Flow characteristic prediction for liquid-liquid system in a stirred tank based on RNG k-ε model

Bin Qin, Chao Chen, Mengxiao Yu, Xin Li and Zhaoyou Zhu*

College of Chemical Engineering, Qingdao University of Science and Technology, Qingdao, China.

*Corresponding author e-mail: huagongyl@163.com

Abstract. The RNG k-ε model was adopted to calculate liquid–liquid turbulent flow in stirred tanks based on Eulerian–Eulerian model. The radial and tangential velocities of numerical calculation were compared with that of reported experiment. The results show that the calculation results are in satisfactory agreement with the experimental data. The complex liquid-liquid flow characteristics in the stirred tank were successfully predicted by the RNG k-ε model which means that the established calculation model can be an alternative method with inexpensive computing costs and high computational accuracy.

1. Introduction

Liquid-liquid stir is widely used in chemical industry for polymerization, extraction, dissolution, etc. The main purpose of stir is to promote the mass transfer and heat transfer of the two phases. The product quality, yield and economy of the processes are significantly affected by the efficiencies of mass/heat transfer in stirred tank. Therefore, it is of great practical significance to study the flow characteristics of the fluids in the stir process.

There are very few experimental studies on liquid-liquid stir because of the high cost of the experiment and the difficulty of the experimental operation. Svensson and Rasmuson [1, 2] studied the effects of disperse phase volume percentage on liquid-liquid flow characteristics with laser Doppler anemometry (LAD) technique and Particle Image Velocimetry (PIV) technique. The flow density, viscosity, and the fluid flow characteristics change with the dispersed phase percentage changes. Laurenzi et al. [3] studied the two-phase turbulent flow fields of a liquid–liquid system in stirred tank which measured by means of PIV technique. The dispersion conditions at different impeller speeds and the flow characteristics of continuous and disperse phases were studied. Cheng et al. [4] applied the planar laser induced fluorescence (PLIF) method to reveal the difference of macro-mixing behavior between the dispersed phase and the continuous phase of liquid-liquid system.

The difficulties of studying the industrial-scaled stir process with experimental methods are focused on the predicted accuracy and safety. Most actual production data cannot be obtained easily by amplifying the experimental data. Hence, it is necessary to develop computational fluid dynamics (CFD) based methods, which are cost-effective and capable of predicting fluid flow characteristics accurately through numerical simulation. Jaworski and Dudczak [5] studied the influence of the size and number of probes on mixing indices in stirred tanks with a CFD method based on standard k-ε model. Kumaresan and Joshi [6] used CFD methods with sliding mesh approach to study the effect of
impeller design on the flow pattern and mixing time for a set of axial flow impellers, and compared the results predicted by CFD methods with the data measured by LAD. Cheng et al. [7] calculated the liquid–liquid flow field in a baffled turbulent liquid–liquid stirred reactor with Rushton turbine by the isotropic standard k–ε model and the anisotropic explicit algebraic stress model (EASM) based on Eulerian–Eulerian model. Van den Akker [8] used the anisotropic Large Eddy Simulations (LES) approach to reproduce the local and transient flow conditions in turbulent mixing processes. The LES approach was regarded to be able to simulate the transient process accurately while it requires a large amount of calculation.

The purpose of this work is to study a liquid-liquid system flow characteristics by a CFD approach based on RNG k-ε model and Eulerian-Eulerian model. Then the root mean square (RMS) velocities, radial and tangential velocities calculated by the CFD approach were compared with the reported experimental data [2]. The validity of the approach was verified and the results of the simulation were discussed in detail.

2. Modeling

2.1. Physical model

A standard stirred tank with a six-blade Rushton turbine was used in this work. Four baffles were set in the stirred tank as shown in Fig. 1. The dimension of the stirred tank is shown in Table 1.

| Item                      | Value | Item                      | Value |
|---------------------------|-------|---------------------------|-------|
| Tank diameter (T)         | 140mm | Blade width (Wb)          | D/5   |
| Liquid depth (H)          | 140mm | Blade length (L)          | D/4   |
| Baffle width (W)          | T/12  | Blade thickness (Tb)      | D/50  |
| Impeller diameter (D)     | T/3   | Disc diameter (Dd)        | 6D/10 |
| Impeller height (Hi)      | T/3   | Disc thickness (Td)       | D/50  |

NaI solution and silicon oil were chosen as continuous aqueous phase and dispersed hydrophobic phase for the liquid-liquid system, respectively. The density and the viscosity of the NaI solution were about 1.34 g/cm³ and 1.4 mPas. The density and the viscosity of the silicon oil were about 0.94 g/cm³ and 11.0 mPas. The silicon oil volume fraction was 7%. The impeller speed was 540 rpm.

