346c CFD-Based Compartmental Mixing Model for Single Phase Stirred Tank Reactors

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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 to predict the performance in a stirred tank reactor. Many phenomenological models 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 6.0) and transferring the data to the compartmental framework to solve the conservation equations for the reacting components. The turbulent dispersion is 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. The model has been used to predict the mixing time of an inert tracer and the predictions have been matched against existing correlation predictions. The predictions are in good agreement at all the impeller speeds studied. Simple kinetic schemes (first and second order reactions) have also been studied to show that the model can capture the essential features of macromixing in a stirred tank reactor. Some of these results for single phase systems will be presented in the final paper.