



## Large Eddy Simulation of Stirred Tank Flows

Somnath Roy  
Ph.D. Candidate

Faculty Advisor: Sumanta Acharya

### ABSTRACT

Impeller stirred tanks (STR) are commonly used in the chemical processing industries (CPI) for a variety of mixing and blending technologies. In the present research, a numerical study of flow and mixing inside turbulently agitated tanks were carried out. An efficient solution algorithm was developed to solve turbulent flow inside stirred tanks where the boundary conditions for moving impeller geometries were prescribed using an immersed boundary method (IBM) and a large-eddy simulation (LES) was used to model effect of unresolved small scales of turbulent flow. Satisfactory agreements with experimental results were obtained. Flow features inside a turbulent stirred tank were explored in order to identify low frequency high amplitude macroinstability (MI) oscillations and changes in the flow field due to MI oscillations were visualized. An active perturbation in impeller speed was introduced which promoted the spreading of impeller jet and enhanced the level of turbulent fluctuations.

### INTRODUCTION

Many commonly used plastic and polymers are derived from hydrocarbon processing techniques in the chemical industry. Due to high viscosities, diffusion time scales are large compared with reaction and polymerization kinetics. So, an efficient mechanical mixing process is extremely important for better production rate. The mixing technologies are estimated to produce several hundred billion dollars of polymer-based products annually. Improvements in existing technologies can therefore potentially translate to several billion dollars in annual cost savings. According to Tatterson et al. (1991), half of the \$750 billion per year output of the U. S. chemical industry is circulated through STRs, and nearly \$1-20 billion per year is potentially lost due to inefficient design of the mixers. Better design of STRs requires a detailed understanding of the associated flow behavior. In this work a numerical study has been carried out to explore the features of STR flows. Changes in the circulation pattern and large scale vortical structures during an MI cycle are observed.

Experiments have been carried out for last 5-6 decades with a goal of achieving better mixing performance. For a turbulent flow in a stirred baffled tank at

high Reynolds number, a common strategy for mixing augmentation is by increasing rate of stirring, i.e., the impeller speed. However, this approach may not be a cost effective one from the energy requirement point of view. Hence, other ways of enhancement of mixing are investigated. For laminar STRs, perturbation in impeller rotational speeds are reported to be a successful way of mixing enhancement by breaking unmixed segregated zones and introducing chaos (Lamberto et al., 2001). The similar idea is exploited for a turbulent STR flow where fluctuation on impeller rotational speed increased the levels of turbulence promoting a better mixedness inside the tank.

### NUMERICAL MODELING

The numerical simulations required accurate modeling of the turbulent flow in the tank over a range of operating conditions (e.g. impeller speed), and in addition, required a computationally efficient solution strategy that can represent moving rigid geometric parts (impellers) in the tank. A methodology is proposed that combines the advantages of the immersed boundary method (IBM) to represent moving rigid geometries with the efficiency of multi-block structured curvilinear meshes for the representation of overall complex domains. This curvilinear-IBM methodology is further combined with the curvilinear coordinate implementation of large eddy simulation (LES) technique to address the issue of modeling unsteady turbulent flows in the STR. The combined IBM-LES methodology is used with a multi-block parallel compressible flow solver CHEM3D. An excellent agreement with experimental observations (Schafer et al., 1997) is obtained for both phase averaged velocity and turbulent kinetic energy (Figure 1) (Tyagi et al., 2003).

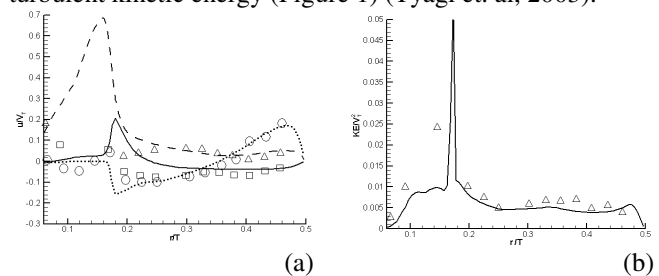


Fig. 1 Comparison of the computed (lines) averaged velocity components (a) and turbulent kinetic energy (b) along the radial direction with the experimental measurements (symbols) (Schafer et al. 1998) at an axial

location of  $z/T = 0.330$ . Axial (Dotted line,  $\circ$ ), Azimuthal (Dashed line,  $\Delta$ ) and Radial (Solid line,  $\square$ ) velocity components.

## BEHAVIOR OF FLOW AND TURBULENCE

From the time averaged and instantaneous flow fields, the trailing edge vortices formed due to the interaction of the fluid streams from the side and top edges of a blade (Schafer et al, 1997) are identified and an enhanced level of turbulent kinetic energy is observed in the vicinity of trailing edge vortices. Time signal for axial velocity is analyzed and low frequency high amplitude oscillations are identified from FFT as well as wavelet analysis. Flow behavior during an entire cycle of MI oscillation is studied. It is observed that the jet stream coming out of a particular impeller blade undergoes a transition from axial to radial resulting into changes in main circulation pattern (Figure 2) during the cycle of an MI oscillation. The trailing edge vortices are also observed to grow, shrink and break down during this cycle due to their interaction with impeller jet. A substantial amount of fluctuating kinetic energy is calculated to be associated with the MI oscillations (Roy et al., 2007).

