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Numerical simulation of macro-mixing in liquid–liquid stirred tanks

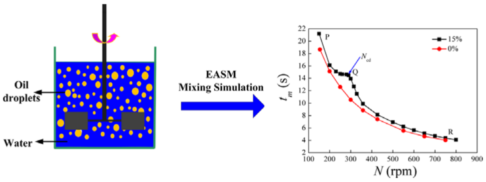
Dang Cheng, Xin Feng, Jingcai Cheng, Chao Yang*

National Key Laboratory of Biochemical Engineering, Key Laboratory of Green Process and Engineering, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, China

HIGHLIGHTS

- The predictive capability for liquid–liquid flows is improved using EASM.
- EASM predicts homogenization curves better than k–ε model.
- The homogenization curves predicted by the EASM are very close to the LES ones.
- The EASM gives better mixing time values than k–ε model.
- Mixing time can be used to determine critical impeller speed.

GRAPHICAL ABSTRACT



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ABSTRACT

Numerical simulations of turbulent immiscible liquid–liquid mixing processes in cylindrical stirred tanks driven by a Rushton turbine are carried out based on an Eulerian–Eulerian approach using in-house codes. An isotropic standard k–ε turbulence model and an anisotropic two-phase explicit algebraic stress model (EASM) are used for flow field simulations. Quantitative comparisons of the homogenization curve and mixing time predicted by the EASM are conducted with reported experimental data and other predictions by the standard k–ε model and large eddy simulation (LES). The comparisons show that the EASM predictions are in satisfactory agreement with experimental data and better than the k–ε model ones. The variation of the continuous phase mixing time with impeller speed can be an effective method to determine the critical impeller speed for complete dispersion of oil phase. The key features of the complex liquid–liquid mixing processes in stirred tanks have been successfully predicted by the EASM, which can be an alternative tool for practical engineering applications with economical computational cost and good accuracy.

1. Introduction

The stirred tanks involving two immiscible liquids are extensively used in chemical and metallurgical industries, such as suspension/emulsion polymerization, heterogeneous/phase-transfer catalytic chemical reaction and hydrometallurgical solvent extraction. Mixing plays a fundamental role in these systems, which controls the processes of blending different liquids, liquid–liquid mass transfer, and chemical reactions etc. The quality of product, yield and economy of the processes is hence significantly affected by mixing. Insufficient or excessive mixing may lead to wastage of processing time and raw materials and/or the formation of by-products (Yeoh et al., 2004).

Mixing is a very complex process in a turbulent stirred tank, which occurs as a result of fluid motion at two (macro- and micro-) typical scales. The presence of a second phase (gas, oil drop or solid) makes the flow and mixing process of the continuous phase even more complicated, especially for high dispersed phase loadings. For liquid–liquid systems, the macro-mixing determines the environmental concentrations for micro-mixing in the continuous phase, which affects the course of chemical reactions directly. It is thus believed that the information related to macro-mixing is very important to control the performance of chemical reactions occurring in the continuous phase in the presence of immiscible oil drops. The macro-mixing is usually characterized by mixing time, i.e., the time required to achieve certain degree of homogeneity of an inert tracer

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* Corresponding author. Tel.: +86 10 62554558; fax: +86 10 82544928.
E-mail address: chaoyang@home.ipe.ac.cn (C. Yang).

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injected into a stirred tank. Moreover, mixing time is a simple and powerful measure to assess the effectiveness of a mixer and one of the most crucial parameters for design, optimization and scale-up of a stirred tank. Therefore, it is necessary to gain a detailed knowledge of the macro-mixing characteristics of turbulent liquid–liquid dispersions.

A large number of experimental works have been devoted to studies on the mixing time in single phase (Nere et al., 2003; Grenville and Nienow, 2004), gas–liquid, solid–liquid and gas–liquid–solid systems (Cheng et al., 2011a), and relevant empirical correlations were well developed during last decades. Whereas, few research efforts have been focused on the mixing time in complex immiscible liquid–liquid systems. Recently, Zhao et al. (2011) measured the continuous phase mixing time in the presence of immiscible oil drops for a wide range of oil volume fractions and viscosities using four different impellers, and the results were combined to an empirical correlation as well. However, the correlation is based on laboratory scale measurements, and its extrapolative use to industrial-scale stirred tanks is risky. Furthermore, it conceals detailed localized information and cannot be used for prediction of homogeneity degree at various locations inside the tank (Jahoda et al., 2007). It is therefore essential to develop computational fluid dynamics (CFD)-based methods, which are powerful and capable of eliminating scaling-up/down problems by numerical solution of the fundamental equations governing fluid flow and tracer transport.

