CFD SIMULATIONS OF SINGLE AND TWO-PHASE MIXING PROESSES IN STIRRED TANK REACTORS

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1. Introduction

Mixing in stirred tanks is a widely used operation aiming to decrease the degree of non-uniformity of any system to which it is applied. Its engineering arrangement and realisation always depends on the system properties. The mixing can be employed to improve the mass transfer along with the heat transfer if needed. When a chemical reaction is designed to occur in a stirred vessel, reactants would require to be successively well mixed for reaction to proceed. If the reaction is relatively fast, the selectivity and the rate and yield will also be determined by the mixer performance.

Modelling a stirred tank using computational fluid dynamics (CFD) requires consideration of many aspects of the process [1]. First of all, the geometry of the stirred tank, even in the case it is very complex, needs to be described by a computational grid, required by the computational model. Second, the motion of the impeller should be treated in a special way, especially when the tank contains baffles or other stationary internals.

In the modelling of the stirred tank reactor two major advance steps have been completed: passive tracer and two-phase gas-liquid mixing. Although, in the case of the passive tracer, the numerical predictions of the liquid phase mixing were the primary task, the system was treated as two-phase flow in order to study the free surface deformation and its impact on the flow. A visualisation technique was applied to obtain an experimental observation of the process to be compared with the numerical predictions obtained using CFX 5.7 CFD software. The two-phase mixing in the stirred tank was studied under the mechanical agitation of a gas-inducing turbine. An X-Ray cone-beam tomography was applied to experimentally assess the process. The numerical predictions for the gas-phase distribution were validated against the experimental observations. The theoretical assessment of the two-phase flow was performed using CFX 10.

2. Experimental set-up

A laboratory scale Büchi Ecoclave 1.6 litre tank, schematically presented in Figure 1, was used to perform the mixing experiments and the numerical simulations. The tank with a diameter of 82 mm was mechanically agitated by a Pfaudler impeller, employed for the passive mixing, and by a gas-inducing turbine stirrer for two-phase flow mixing. The Pfaudler impeller with a diameter of 58 mm and the gas-inducing turbine with a diameter of 45 mm were both mounted at a clearance of 27 mm. In the case of the passive tracer mixing, the liquid level height was chosen to be equal to the tank diameter and in the case of the two-phase flow mixing it was 232 mm.

A video technique was applied to experimentally study the passive tracer mixing process. The initially stratified lighter (alcohol) coloured component and the heavier (water) transparent one were brought into motion by the rotating impeller. The mixing process was recorded on a digital camcorder and subsequently the images were digitally processed. To obtain the colour-calibration curve, the procedure was repeated for a number of different initial concentrations of the lighter liquid. Different points, at which the optical distortions were minimal, were chosen to acquire the mixing curves of the concentration change in time. The comparison points were located close to the impeller shaft and the tank wall.

