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CFD PREDICTION OF LIQUID HOMOGENISATION IN A GAS-LIQUID STIRRED TANK

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Abstract. In this work, simulations of liquid homogenisation were performed for a two phase gas-liquid stirred tank using CFD. The predictions were compared with experimental results obtained in a baffled cylindrical vessel stirred by a pitched-blade impeller. The impeller speed was 300 rpm. The CFD simulations were performed in 3D using the Fluent 6.3 numerical software. For the solution, a simplified numerical setup of mono-dispersed bubbles, constant drag coefficient and the k-ε turbulence model have been applied. Despite the assumed simplifications, the numerical predictions exhibit a good agreement with the experimental data.

Key words: CFD; Liquid homogenisation; Stirred tank; Gas-liquid;

1. INTRODUCTION

Homogenisation of miscible liquids is the most frequently used operation in mixing processes in all branches of chemical, biochemical, food or pharmaceutical industries. Homogenisation of one-phase stirred systems (only liquid phase) is currently well experimentally explored and there are empirical correlations for calculation of mixing time for one-impeller systems [1-3]. The proposal of suitable correlations for determination of mixing time in different arrangements, e.g. more impellers, non-standard configurations, multi-phase mixing; is questionable due to great number of variables. Use of the empirical correlations is limited, because they cannot be used for prediction of evolution of degree of homogeneity at various locations inside a tank in time. For these reasons, various models containing the progress of liquid homogenisation in stirred tanks have been developed. The cells or dispersion models [4-6] were used previously, but CFD (Computational Fluid Dynamics) methods based on a solution of the Navier-Stokes equations have now become a powerful tool for prediction of fluid flow and mixing time in stirred tanks.

An advantage of the CFD-based methods is that the fundamental equations governing fluid flow are solved and can be used for prediction of mixing characteristics of industrial sized mixers or equipment for which no empirical correlations are available. Two alternative methods are usually employed for fluid flow simulation of stirred tanks: the Reynolds-averaging (RANS) method with RANS-based turbulence models (for example the k-ε models) or the unsteady Large Eddy Simulation (LES) approach. Subsequent unsteady solution of a tracer transport equation leads to the prediction of the evolution of the tracer concentration (liquid homogenisation) inside the tank in time [7-10].

Liquid flow in multiphase mixed systems have been studied mainly experimentally, usually together with other characteristics like distribution of solid particles, gas hold-up or mass exchange among phases. Authors who simulated multiphase flows in stirred tanks mainly focused on the dispersed phase, i.e. solid particles or gas bubbles. Results from CFD simulation of time evolution of liquid homogenisation in multiphase stirred systems have been presented only rarely [11]. The presence of an additional phase (solid or gas phase) affects the dynamics of the continuous phase (liquid) and the interactions among the phases involve various momentum exchange mechanisms such as drag, lift and the added mass force. Nevertheless, the contribution of the drag force is dominant, while the effect of the other forces could be ignored. It has been reported that the other forces have no considerable effect on either gas-liquid [11-13], solid-liquid [14-16] or gas-solid-liquid [17] hydrodynamics in stirred tanks. In the case of gas-liquid systems, authors often used a simplified conception in which spherical bubbles have the same size [11, 12]. For more accurate results of distribution of gas bubbles in a tank, modelling of coalescence and break-up phenomena is recommended [18, 19].

The objective of this article is to present CFD simulations of two-phase (gas-liquid) flow and liquid homogenisation in an aerated agitated charge in a standard tank equipped with radial baffles and a rotational impeller. This research directly relates onto our previous papers [9, 10] aimed at prediction of liquid homogenisation in mechanically stirred tanks using the CFD method. The preceding works were focused on a single liquid phase and this study extends the previous investigations using an additional gas phase.

2. EXPERIMENTS

Experiments were carried out in a fully-baffled, flat-bottomed cylindrical tank of inner diameter $T = 0.29$ m and baffle width of $T/10$, see Fig. 1. The tank was equipped with one impeller and filled with tap water to a height H equal to T. The impeller was a 6-bladed 45° pitched blade turbine (PBT) pumping towards the tank bottom and its diameter was $D = T/3$. The off-bottom clearance of the impeller was one third of the tank diameter, $C = T/3$. The impeller was attached to a centric shaft, moving at a constant rotational speed of 300 rpm. This corresponds to a Reynolds number for mixing of $4.66 \cdot 10^4$. The gas (air) was introduced using a ring sparger of diameter of 0.06 m which was located at $D/2$ from the bottom of the tank. Volumetric gas flow rate varied from 1 l/min to 7.75 l/min.