Various alternative methods can be employed to model turbulent macro-mixing processes. The most popular are the Reynolds-averaged Navier–Stokes (RANS) approach with turbulence models and the large eddy simulation (LES) approach. Although the LES method was generally revealed to be able to mimic the transient experimental responses of probes monitoring local tracer concentrations quite accurately and give more realistic mixing time values (Van den Akker, 2006; Jahoda et al., 2007), its tremendous computational cost, e.g., more than 2 months for a typical job (flow field simulation plus mixing) in very small lab-scale stirred tanks (Yeoh et al., 2005; Hartmann et al., 2006) is still a major constraint for industrial/pilot scale applications and therefore is not yet fine-tuned for quick process design validation (Kasat et al., 2008). Overall, improvement is expected with the LES approach for flows in which the rate-controlling processes occur in the resolved large scales, while the appeal of LES is weak when the rate-controlling processes occur below the resolved scales (Pope, 2004). Moreover, the flow field simulations by LES have not yet been quantitatively validated for the complex immiscible liquid–liquid flows in stirred tanks. Coroneo et al. (2011) performed systematic and stringent evaluation of the contribution of numerical issues to the accuracy of the most widespread $k-\varepsilon$ model, and confirmed that Reynolds averaging of the convection–diffusion equation was an acceptable approximation. For these reasons, the computationally efficient RANS approach with appropriate turbulence models might be the main tool in practical industrial applications.

The RANS approach with a turbulence model based on the fully predictive strategy, i.e., the sliding mesh or the multiple frames of reference (MFR) framework, or sometimes a combination of the two, or the inner-outer iterative procedure, has been widely used to model the turbulent macro-mixing processes in stirred tanks. Most of them were devoted to single phase systems (Jaworski and Dudczak, 1998; Osman and Varley, 1999; Jaworski et al., 2000; Do et al., 2001; Bujalski et al., 2002a, 2002b; Murthy Shekhar and Jayanti, 2002; Montante and Magelli, 2004; Montante et al., 2005; Kukukova et al., 2005; Mostek et al., 2005; Javed et al., 2006; Kumaresan and Joshi, 2006; Ochieng et al., 2008; Coroneo et al., 2011), and very few were focused on multiphase (gas–liquid and solid–liquid) stirred reactors (Khopkar et al., 2006b; Jahoda et al., 2009; Kasat et al., 2008). From the above survey, it is noted that nearly all the simulation works used the standard $k-\varepsilon$ model to handle turbulence. In the past decades, the standard $k-\varepsilon$ turbulence model has been the most commonly used model for stirred tank simulations. The primary weakness of the $k-\varepsilon$ model is that it fails to predict accurately the flow in anisotropic turbulence regions for its assumption of isotropic turbulence and spectral equilibrium. Further, it is clear that modeling of the transport equations for k and ε leads to difficulties to account for streamline curvature, rotational strains, and other body-force effects (Joshi et al., 2011). The impeller zone is the main source of anisotropic turbulence in stirred tanks, where the agitation power is transferred into the tank. Zhao et al. (2011) reported that the shortest mixing time was observed when the tracer was injected into the liquid from the impeller zone as compared to the cases when the tracer was injected from the liquid surface or the tank bottom. This observation further illustrates that the impeller zone is very important for the mixing process, suggesting that modeling of anisotropic turbulence is especially crucial for prediction of the overall mixing performance of stirred tanks.

As the anisotropic turbulence model is concerned, Reynolds stress model (RSM) and algebraic stress model (ASM) are widely shown to perform well in prediction of single phase flow fields (Murthy and Joshi, 2008). Since Reynolds stress components are solved directly from a differential equation or an algebraic equation rather than being modeled by an isotropic hypothesis like the $k-\varepsilon$ model, anisotropic turbulence can be successfully predicted. However, both RSM and ASM are not computationally robust and have difficulty to reach converged solutions. To overcome these problems, Pope (1975) proposed an explicit algebraic stress model (EASM) for two-dimensional flows based on the RSM or the ASM by using a tensor polynomial expansion theory, in which the Reynolds stress components were expressed as an explicit algebraic correlation of mean strain rate tensor, rotation rate tensor and turbulence characteristic quantities. Following Pope's theory, Gatski and Speziale (1993) and Wallin and Johansson (2000) developed three-dimensional EASMs. Recently, Feng et al. (2012a, 2012b) simulated single phase and solid–liquid two-phase flows successfully with improved computational stability and greatly reduced computational cost using Wallin and Johansson's explicit algebraic stress model (EASM). Considerably improved agreement with experimental data was found in terms of mean as well as turbulence quantities compared to those predicted by the $k-\varepsilon$ and ASM models. Since the EASM performs well in predicting single and solid–liquid flows in stirred tank, it is expected to perform as well for description of immiscible liquid–liquid flows. Feng et al. (2012c) also made an attempt to simulate two-phase liquid–liquid flows in stirred tanks using the two-phase EASM, and comparisons with experimental data and $k-\varepsilon$ predictions in terms of mean velocities and the dispersed phase holdup distributions were conducted. The results were encouraging, but the quantitative comparisons were limited owing to the experimental measurement and CFD simulation of immiscible liquid–liquid flows in stirred tanks were only rarely reported (Wang and Mao, 2005; Svensson and Rasmuson, 2004, 2006; Laurenzi et al., 2009; Cheng et al., 2011b). Therefore, the EASM deserves further evaluation in order to assess comprehensively its performance for describing turbulent liquid–liquid flows in stirred tanks. As the macro-mixing process is closely related to the mean flow field and the turbulence, the EASM can be further verified using macro-mixing experimental data, which can be easily measured.

To the best of the authors' knowledge, numerical simulation of the continuous phase mixing characteristics and assessment of the predicted macro-mixing data using both the isotropic standard $k-\varepsilon$ turbulence model and the anisotropic EASM against experimental values of liquid–liquid systems have not yet appeared in the