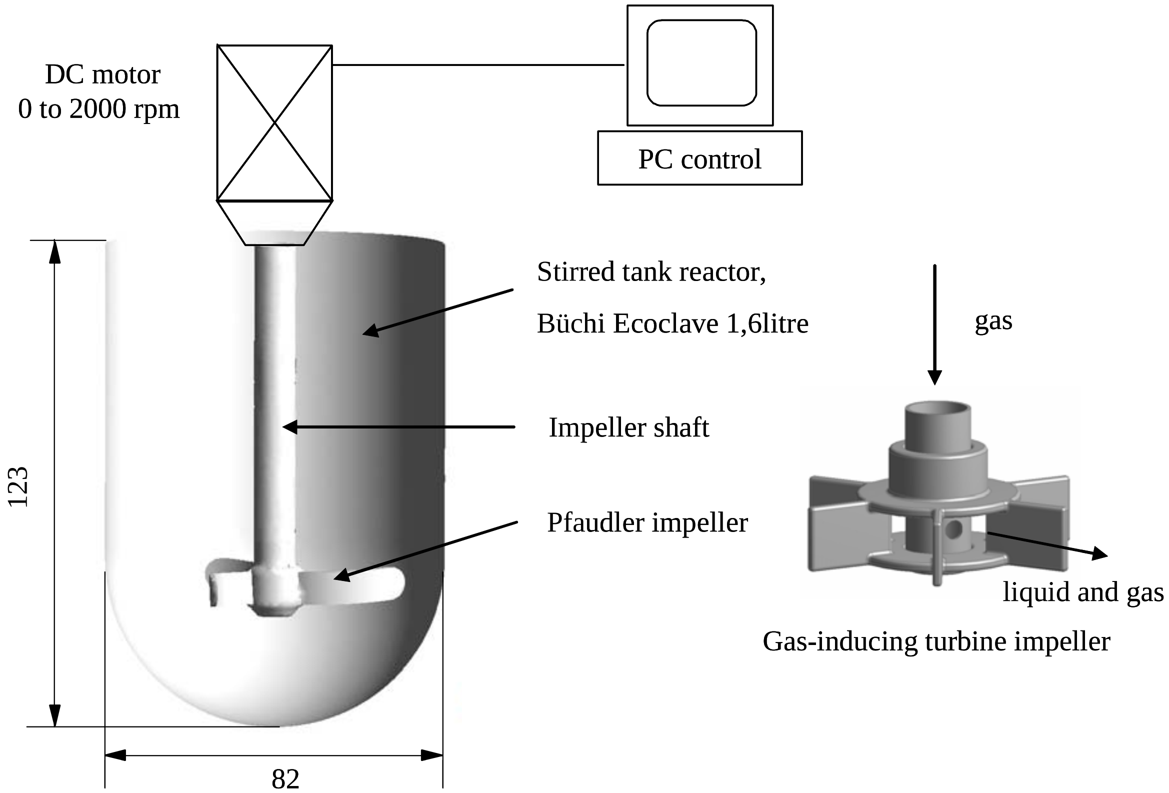

Fig. 1: Schematic view of the experimental rig and the gas-inducing turbine

The system under investigation comprises air as gas phase and isopropanol as liquid phase at room temperature. Both isopropanol and air, which were initially stationary, were brought into motion by the rotating impeller. Measurements carried out with the X-Ray cone beam tomography, were taken at five different stirrer speeds with thresholds of 50 rpm starting from 1000 rpm at which the gas inducement occurs for the given operating conditions. The final stirrer speed was 1200 rpm at which the central vortex virtually reaches the impeller. Additionally, video observations, performed with a digital camcorder, were taken to study the unsteady behaviour of the central vortex.

The X-Ray cone-beam tomography is a potential method to measure the phase distributions in stirred vessels. Three-dimensional information can be gathered within only one tomographic scan [2]. The reconstruction of a rotationally symmetric distribution field is even possible from a single radiographic image. Such an experimental approach was carefully examined and applied to obtain the quantitative measurements of gas-fraction profiles in a stirred tank reactor. Additionally, a moving slit technique was adapted to estimate the inherent scattered radiation offset, which emerges while uncollimated X-Rays penetrate the fluid-filled tank. An additional reference measurement was introduced and used to remove beam-hardening artefacts. An absolute quantification was possible due to the knowledge of the ratio of the fluids and the reference-materials X-Ray absorption coefficients. Phantom measurements inside the vessel were conducted for performance evaluation. A systematic measurement error of less than 1.5% absolute gas fraction for local gas fractions up to 30% was achieved while maintaining a spatial resolution of better then 1 mm.

3. Theoretical assessment of the mixing process in the stirred tank reactor

3.1 Passive tracer mixing

The passive tracer mixing simulations were carried out to numerically assess the mixing behaviour of different density liquids. Such a process is a common operation in the process industry and occurs when a higher density liquid is injected into a tank filled with a lighter density one or in the case of impeller malfunctioning when the different density liquids can get stratified. The process might prove to be of significant importance, particularly in the case of reacting liquids for large-scale reactors operating in the industry.