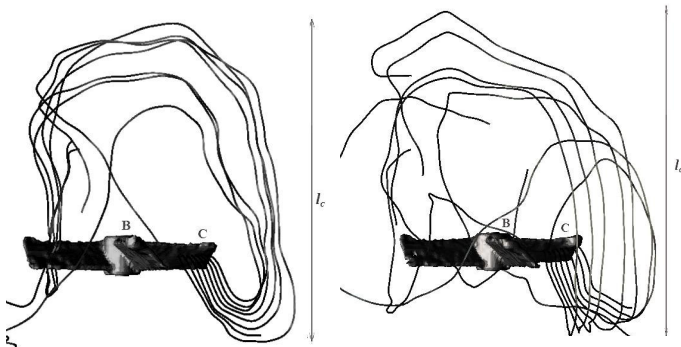


Fig. 2: Three-dimensional streamlines showing impeller jet stream coming out of impeller-blade C at different phases of an MI cycle.  $l_c$  is the length of the main circulation bubble.

## IMPELLER SPEED PERTURBATION

Two fixed impeller speed cases with 3 RPS and 4 RPS are compared with a variable impeller speed condition where the impeller speed is modulated as a square wave between 2 and 4 RPS with a time period of 15 sec. Mean flow field data is obtained by averaging phase averaged data of six different equispaced vertical. Mean velocity vectors from CFD results for three different cases are shown in Figure-3. Variable impeller-speed shows an enhancement in impeller jet width and shrinkage in the sizes of segregated zones. This enhancement in jet width is due to increase in the level of turbulence which results from the perturbation of the flow field. The higher turbulence levels with the step-perturbation are responsible for greater turbulent diffusion of the impeller-jet momentum, and this, in turn contributes to the greater spreading of the impeller-jet stream. Enhancement in turbulence contributes to rotational velocity of fluid elements and diffusion of vorticity, thus augments to the size and strength of trailing edge vortices. Spreading of the radial jet as well as the propagation of the trailing edge vortices improves mixing inside the tank by

shrinking poorly mixed segregated zones. Mixing at the molecular level is augmented by achieving higher levels of turbulent kinetic energy dissipation due to the step perturbation (Roy et al., 2008).

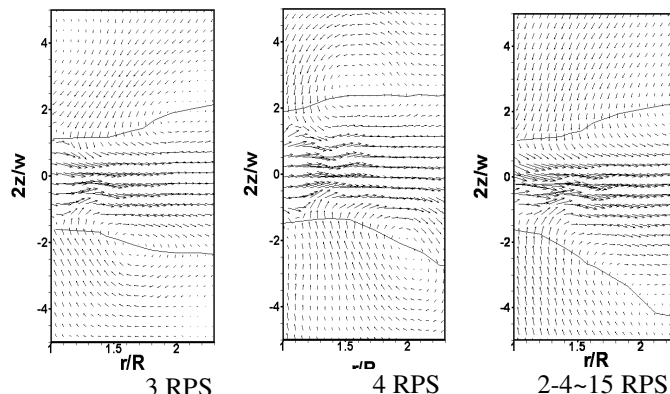


Fig. 3: Mean velocity vectors for different rotating speeds.

## ACKNOWLEDGMENTS

This work was supported by DOW Chemical Company and the Louisiana Board of Regents. Computational work has been done using super computing facilities of LSU and LONI.

## REFERENCES

1. Lamberto, D. J., Alvarez, M. M. and, Muzzio, F. J., (2001) Computational Analysis of Regular and Chaotic Mixing in a Stirred tank Reactor, *Chem. Engg. Sci.*, 56, 4887-4899.
2. Roy, S., and Acharya, S. (2007), Study of Flow and Turbulence inside a Turbulent Stirred Tank and Investigations on the Effect of Macroinstability on Trailing Edge Vortex Structures, *ASME-Intl Mech. Engg. Congress and Expo. (IMECE)*, 2007, Seattle.
3. Roy, S., Acharya, S., and Gao, D.(2008), Active Enhancement of Mixing through Impeller-speed Perturbation in a Stirred Tank, *ASME-Intl Mech. Engg. Congress and Expo. (IMECE)*, 2008, Boston.
4. Schafer, M., Yianneskis, M., Wachter, P. and Durst, F., 1998, Trailing Vortices around a  $45^\circ$  Pitched-blade Impeller, *AIChE J.*, 44, 1233-1246.
5. Tatterson, G. B., Brodkey, R., Calbrese, R. V., (1991). Move Mixing Technology into the 21<sup>st</sup> Century, *Chemical Engineering Progress*, 6, 45-48.
6. Tyagi, M., Roy, S., Harvey, A., and Acharya, S., (2007), Simulation of Laminar and Turbulent Flows in Impeller Stirred Tanks Using Immersed Boundary Method and Large Eddy Simulation with Multi-Block Curvilinear Geometry, *Chem. Engg. Sci.*, 62, 2007, 1351-1363.