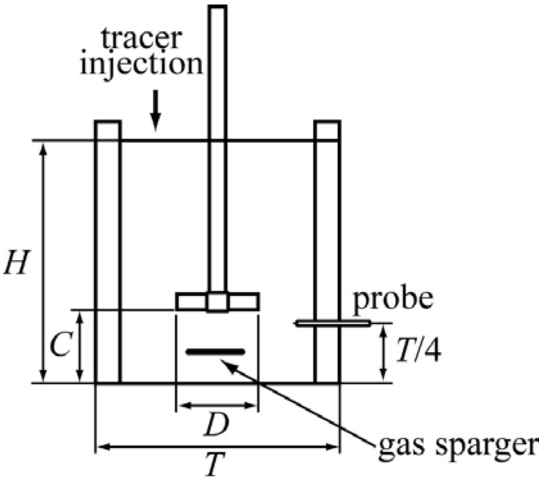

Fig. 1 Geometry of the stirred tank

For measurement of tracer concentration curves (liquid homogenisation), a conductivity method was used. Detection volume of the conductivity probe was 0.55 cm^3 and the probe was placed between the baffles, with off-bottom clearance of $T/4$ and at a distance of $T/20$ from the tank wall. A mesh cage around the probe allowed a signal to be obtained without being disturbed by the presence of bubbles. Approximately 4 ml of the tracer (saturated solution of NaCl) were injected in each experiment. It was injected on the free liquid surface, at a horizontal distance of $T/4$ from the tank wall, opposite the probe, see Fig. 1. Output signal from the probe was processed by a conductivity meter, digitised by A/D converter and registered by a computer for further processing. The registered values of voltage from the conductivity meter were directly proportional to the tracer concentration. For each set-up, approximately ten measurements were made. Time traces, presented in the form of normalised concentrations, were used for determination of experimental mixing times. The mixing time (t_m) was defined as the time necessary to reach a permanent level of variation of the normalised terminal concentration of within ± 5% of the final value.

3. CFD SIMULATIONS

In this paper, the commercial CFD software FLUENT 6.3 was employed to numerically investigate the homogenisation process in the stirred tanks using the Reynolds Averaged Navier-Stokes method with the standard k-ε turbulence model. The Multiple Reference Frames (MRF) technique was used for simulation of the impeller motion.

Presented CFD simulations consist of three main steps. At first, the geometry of the tank was defined and a computational grid was made in the pre-processor Gambit 2.3. The mesh contains approximately 475,000 hexahedral cells. From assessment of the grid quality, we found out that more than 99% of the cells had excellent or good quality and only 0.02% of the cells were low quality. We utilized our previous experience in the computational grid formation obtained during liquid flow simulations of a single-phase stirred system [9].

Next, the unsteady simulations of the mixture (gas-liquid) flow fields were performed. The Eulerian-Eulerian model was used in which a set of momentum and continuity equations is solved for each phase. The model of Schiller and Naumann has been employed for the drag coefficient calculation. For simplification of the solution, a mono-disperse gas-phase with the effective bubble size of 4 mm was used for all simulations [11].

After the flow field had fully developed (about 15 s of real time was simulated), a simulation of the tracer homogenisation was performed. The tracer, having the same physical properties as the bulk, was added just under the free liquid surface opposite the probe. The molecular diffusivity was assumed to be equal to 10^{-8} m^2 s^{-1}, a typical value for liquids. The turbulent Schmidt number was kept default, $Sc_t = 0.7$. The tracer mass fraction in the vessel was recorded during the time-dependent simulation. A virtual probe was placed at a point, at the same position as the real probe. The average mass fraction value, calculated from the adjacent cell centres, was recorded after each time step, which was set to 0.01 s. The value of species residual for a converged solution was set equal to 10^{-7}.