The CFD analyses were performed with the CFX 5.7 numerical package. Although the non-baffled vessel exhibits an axi-symmetric behaviour on a macro-mixing scale, the process was regarded as three-dimensional in order to demonstrate the local instabilities associated with the blade passage. The dynamic mixing behaviour of two miscible liquids with different densities was numerically predicted from initially stratified conditions to complete mixing. Time steps of 0.01 seconds were found to satisfy the convergence criteria for the transient run. The gas phase was involved in the simulations to investigate the effect of the free surface deformation on the mixing process, which was modelled using the free surface model [3]. A single velocity field was assumed for the two-phase flow, imposed by the homogeneous two-phase flow model [3]. The multicomponent model [3] was applied to the liquid phase in which the two different density liquids were present. The suitability of the different turbulence models was also addressed but the k-ε turbulence model was finally employed. In order to obtain grid independent results, the numerical simulations were performed on different size grids. However, the grid elements size, in total just above 400 000 for the whole tank, was kept relatively low because of the dynamic behaviour of the liquid surface central vortex. Two domains, one stationary and one rotating with Transient Rotor interaction scheme [3], were used to represent the tank with the rotating impeller. Additionally, the impeller acceleration from stationary to 200 rpm was modelled.

A comparison between the experimentally observed and theoretically predicted integral mixing curves at four different locations is presented in Figure 2. Since the video visualisation technique provides integral mixing curves at the chosen locations, the predicted concentration values were exported and averaged along lines going through the tank and corresponding to these locations. The points located in the initially stratified isopropanol layer are not presented here since the colour change in time is strongly influenced by the liquid phase surface deformation. It is visible from Figure 2 that the CFD predictions qualitatively reproduce the visual observations. In all of the mixing curves, the mixing rate of the different density liquids is a bit over predicted, which indicates that the density layer is more rapidly destroyed when compared to the visual observations. Closer match between the experiment and the simulations is demonstrated for the lower part of the tank beneath the impeller (Figure 2(b)), which might be due to the radial pumping characteristics of the impeller. In this case, relatively stagnant zone, regarded as low mixing rate one, is present below the impeller because of the lack of baffles. This property of the non-baffled tank is captured by both the experiment and the numerical prediction. The complete mixing is predicted to happen at 13 seconds after the impeller start up, close to the experimentally measured value of 15 seconds.