![Figure 1. Geometric construction of the stirred tank.](image)

2.2. Mathematical models

A high quality 3D grid of stirred tank was established by the ANSYS ICEM software. The fine grid with 3,778,105 elements was employed in the simulations. The calculation domain is divided into two parts: the center rotation dynamic domain containing the blades with structured grid and the surrounding static domain with unstructured grid.

The reliability of numerical simulation plays an important role in the study of flow field. Fluent 17.0 was used for numerical simulation in this work. The gradient discretization method was Least Squares Cell Based. The momentum discretization method, the volume fraction discretization method,
Turbulent Kinetic Energy discretization method and Turbulent Dissipation Rate discretization method were all discretized by First Order Upwind scheme.

2.2.1. Governing equations. Eulerian-Eulerian model was adopted to calculate the liquid-liquid flow and the phase interactions in the stirred tank. Governing equations are shown as Eq.1 and Eq.2:

\[ \frac{\partial}{\partial t}(\alpha \rho \mu \bar{u}) + \nabla \cdot (\alpha \rho \mu \bar{u} \bar{u}) = 0 \]  

(1)

\[ \frac{\partial}{\partial t}(\alpha \rho \mu \bar{u}) + \nabla \cdot (\alpha \rho \mu \bar{u} \bar{u}) = -\alpha \nabla p + \nabla \cdot \tau + \alpha \rho g + \bar{F} \]  

(2)

Where \( \bar{u} \) is velocity, \( \alpha \) is volume fraction, \( \rho \) is density, \( g \) is gravity, \( p \) is pressure, \( \tau \) is stress tensor. The \( \bar{F} \) is the integration of the forces of phase interactions. The drag force was mainly considered [9] and schiller-naumann model was adopted in this work.

2.2.2. Turbulence models. RNG k-\( \varepsilon \) model was built for fluid turbulence characteristics and widely used to study stir process. It is found that the calculation accuracy of the model can be satisfied with the calculation requirements and the calculation cost is low [10]. The transport equations for the RNG k-\( \varepsilon \) model are expressed as Eq.3 and Eq.4:

\[ \frac{\partial}{\partial t}(\rho k) + \nabla \cdot (\rho k \bar{u}) = \frac{\partial}{\partial x_i}(\rho \mu_{eff} \frac{\partial k}{\partial x_i}) + G_i + G_\varepsilon - \rho \varepsilon - Y_M + S_i \]  

(3)

\[ \frac{\partial}{\partial t}(\rho \varepsilon) + \nabla \cdot (\rho \varepsilon \bar{u}) = \frac{\partial}{\partial x_i}(\rho \mu_{eff} \frac{\partial \varepsilon}{\partial x_i}) + C_1 \varepsilon \left( \frac{G_i}{k} + C_3 \varepsilon \right) - C_2 \rho \frac{\varepsilon^2}{k} - R_s + S_i \]  

(4)

The \( G_k \) represents the generation of turbulence kinetic energy due to the mean velocity gradients and it is calculated by Eq.5:

\[ G_i = -\rho u_i \frac{\partial u_i}{\partial x_j} \]  

(5)

The \( G_\varepsilon \) represents the generation of turbulence kinetic energy due to buoyancy and it is calculated by Eq.6:

\[ G_\varepsilon = \beta_g \frac{\mu}{\rho} \frac{\partial T}{\partial x_j} \]  

(6)

The \( Y_M \) represents the contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate and it is calculated by Eq.7:

\[ Y_M = 2 \rho \varepsilon M^2 \]  

(7)

The quantities \( \alpha_k \) and \( \alpha_\varepsilon \) are the inverse effective Prandtl numbers for k and \( \varepsilon \). \( C1\varepsilon \) and \( C2\varepsilon \) are model constants, where \( C1\varepsilon = 1.42 \) and \( C2\varepsilon = 1.68 \).

3. Results

3.1. RMS velocities

In order to study the flow characteristics of the liquid-liquid multiphase system in a stirred tank, the RMS velocities of the continuous phase were calculated by a CFD approach based on RNG k-\( \varepsilon \) model and Eulerian-Eulerian model. The comparison between simulation results and experimental results reported by Svensson and Rasmuson [2] were shown in Fig. 2.
Figure 2. Comparison of simulation results (left) and experimental measurements (right) for RMS velocities of the continuous phase.

