, only a few studies on CFD predictions have been reported, including mixing time in gas–liquid reactors such as bubble columns (Rampure et al., 2007; Ekambaram and Joshi, 2003; Joshi, 2001; Thakre et al., 1999) and loop reactors (Roy et al., 2006). However, no study on mixing time with CFD is found in gas–liquid stirred tanks. The object of this work is to make use of CFD to predict the mixing time in a gas-liquid stirred tank. In this work, a two-phase flow model was first used to calculate the flow field, $k$ and $e$ distributions, and afterwards the model was extended.
for the prediction of mixing time in the stirred tank. In order to validate the numerical predictions, experiments were also carried out at same conditions.

2. Experimental section

2.1. Experimental setup

Experiments were carried out in a flat-bottom transparent acrylic cylindrical tank. The equipment and the specific dimension of the vessel used in this study are shown in Figs. 1 and 2, respectively. The cylindrical tank had a diameter of $T = 0.24$ m and was filled with an aqueous solution up to $H = T$. It was equipped with four standard wall baffles of width $T/10$ and a standard six-bladed Rushton turbine impeller of diameter $D = T/3$. The ring sparger with 16 holes in 1.5 mm diameter was located in the height of 0.055 m from the tank bottom. The operating system was air-water.

2.2. Determination of mixing time

The tracer response technique was used in this work to obtain mixing time. The tracer was 10 mL of 4.3 M NaCl solution for each measurement and was added into the liquid surface instantaneously. A monitoring conductivity electrode was located at various positions and the longest time was chosen as the mixing time under the given condition. As bubbles in the reactor would significantly affect the conductivity, the electrode was surrounded by a mesh. The mixing time is defined as the period of time necessary for a system to achieve the desired level of homogeneity which can be expressed in terms of the degree of mixing, $Y$:

$$Y = \frac{c(t) - c_0}{c_\infty - c_0}$$

where $c(t)$ is the tracer concentration at time $t$, $c_0$ and $c_\infty$ are the initial and final average concentrations of tracer, respectively. In this work, we take $Y = 0.95$.

![Fig. 1. Schematic of experimental apparatus: 1. Stirred tank, 2. Rushton turbine, 3. sparger, 4. motor, 5. speed controller, 6. electrode, 7. conductivity meter, 8. computer.](image1)

![Fig. 2. (a) Geometry of the tank; (b) Rushton impeller.](image2)

3. Mathematical model

3.1. Governing equations

For a two-phase flow, the equations of continuity, momentum at steady state, can be written as the following expressions:

Continuity equation:

$$\frac{\partial}{\partial x_j} \left( \rho_k c_{jk} \mu_k \right) = \frac{\partial}{\partial x_j} \left( \frac{\mu_k}{\sigma_k} \frac{\partial \gamma_k}{\partial x_j} \right)$$

(2)
Momentum equation:

\[
\frac{\partial}{\partial x_j} \left( \rho K u_{ij} u_{kl} u_{lk} \right) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \frac{\mu L}{\alpha L} \frac{\partial u_{ij}}{\partial x_j} + \frac{\mu L K}{\alpha L} \frac{\partial u_{ij}}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left( \frac{\mu L}{\alpha L} \frac{\partial u_{ij}}{\partial x_j} - \frac{\partial u_{ij}}{\partial x_j} \right) - \frac{2}{3} \frac{\partial K}{\partial x_i} + \rho K u_{ij} \frac{\partial u_{ij}}{\partial x_i} + F_{ij}
\]

The transport equations for \( k \) and \( \varepsilon \) are

\[
\frac{\partial}{\partial x_j} \left( \rho L u_{ij} u_{ik} \right) = \frac{\partial}{\partial x_j} \left( \frac{\mu L}{\alpha L} \frac{\partial u_{ij}}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left( \frac{\mu L}{\alpha L} \frac{\partial u_{ij}}{\partial x_j} + \frac{\partial u_{ij}}{\partial x_j} \right) + C_L + G_{C} - \rho L u_{ij} u_{ij}
\]

where \( C_L \) denotes the phase \( (K = G, L) \) and \( S_{K,\phi} \) for different transport variables are given in Table 1, in which

