

STIRRED REACTORS

I-17. Quantification of Solids Distribution and Solids Flow Field in Solid-Liquid Stirred Tank Reactors

A. Problem Definition

Liquid-solid stirred tank reactors find extensive use in the chemical process industry. Relevant examples include multiphase catalytic reactions, adsorption, crystallization, dissolution, leaching and precipitation. An important aspect in the design and operation of slurry reactors is the determination of the state of full particle suspension, at which point no particles reside on the vessel bottom for a long time. Such a determination is critical to enhance the performance of the reactor, because until such a condition is achieved the total surface area of the particles is not efficiently utilized. Considerable amount of research work has been done to determine the minimum impeller speed N_{js} required to suspend all the particles from the bottom of the reactor. The pioneering work of Zwietering (1958)¹ based on visual observations for the just-suspended condition (no particle settles at the tank bottom for more than 1 second) is still the most widely used correlation for operation of solid-liquid stirred tank reactors. However, the state of suspension of solid particles in the reactor is completely governed by the hydrodynamics and turbulence prevailing in the reactor. The interaction of the particle with the liquid flow field (in terms of lift, drag, buoyancy and gravity forces) and also the interactions with other particles (significant for dense systems) determine the motion of the solid particles within the reactor. Although many experimental efforts have been focussed on developing correlations for “just-suspension speed”, a systematic experimental study to characterize the hydrodynamics in slurry reactors can hardly be found in the literature. Recently Fishwick et al. (2005)² used the positron emission particle tracking to study the hydrodynamics in solid-liquid stirred tanks, but their study is limited to very dilute system (1% w/w). Also, extensive validations of CFD simulations with experimental results in terms of time-averaged velocity, solid hold-up and solids turbulent kinetic energy profiles for solid-liquid stirred tank are scarcely available. It is, therefore, still necessary to obtain detailed hydrodynamic information experimentally for these systems so that available CFD codes and closure models can be validated extensively before they can be confidently used for the design and scale-up of industrial reactors.

B. Research Objectives

The hydrodynamics in liquid-solid stirred tank reactors is experimentally studied using two non-invasive techniques, Computer Automated Radioactive Particle Tracking (CARPT)³ and Computed Tomography (CT)³. This will provide information regarding solid flow patterns, time-averaged velocity profiles and solids turbulent kinetic energy profiles (CARPT) and solid hold-up distribution and hold-up profiles at different cross-sections in the reactor (CT). The detailed hydrodynamic information thereby obtained will be used to evaluate CFD models extensively in terms of the quantities mentioned and different available drag closures will be evaluated to understand which provides better prediction of experimental data.

C. Accomplishments

Experiments to characterize the solids distribution and solids-flow field in a solid-liquid stirred tank reactor equipped with a six-bladed Rushton turbine (Fig.1) using CT (Fig.2a) and CARPT (Fig.2b) are performed. For the experimental study, water ($\rho=1000 \text{ kg-m}^{-3}$) is used as the liquid phase and glass beads ($\rho=2500 \text{ kg-m}^{-3}$) of mean diameter 0.3 mm are used as the solid phase. Experiments are carried out for overall solid hold-up of 1% to 7% which corresponds to 2.5 to 19% solid loading (wt/wt) respectively. Two different impeller speeds were used for each hold-

up, one above and one below the “just suspension speed” predicted by Zwietering correlation. For CT experiments, the scans were taken at three different axial locations in the reactor, $Z=0.015\text{m}$ (close to bottom), $Z=0.05\text{m}$ (just below impeller) and $Z=0.13\text{m}$ (between impeller and top surface).

The evaluation of CFD models for solid-liquid stirred tanks based on the experimental data obtained is currently underway. The Euler-Euler model available in Fluent is being tested here and LES simulations are being carried out by Prof. Derksen at the University of Delft. Different drag closures currently available are also being evaluated in the Euler-Euler framework.

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D. References

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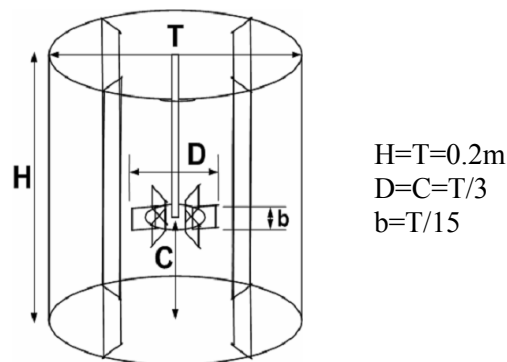


