

MIXED TANKS

I-20. CFD-Based Compartmental Mixing Model for Stirred Tank Reactors

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 because perfect mixing at all length scales can never be achieved and concentration gradients do exist within the reactor over finite distances and times. This has serious consequences for scale up when some of the reaction time scales are small compared to the time scale of mixing. Since chemical reactions are molecular events, the product distributions are affected by the concentration inhomogeneities within the reactor.

Mixing in a stirred tank reactor takes 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 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. Many phenomenological models^{1,2,3} have been developed so far to describe the effects of mixing on the product distribution and selectivity of industrial reactions but detailed flow descriptions have not been included in these models. An alternative is to use the commercial CFD codes available to solve the flow field as well as the concentration field in a stirred vessel. But, the CFD solutions are computationally intensive which might be of serious concern for the prediction of product distribution for multiple reactions or complex reaction schemes. An improved methodology and the objective of this work would be to bridge the existing gap between CFD and the phenomenological models, by developing a compartmental model that incorporates the flow field simulated by CFD. This can be accomplished by solving the flow field using CFD (FLUENT) and transferring the data to the compartmental framework to solve the conservation equations for the reacting components. The turbulent dispersion can be estimated from the kinetic energy and the dissipation rates obtained from the CFD solution of the flow. This enables to couple the flow field, turbulent mixing and kinetics.

B. Research Objectives

The objective of this work is to develop a compartmental model using detailed flow descriptions from Computational Fluid Dynamics and evaluate the effects of mixing on the performance of single phase stirred tank reactors.

C. Accomplishments

The compartmental approach to modeling a stirred tank reactor divides the reactor into small, interconnected and perfectly mixed compartments. The flows among the compartments mimic the overall flow pattern in the system. In the CFD-based approach, the complete CFD

solution of the flow and turbulence parameters provides the input for the compartmental mixing model. A scheme to calculate the number of compartments necessary for a given reactive system has been devised based on the time scales associated with the process, such that in each compartment Damkohler Number (Da) is less than one.

The flow field in the tank is solved in FLUENT 6.0 framework using the Multiple Reference Frame model and the standard k - ϵ model for turbulence. The model has been used to predict the reactor performance for a second order, competitive-consecutive reaction scheme⁴ and the effect of feed location and mixing for the homogeneous, multiple-reaction system is shown. Two feed lines are used, one near the top surface and the other below the impeller. The predicted and experimentally observed yields of the desired product at the end of the reaction are in reasonable agreement for both the feed locations (Figure 1). The conventional perfectly mixed model would predict a yield of 75.5% when there is no mixing limitation.

In order to check the sensitivity of the predictions on the exchange coefficient term, simulations are done by dropping the exchange terms completely (retaining only the mean flow) and also by increasing the exchange coefficients by a factor of 2. The results show that this term has significant influence when the feed is far from the impeller but convection dominates when the feed line is close to the impeller. As a result, the top-feeding turns out to be quite sensitive to the exchange term, while the bottom one is almost independent of the exchange term.

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D. References

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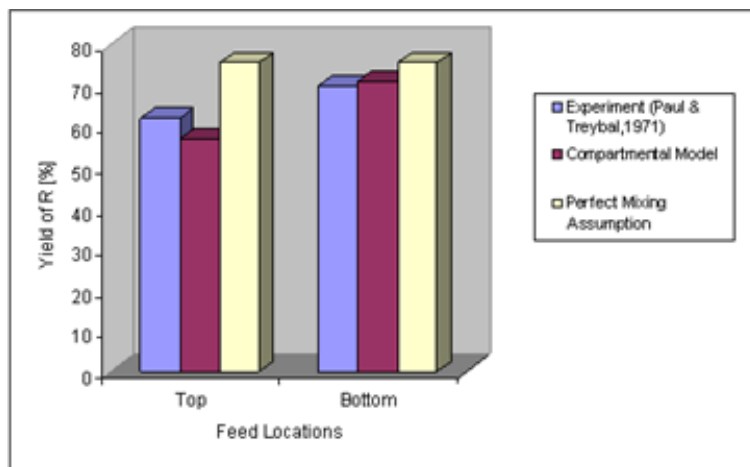


Figure 1: Comparison between measured and predicted yield of R at the end of the reaction for the two feed locations