\[
G_{L} = 2n_{L} \mu_{L} \left[ \left( \frac{\partial u_{ij}}{\partial r} \right)^2 + \left( \frac{1}{r} \frac{\partial u_{ij}}{\partial \theta} \right)^2 + \left( \frac{\partial u_{ij}}{\partial z} \right)^2 \right] + n_{L} \mu_{L} \left( \frac{\partial u_{r}}{\partial r} + \frac{1}{r} \frac{\partial u_{\theta}}{\partial \theta} \right)^2 + n_{L} \mu_{L} \left( \frac{\partial u_{z}}{\partial z} + \frac{1}{r} \frac{\partial u_{\theta}}{\partial \theta} \right)^2 + n_{L} \mu_{L} \left( \frac{\partial u_{z}}{\partial z} + \frac{1}{r} \frac{\partial u_{\theta}}{\partial \theta} \right)^2 + n_{L} \mu_{L} \left( \frac{\partial u_{z}}{\partial z} + \frac{1}{r} \frac{\partial u_{\theta}}{\partial \theta} \right)^2
\]

(10)

and \( G_{C} = 0 \).

3.3. Boundary and initial conditions

(1) Along the axis: Axisymmetry in \( u_{G,r}, u_{L,r}, u_{G,\theta}, u_{L,\theta}, u_{G,z}, u_{L,z}, K \) and \( \varepsilon \).

(2) At the top free surface of the computational domain, the axial gradients of the dependent variables are set to zero.

(3) Wall function: The velocities along the wall satisfy the no-slip boundary conditions, and the wall function method is used to calculate the wall shear stress and the values of \( k \) and \( \varepsilon \) close to the wall.

(4) At the inlet: When the gas get into the stirred tank through the sparger, the gas velocity was ignored. A source term was added into the continuity equation when the grids were located at the sparger.

3.4. Numerical solution

The set of equations given in Table 1 was first solved by the control volume technique to get the flow field, \( k \) and \( \varepsilon \) distributions. After that, the flow results were used to study the mixing process in the stirred tank. The transport equation for tracer concentrations in a three-dimensional axisymmetric cylindrical co-ordinate system is given by the following equation:

\[
\frac{\partial}{\partial r} \left( r x_{1} D_{e f f} \frac{\partial c}{\partial r} \right) + \frac{\partial}{\partial \theta} \left( r x_{2} D_{e f f} \frac{\partial c}{\partial \theta} \right) + \frac{\partial}{\partial z} \left( D_{e f f} \frac{\partial c}{\partial z} \right) = \frac{1}{r} \frac{\partial}{\partial r} \left( r x_{1} \frac{D_{e f f}}{r} \frac{\partial c}{\partial r} \right) + \frac{\partial}{\partial \theta} \left( D_{e f f} \frac{\partial c}{\partial \theta} \right) + \frac{\partial}{\partial z} \left( D_{e f f} \frac{\partial c}{\partial z} \right)
\]

(11)

where \( D_{e f f} \) is the effective diffusion coefficient and can be given by (Roy et al., 2006)

\[
D_{e f f} = \mu_{e f f} + D_{m}
\]

(12)

in which \( \mu_{e f f} \) are turbulent diffusion coefficient and can be got from the results of the flow field. \( D_{m} \) is molecular diffusion coefficient and taken as 0.00005 m² s⁻¹ (Roy et al., 2006).
Table 1
General variables \( \phi_x, F_{xy,0} \) and \( S_{xy} \) in Eq. (9).

<table>
<thead>
<tr>
<th>Equations</th>
<th>( \phi_x )</th>
<th>( F_{xy,0} )</th>
<th>( S_{xy} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Continuity equation</td>
<td>1</td>
<td>0</td>
<td>( 1 \frac{\partial}{\partial t} \left( \frac{\mu_x \cdot \frac{\partial \epsilon_x}{\partial t}}{\alpha_t} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{\mu_x \cdot \frac{\partial \epsilon_x}{\partial r}}{\alpha_t} \right) )</td>
</tr>
<tr>
<td>Radial momentum</td>
<td>( u_{r,0} )</td>
<td>( \mu_{xy,0} )</td>
<td>( \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{\mu_x \cdot \frac{\partial \epsilon_x}{\partial r}}{\alpha_t} \right) + \frac{1}{\alpha_t} \frac{\partial \epsilon_x}{\partial r} )</td>
</tr>
<tr>
<td>Tangential momentum</td>
<td>( u_{t,0} )</td>
<td>( \mu_{xy,0} )</td>
<td>( \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{\mu_x \cdot \frac{\partial \epsilon_x}{\partial r}}{\alpha_t} \right) + \frac{1}{\alpha_t} \frac{\partial \epsilon_x}{\partial r} )</td>
</tr>
<tr>
<td>Axial momentum</td>
<td>( u_{z,0} )</td>
<td>( \mu_{xy,0} )</td>
<td>( \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{\mu_x \cdot \frac{\partial \epsilon_x}{\partial r}}{\alpha_t} \right) + \frac{1}{\alpha_t} \frac{\partial \epsilon_x}{\partial r} )</td>
</tr>
<tr>
<td>Turbulent kinetic energy</td>
<td>( k )</td>
<td>( \mu_{xy,0} )</td>
<td>( \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{\mu_x \cdot \frac{\partial \epsilon_x}{\partial r}}{\alpha_t} \right) + \frac{1}{\alpha_t} \frac{\partial \epsilon_x}{\partial r} )</td>
</tr>
<tr>
<td>Turbulent energy dissipation</td>
<td>( \varepsilon )</td>
<td>( \mu_{xy,0} )</td>
<td>( \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{\mu_x \cdot \frac{\partial \epsilon_x}{\partial r}}{\alpha_t} \right) + \frac{1}{\alpha_t} \frac{\partial \epsilon_x}{\partial r} )</td>
</tr>
</tbody>
</table>