4. RESULTS AND DISCUSSION

Figure 2 shows a comparison of velocity magnitude profiles for both liquid and gas phases for two different volumetric gas flow rates: 1 and 6 l/min. The CFD simulations correspond to the fact that the gas phase introduced under the rotational impeller influences the discharge liquid flow from the impeller and liquid motion in the tank. In the case of the low volumetric gas flow rate (Fig. 2a), the liquid flow pattern for an axial type of impeller is similar to the case of a one phase system. The liquid flow is dominant. The liquid phase has enough energy to snatch the gas bubbles, see Fig. 2b. When the gas flow rate increases, the bubble flow becomes more dominant, see Fig. 2d, and the resulting discharge liquid flow from the axial PBT is similar to the radial type of impeller. One more symmetrical circulation loop in the area above the impeller is apparent, see Fig. 2c.

Figure 3 shows the time traces of the normalised tracer concentrations for all investigated configurations. The CFD predictions of liquid homogenisation agree well with experiments, namely for greater volumetric gas flow rates (6 and 7.75 l/min). For these flow rates, the calculated mixing time is practically identical with the one obtained experimentally, see Fig. 4. However, the predicted liquid homogenisation is worse for configurations where the liquid flow is dominant (low volumetric gas flow rates). Here, we obtained similar results as in the case of a one phase system [10]. It could be due to simplification of the MRF technique, where the motion of the liquid and tracer introduced into the rotating frame is inaccurate (the rotational motion of the impeller is compensated by additional forces inside the impeller area). Dominant bubble flow could reduce this inexactitude.