It can be seen that the simulation results were in good agreement with experimental results which means that the CFD approach predicted the RMS velocity distribution well. The velocity at impeller disc height was higher than that in other areas, and the further away from the impeller, the smaller the velocity. Moreover, there are large vortex occurred in the tank which reflect that the efficiency of mixing is good. The locus of the vortex center predicted by the CFD approach and measured by PIV technique can be seen clearly in the vertical planet in Figure 2, which explained that the RNG k-ε model can predict the vortex center in liquid-liquid stir accurately.

3.2. Tangential and radial velocity
The tangential and radial velocities predicted by simulation and measured by experiment were compared. It can be seen in Fig. 3 that the CFD approach can give exact prediction of the velocities.

The data predicted by simulation was in good agreement with experimental data. The tangential velocity at impeller disc height predicted by simulation near the impeller was not as good as far from the impeller. The tangential velocity was in better agreement than the radial velocity with experimental data. It is can be seen in Fig. 3 clearly that the radial velocity and the tangential velocity at impeller disc height were greatly affected by the change of the depth from wall. The absolute values of the radial velocity and the tangential velocity at impeller disc height increase significantly with the increase of the depth. It shows that the closer to the impeller, the larger the kinetic energy of the fluid. The radial velocity and the tangential velocity at 10 mm above the tank bottom were relatively stable with the change of the depth.
Figure 3. Comparison of simulation predictions and experimental data of radial velocities and tangential velocities for the continuous phase at:
impeller disc height (a, c); 10 mm above bottom(b, d).

4. Conclusion
Liquid-liquid stir in the stirred tank with a six-blade Rushton turbine was simulated by a CFD approach based RNG k-ε model and Eulerian–Eulerian model in this work. The data predicted by simulation were compared with the data measured by experiment. The RNG k-ε model gave reasonable predictions of the RMS velocity, the tangential velocity and the radial velocity. The overall trends of the simulation results are in good agreement with the experimental data. The vortex center in liquid-liquid stir can be predicted accurately with the RNG k-ε model. The radial velocity and the tangential velocity at impeller disc height increase significantly with the increase of the depth from wall. Through the calculation data and the experimental data, it can be concluded that the fluid near the impeller has larger kinetic energy and it is greatly affected by the impeller.

References
[1] F.J.E. Svensson, A. Rasmuson, LDA-measurements in a stirred tank with a liquid-liquid system at high volume percentage dispersed phase, Chem. Eng. Technol. 27 (2004) 335-339.
[2] F.J.E. Svensson, A. Rasmuson, PIV measurements in a liquid–liquid system at volum percentages up to 10% dispersed phase, Exp. Fluids. 41 (2006) 917–931.
[3] F. Laurenzi, M. Coroneo, G. Montante, A. Paglianti, F. Magelli, Experimental and computational analysis of immiscible liquid–liquid dispersions in stirred vessels, Chem. Eng. Res. Des. 87 (2009) 507–514.
[4] D. Cheng, X. Feng, J. Cheng, C. Yang, Z. Mao, Experimental study on the dispersed phase macro-mixing in an immiscible liquid–liquid stirred reactor, Chem. Eng. Sci. 126 (2015) 196–203.
[5] Z. Jaworskia, J. Dudczaka, CFD modelling of turbulent macromixing instirred tanks. Effect of the probe size and number onmixing indices, Couput. Chem. Eng. 22 (1998) S293-S298.
[6] T. Kumaresan, J.B. Joshi, Effect of impeller design on the flow pattern and mixing in stirred tanks, Chem. Eng. J. 115 (2006) 173–193.

[7] D. Cheng, X. Feng, C. Yang, Z. Mao, Modelling and experimental investigation of micromixing of single-feed semi-batch precipitation in a liquid–liquid stirred reactor, Chem. Eng. J. 293 (2016) 291–301.

[8] H.E.A. Van den Akker, The Details of Turbulent Mixing Process and their Simulation, Adv. Chem. Eng. 31 (2006) 151-229.

[9] M. Ljungqvist, A. Rasmuson, Numerical simulation of the two phase flow in an axially stirred reactor, Chem. Eng. Res. Des. 79 (2001) 533-546

[10] Z. Hao, J. Xu, H. Bie, Z. Zhou, Numerical simulation of the effects of baffle on flow field in a stirred tank, Adv. Mater. Res. 732-733 (2013) 432-435.