*The terms are included when a non-inertial reference frame is used.

4. Computational grid

Four computational grids of different sizes were used in the numerical simulation to test the effect of the grid independence on the predicted results in this work: \( 24 \times 48 \times 60 \) (grid 1), \( 30 \times 60 \times 75 \) (grid 2), \( 36 \times 72 \times 75 \) (grid 3) and \( 36 \times 72 \times 90 \) (grid 4) \((r \times \theta \times z)\). The computation was considered converged when the normalized residuals for each primary variable dropped well below \( 10^{-4} \). The gas holdup \( z_g \) and mixing time obtained with different meshes are presented in Fig. 3, which shows that the effect of the grids on the simulation procedures is negligible when the grid of \( 36 \times 72 \times 75 \) (grid 3) was used and similar results were also derived for liquid
velocities at different radial positions \( (u_{L,r}, u_{L,\theta} \text{ and } u_{L,z}) \). Thus, the finer grid of \( 36 \times 72 \times 90 \) was used in all the subsequent simulations.

5. Results and discussion

5.1. Liquid velocity and gas holdup

The accuracy of liquid velocity and gas holdup simulated by different models would significantly affect mixing time value. In order to verify the accuracy of the model used in this paper, we simulated Lu and Ju’s (1987) vessel and compared with their experiments. As shown in Figs. 4 and 5, the simulations agree well with experimental results. In Fig. 5, it can be seen that there is large discrepancy with experimental data in the impeller zone, which may be because that the \( k-e \) model used in our work is established on the basis of isotropic turbulent flow. The \( k-e \) model cannot correctly describe the strongly anisotropic flow in the impeller zone. However, there is still no proper model to describe accurately the complex two phase flow in the impeller zone.

5.2. Mixing time

5.2.1. Typical tracer response

Comparison between the experimental and predicted tracer response was shown in Fig. 6. It can be seen that the simulation curve was in accordance with the experimental curve very well. It means that the tracer disperse process in a gas–liquid stirred tank can be accurately predicted by the CFD model.

5.2.2. Effect of feed position

As shown in Table 2, three different feed positions were considered in order to investigate the effect of feed position on mixing time. It can be seen that when the feed position was located at P3, the smaller mixing time was achieved than that at the other two positions considered in this paper. This is due to that P3 is located nearby the impeller, where the liquid velocity is so high in this region and the tracer can be dispersed to the other region quickly.

5.2.3. Effect of impeller speed

Impeller speed is a very important parameter which affects the velocity, gas hold-up and mixing time in a stirred tank. The impeller speeds of 300–600 rpm were considered in this study as shown in Fig. 7. It is obvious that increasing impeller speed resulted in decreasing mixing time. Increasing impeller speed, the degree of turbulent intensity was strengthened and the liquid circulation speed was increased, which resulted in decreasing the mixing time in the stirred tank. It can be seen that the simulated results are also in good agreement with the experimental data.
5.2.4. Effect of gas flow rate