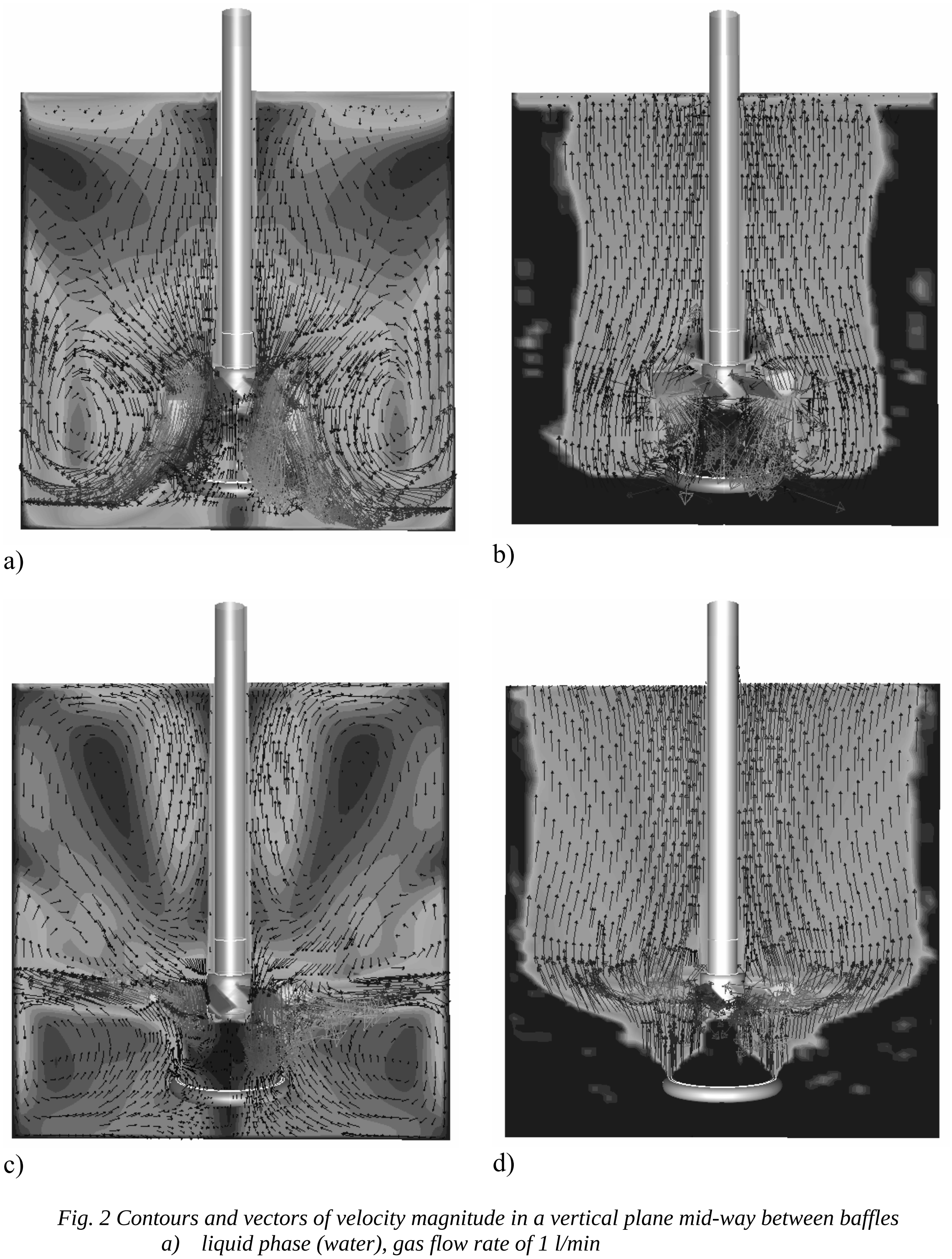

Fig. 2 Contours and vectors of velocity magnitude in a vertical plane mid-way between baffles

- *a) liquid phase (water), gas flow rate of 1 l/min*
- *b) gas phase (air), gas flow rate of 1 l/min*
- *c) liquid phase (water), gas flow rate of 6 l/min*
- *d) gas phase (air), gas flow rate of 6 l/min*