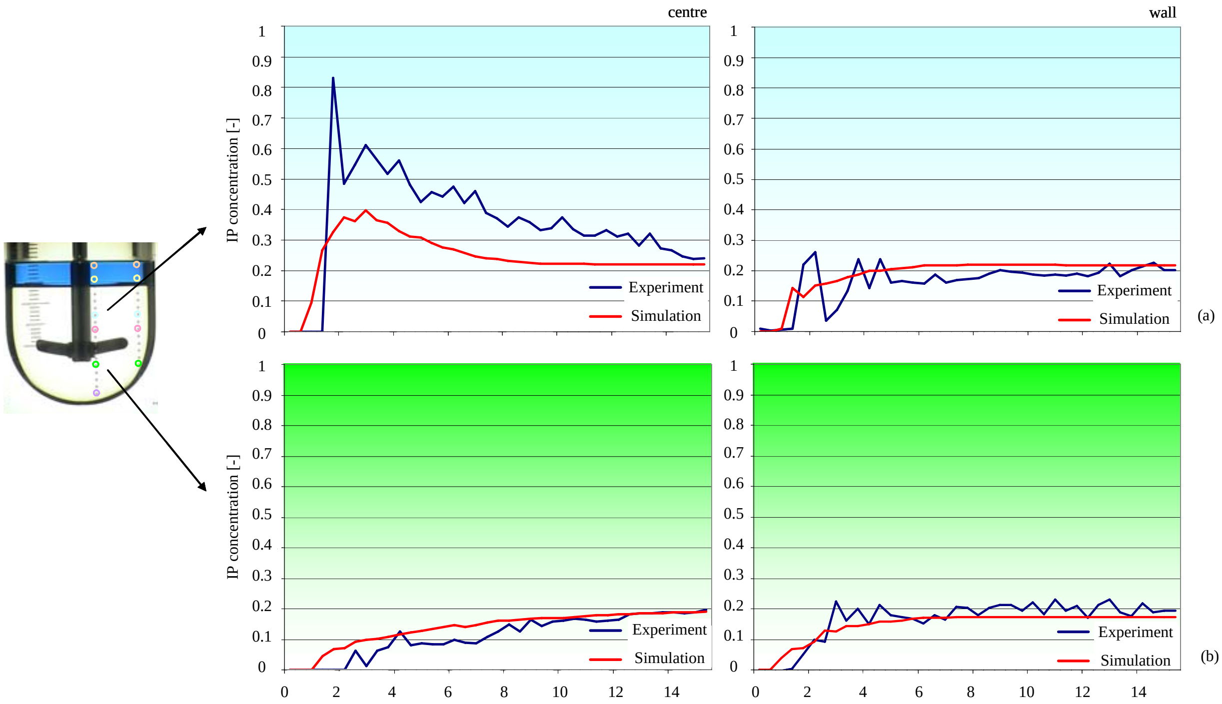

Fig. 2: Integral mixing curves at different locations

3.2 Two-phase flow in the stirred tank reactor

Gas-liquid mixing in stirred tank reactors is a common process in the industry. It is regarded as one of the most difficult to tackle because of its complexities in terms of flow regimes and multiphase operations. Traditionally the gas-liquid stirred tank reactor is equipped with an impeller responsible for dispersing the gas phase, which is usually supplied via a single dip pipe or a ring sparger mounted beneath the impeller. The gas-inducing impellers provide an alternative gas injection, in which case the gas is sucked via a hollow shaft and fed directly into the stirrer region. More gas bubbles are broken up into small bubbles when such a configuration is applied, which consequently provides higher mass transfer.

The computational fluid dynamics analyses of the stirred tank reactor were performed with CFX 10.0 numerical software. A full three dimensional approach was adopted in order to capture the spatial behaviour of the central vortex. Four steady state simulations at stirrer speed from 200 to 800 rpm were conducted to obtain an initial guess of the flow field and the phase distribution for the simulation at 1000 rpm. The numerical predictions above 1000 rpm used the previous simulation results as an initial guess. Starting from 1000rpm, five simulations were performed at stirrer speed thresholds of 50 rpm to be compared with X-Ray cone-beam tomography measurements. The tetrahedral mesh with above 1500000 elements was globally refined since a detailed view in the whole geometry is required. The stirred tank was broken down into four domains, three rotating and one stationary. A Frozen Rotor interaction scheme was used in the simulations to bond the multiple frames of references domains. The inhomogeneous two-phase flow model with the particle transport model was applied to the system with momentum transfer described by the drag force and turbulence transfer modelled by Sato enhanced eddy viscosity model [4]. The gas phase was modelled as dispersed fluid with a mean diameter of 1 mm and the liquid phase as continuous fluid. Different turbulence models and their suitability were considered for the liquid phase. The gas-phase turbulence was modelled using the dispersed phase zero equation. The flow was regarded as buoyant and implemented using the density difference model.