Gas flow rate is another parameter affecting the mixing time in a gas–liquid stirred tank. There are major contradictions in the literature as to the effect of gas flow rate on the mixing time. An increase in gas flow rate can increase, decrease, or not affect the mixing time. Bouaifi and Roustan (2001) studied the mixing behavior in a stirred tank with various axial and mixed dual-impellers and found that the mixing time increased when the gas flow rate increased at any given configuration and constant impeller speed. However, Shewale and Pandit (2006) also investigated the effect of gas flow rate on mixing time at the impeller speed of 0–8 rad s⁻¹ but got the contrary results. The effect of gas flow rate on mixing time investigated in this work is shown in Fig. 8. It can be seen that the mixing time increased with an increase in the gas flow rate \( Q_G \) from 0 to 0.6 m³ h⁻¹. When \( Q_G \geq 0.6 \) m³ h⁻¹, the value of mixing time leveled off with increasing the gas flow rate. The trend of our experimental and simulated results shows good agreement with Lu et al. (1997)'s experiments. Pandit and Joshi (1983) reported that the mixing time increased with an increase in the \( Q_G \) at any impeller speed that was greater than \( N_F \) (the critical impeller speed for the onset of flooding). \( N_F \) can be calculated by the following expression (Lu and Chen, 1986):

\[
N_F = 0.54Q_G^{0.3}D^{-1.8}
\]

For \( Q_G = 0.6 \) m³ h⁻¹, \( N_F = 224.7 \) rpm, and for \( Q_G = 1.2 \) m³ h⁻¹, \( N_F = 276.6 \) rpm. The values of \( N_F \) are all lower than the operating impeller speed investigated in this work. As shown in Fig. 8, the mixing time of gas–liquid phase was higher than that of single phase, this may be because that the presence of gas reduces the impeller pumping capacities and prolongs the mixing time. When \( Q_G \) changed

---

**Table 2**

<table>
<thead>
<tr>
<th>Position</th>
<th>( r ) (m)</th>
<th>( \theta ) (°)</th>
<th>( z ) (m)</th>
<th>( t ) (s)</th>
<th>Experimental</th>
<th>Predicted</th>
</tr>
</thead>
<tbody>
<tr>
<td>P1</td>
<td>0.055</td>
<td>45</td>
<td>0.231</td>
<td>13.3</td>
<td>13.2</td>
<td></td>
</tr>
<tr>
<td>P2</td>
<td>0.055</td>
<td>45</td>
<td>0.190</td>
<td>12.7</td>
<td>12.85</td>
<td></td>
</tr>
<tr>
<td>P3</td>
<td>0.055</td>
<td>45</td>
<td>0.155</td>
<td>11</td>
<td>10.1</td>
<td></td>
</tr>
</tbody>
</table>

---

**Fig. 5.** Prediction of gas holdup compared with the experimental data by Lu and Ju (1987).

**Fig. 6.** Comparison between experimental and predicted tracer response as a function of time (\( Q_G = 0.6 \) m³ h⁻¹, \( C = T/3, P1 \)).

**Fig. 7.** Effect of impeller speed on mixing time (\( Q_G = 0.6 \) m³ h⁻¹, \( C = T/3, P1 \)).

**Fig. 8.** Effect of gas flow rate on mixing time (\( C = T/3, P1 \)).
from 0.6 to 1.2 m$^3$ h$^{-1}$ in our work, the value of gas flow rate did not affect the value of mixing time, possibly because that the impeller still pumped considerable amount of fluid in radial direction when $Q_G > 0.6$ m$^3$ h$^{-1}$, and the aerated rate did not affect the mixing quality under this circumstance.

6. Conclusions

A CFD model was successfully developed to predict the mixing time in a gas–liquid stirred tank agitated by a Rushton turbine for the first time in this paper. The mean liquid velocity and gas holdup of Lu and Ju’s (1987) vessel were also simulated and good agreements were got. Comparison between the predicted and experimental results of the tracer response curves during the turbulent mixing process was investigated, and the curve from numerical simulation was in accordance with the experimental result very well. It means that the tracer disperse process in a gas–liquid stirred tank can be accurately predicted by the CFD model. The effects of operating conditions such as impeller speed, feed position and gas flow rate on mixing time were considered experimentally and numerically. It can be concluded that the mixing time was significantly different at different feed positions. The mixing time was decreased with an increase of the impeller speed. With increasing the gas flow rate, the mixing time first increased and then leveled off. A good agreement was also observed between the CFD simulation and experimental results of the mixing time in a gas–liquid stirred tank. This work illustrates that the CFD model can accurately describe the macro-mixing process in a gas–liquid stirred tank, and it was very useful for the design and scale-up of multiphase stirred tanks.

### Acknowledgments

The authors acknowledge the National Natural Science Foundation of China (20676134, 20490206), 973 Program (2007CB613507), the National Project of Scientific and Technical Supporting Program (2008BAF33D03) and the Project of Scientific and Technical Supporting Program in Jiangsu Province (BE2008086).

### References