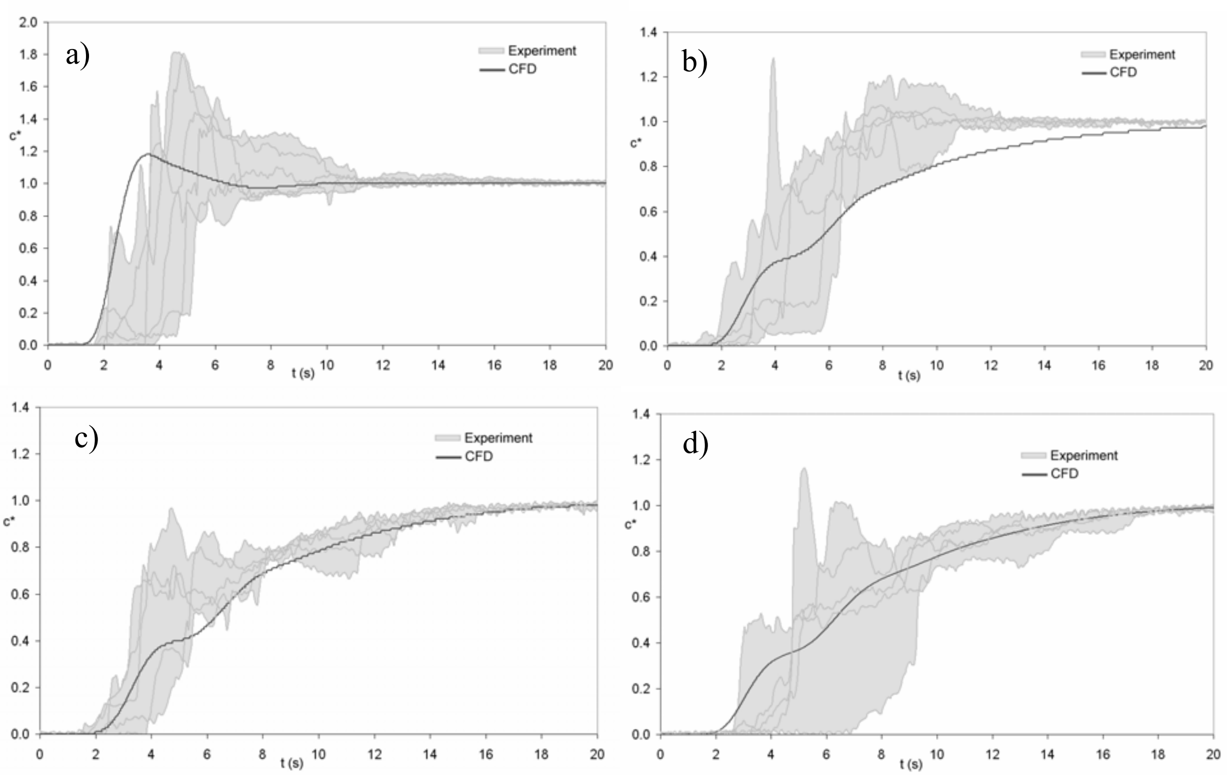

Fig. 3 The time traces of normalised concentration for various volumetric gas flow rates a) Q_g = 1 l/min; b) Q_g = 4 l/min; c) Q_g = 6 l/min; d) Q_g = 7.75 l/min

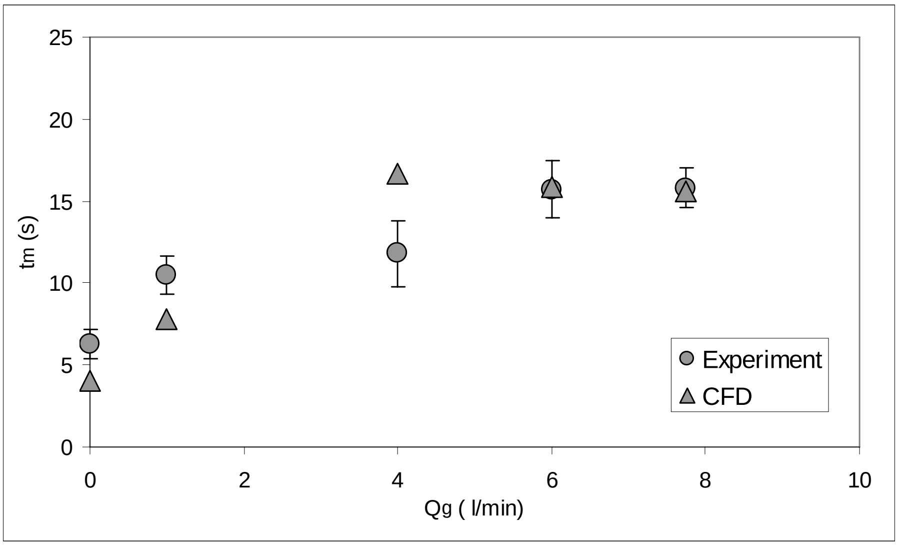

Fig. 4 Comparison of predicted mixing times with experimental data including experimental error bars with the standard deviation

The MRF technique and the standard k-ε turbulence model present the simplest way to CFD prediction of liquid patterns in stirred tanks. The predicted mixing times are usually shorter than experimentally obtained, but the main advantage of this method is relatively low computational time with acceptable results. In the case of single-phase stirred systems, an excellent agreement with experimental evolution of liquid homogenisation was obtained using the Sliding Mesh technique and the Large Eddy Simulation turbulence model [11]. Using the LES model for prediction of gas-liquid flow patterns is tied together with the Volume of Fluid (VOF) method in the Fluent solver, making the solution very time demanding.

5. CONCLUSIONS

Three-dimensional CFD simulations of a gas-liquid two-phase flow in a laboratory-scale stirred tank equipped by a pitched-blade impeller have been performed. The flow of phases and the evolution of tracer homogenisation were predicted using the RANS technique with the standard k-ε turbulence model and the Eulerian-Eulerian approach. Despite simplifications (MRF technique, mono-dispersed bubbles, no bubbles coalescence or break-up), the results are in a very good agreement with experiments, particularly when the bubble flow is dominant.

A further study could address the Sliding Mesh method for modelling of impeller rotational motion instead of the MRF technique, different models for the drag force, solution of the bubble size distribution using appropriate models for bubble break-up and coalescence and calculation of other mixing characteristics of gas-liquid stirred systems like gas hold-up or gas power number.

6. ACKNOWLEDGEMENTS

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7. NOMENCLATURE

C	impeller off-bottom clearance	m
c^*	dimensionless concentration	-
D	impeller diameter	m
H	liquid height	m
T	tank diameter	m
t_m	mixing time	s
Q_g	volumetric gas flow rate	$m^3.s^{-1}$

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