Fig.1: Reactor Schematic and Dimensions

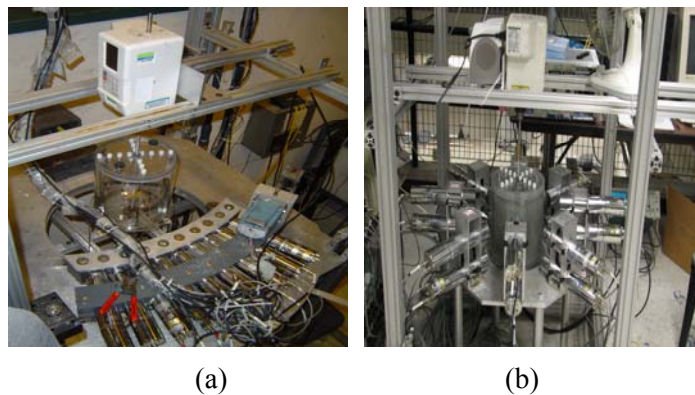


Fig.2: (a) CT experimental set-up; (b) CARPT experimental set-up

I-18. Compartmental Model for Stirred Tank Reactors: Evaluation of Turbulence Models

A. Problem Definition

Mechanically agitated reactors are widely used in variety of process industries. Traditional designs often assume perfect mixing in these reactors which, however, depends on the relative rates of chemical reactions with the rates of mixing induced by stirring, i.e. an evaluation of characteristic reaction and mixing times. This assumption often fails, which can have serious consequences for scale up, since the product distributions can be significantly affected by the concentration inhomogeneities within the reactor.

Mixing in stirred vessels take place through convection and turbulent exchanges (at larger length scales in the inertial subrange; macromixing), as well as by molecular diffusion (at smaller length scales below the Kolmogorov scale; micromixing). In the turbulent regime, i.e. at large impeller speeds, actual reactor performance depends highly on the flow field and turbulence that exists within the reactor. Hence detailed flow descriptions are essential to describe the mixing effects and predict the performance in a stirred tank reactor, which, however, remain unaccounted in many of the phenomenological models^{1,2,3} currently available. An alternative is to use the commercial CFD codes to solve the flow field as well as the concentration field in the reactor, which can become computationally intensive and that might be of serious concern for the prediction of product distribution for multiple reactions or complex reaction schemes of industrial operations. An improved methodology (in terms of reduced computational expense and time) can be devised if the CFD solution for the flow in the reactor is used along with the compartmental approach, thereby decoupling the flow and kinetics of the system, but still accounting for the effect of hydrodynamics on the mixing behavior of the system⁴. Turbulent dispersion is accounted using the gradient-diffusion model, where the turbulent diffusivity is estimated from the kinetic energy and the dissipation rates obtained from the CFD solution of the flow in the reactor⁴.

In our earlier work⁴, it has been shown that the CFD-based compartmental approach can be used to predict effect of mixing on the reactor performance and the effect of feed locations were nicely captured. A sensitivity analysis of the dispersion term on the model predictions showed that this term has a significant influence on the model predictions when the feed location is far from the impeller, whereas it has almost no influence when the feeding is close to the impeller where convection dominates the mixing behavior of the system. Hence, a better prediction of the dispersion coefficient, which is being calculated from the turbulent kinetic energy and kinetic energy dissipation rates, would be useful and would lead to better predictions. It is well known that the $k-\varepsilon$ model does not have the capability of predicting the turbulence quantities accurately and therefore, advanced modeling approaches to simulate the flow field is necessary.

B. Research Objectives

The objective of this work is to compare and evaluate the effect of turbulence model used to solve the CFD flow field on the predictions obtained using the CFD-based compartmental model for single phase stirred tank reactors. Large Eddy Simulation (LES) offers a viable alternative to the Direct Numerical Simulations (DNS) in order to resolve various length scales associated with turbulence. LES can resolve the large scale structures but does not solve for the sub-grid scales directly. To model the sub-grid length scales, sub-grid scale (SGS) models are used. Large eddies are more dependent on the geometry and boundary condition of a flow while small eddies tend to be more isotropic and less geometry dependent, which is the rationale behind using the LES

model to describe turbulent flows⁵. Though computationally lot more expensive than the RANS based $k-\varepsilon$ model, the LES model will be used in the present work to obtain the time-averaged flow field and to estimate the kinetic energy and dissipation rates of turbulence, because of its accuracy to provide the turbulence parameters. These quantities will be used to calculate the turbulent diffusivities in the compartmental modeling approach.

C. Ongoing Work

The flow field in the tank is solved in FLUENT 6.2 framework using the LES model. The Sliding Mesh model is used to model the impeller rotation. As a first step, simulation is being carried out for a tank of diameter 0.2m equipped with a Rushton turbine rotating at 150 RPM ($Re_{imp} \sim 12,000$). Experimental data for mean velocity and turbulent kinetic energy profiles obtained using CARPT⁶ will be compared with those obtained with the RANS based standard $k-\varepsilon$ model and the LES model. Similar comparison of mean and turbulent quantities will also be done with LDA data available in the literature⁷. The time-averaged LES results will then be used to provide input to the compartmental model in terms of mean flow and turbulence parameters. The consecutive-competitive reaction scheme studied by Paul and Treybal (1972)⁸ will be used to evaluate the effect of the turbulence model used on the performance predictions obtained using the compartmental approach.

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