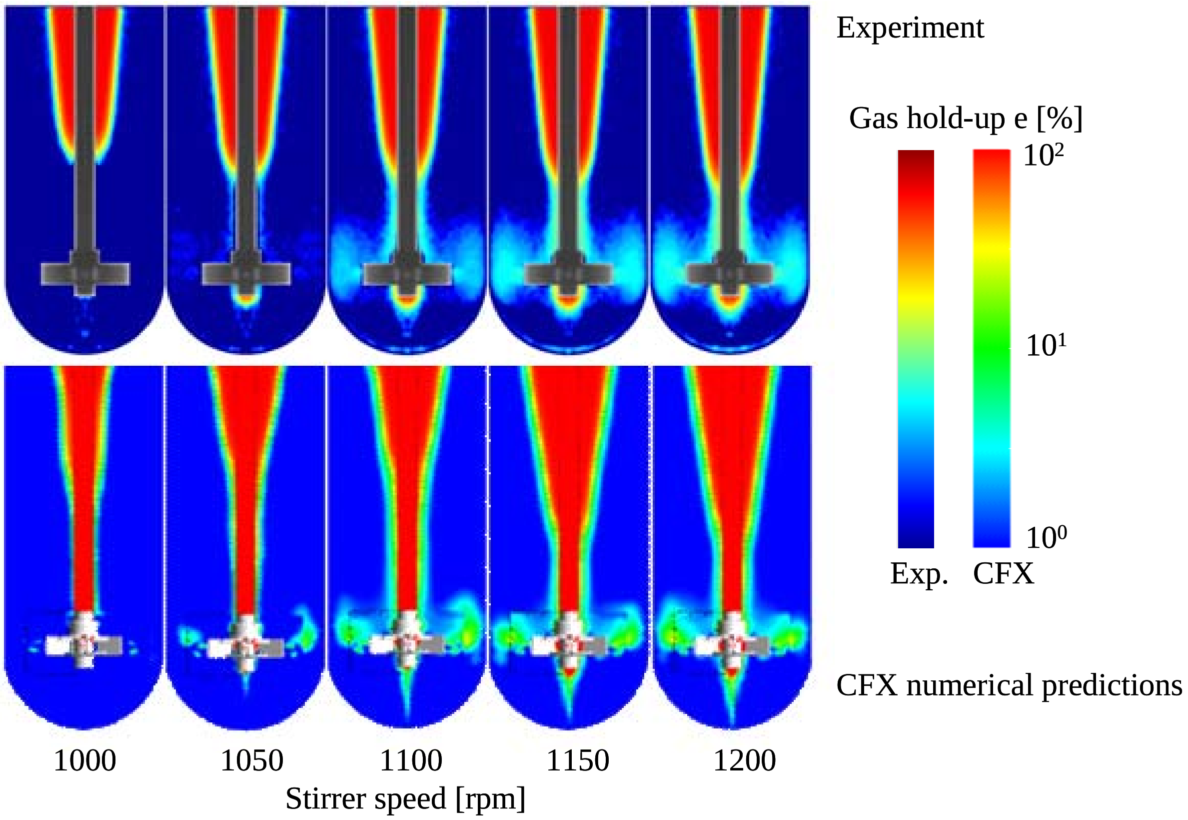

Fig. 3: Gas hold-up in stirred tank reactor at different impeller speeds

A comparison between the experimentally measured and numerically predicted gas hold-up distribution at different stirrer speed is presented in Figure 3. It is clearly visible that the CFD predictions closely mimic the experimental observations. The central vortex depths as well as its spread out closely correspond to the ones experimentally observed except for the lower stirrer speeds of 1000 and 1050 rpm, for which the dept is slightly under predicted. For impeller speed above 1050 rpm, the predicted central vortex depth and shape boundaries match exactly the experimentally measured ones. At stirrer speed of 1050 rpm and above, gas is captured beneath the impeller shaft as indicated in both the experimental and numerical results. It is clearly indicated in Figure 3 that the gas hold-up significantly increases with the stirrer speed as more gas gets induced by the rotating impeller. A slightly higher gas hold-up beneath the impeller shaft is experimentally measured. This might be associated with the time-spatial averaging procedure applied in the experiment.

4. Conclusions

The hydrodynamics of the different density liquids system is of particular importance for many chemical and biochemical reactions engineered to take place in stirred tank reactors. Although the initial conditions were to some extend idealised in order to avoid some complications raised by the presence of an injection, the studies showed strong influence of the density difference on the homogenisation. Such so called idealised conditions, however, also might occur in the stirred vessel, especially in the case of impeller malfunctioning. In case of impeller stoppage, i.e. breakdown, different density liquids present in the vessel might get stratified. The CFD is also capable of capturing the two-phase flow in detail, which can provide valuable information for the industry. In particular, the spatial gas phase distribution, which can also have time-dependent behaviour, can have a crucial impact on the reactor performance. Different local gas hold-up in the vessel would determine different local mass transfer, which consequently would affect reaction rates and/or selectivity. The above described results demonstrate the potential of the CFD to assess in detail the fluid flow phenomena in the stirred tank reactor. The CFD based software in that sense can prove to be an essential tool for the reactor design, optimization and scale-up as well as for hazard analyses.

References

[1] E. Marden Marshall and A. Bakker (2002), Computational Fluid Mixing, Fluent Inc., Lebanon, New Hampshire, USA
[2] S. Boden, U. Hampel, M. Speck (2005), Quantitative Measurement of Gas Distribution in a Stirred Chemical Reactor with Cone-Beam X-ray Computed Tomography, Proceedings of the 4th World Congress on Industrial Process Tomography (05.-08.09.2005), Aizu, Japan), p. 813-818
[3] ANSYS CFX User Manual (2005), ANSYS Inc.
[4] Y. Sato and K. Sekoguchi (1975), Liquid velocity distribution in two-phase bubbly flow, Int. J. Multiphase Flow, 2, p79