Predicting Residence Time Distribution with FLUENT

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In chemical reaction engineering, the concept of residence time distribution (RTD) is fundamental to reactor design. RTD is the exit age distribution of fluid molecules leaving a reactor. The residence time is the total time spent by the fluid molecules within the reactor. The RTD for process equipment is typically measured using stimulus-response tracer experiments to detect design flaws such as bypass, channeling, and dead zones, in addition to characterizing a reactor's mean residence time and standard deviation. This measurement has been done, historically, when a complete velocity distribution map for the fluid in the vessel is not available. Because CFD is capable of predicting the complete velocity distribution in a vessel, it provides an alternative, indeed, simpler means of determining the RTD. As part of a Department of Energy Chemical Industry of the Future project for modeling crystallization, Fluent is working with the University of Utah to predict RTD using FLUENT, with the results being compared to experimental measurements.

On the experimental side, a 1.4 liter stirred tank with complex multiple feed tube geometry has been used to measure the residence time distribution as a function of flow rate. The vessel is driven by a Rushton impeller and is either baffled or not baffled for the different cases studied. At both ideal and non-ideal conditions, experiments and simulations of the RTD have been performed.

For the CFD work, there are multiple approaches for predicting residence time distribution. In one approach, the tracer fluid is represented by a large number of discrete particles and Lagrangian particle tracking analysis is done with the discrete phase model (DPM). A histogram of time at the outlet is the residence time distribution. One drawback of this method, however, is that a large number of particles are required to ensure proper statistics. Alternatively, the tracer fluid can be treated as a continuum by solving a transport equation for the tracer species. It is the latter continuum approach that has been used for the crystallization project.

A single-species flow field was first obtained using the k-ε turbulence model. A passive tracer was then introduced with a step change in its concentration in the feed. The tracer was modeled using a user-defined scalar transport equation. The surface-area averaged tracer concentration was monitored as a function of time at the outlet. The results provided the exit age distribution of the tracer in the reactor, and therefore, represent the RTD. The FLUENT predictions were found to be in excellent agreement with the experiment over a broad range of flow rates and impeller RPM values, for both baffled and non-baffled tanks.

Since residence time distributions are routinely, and rather easily measured for process equipment, the RTD predictions allow a rather painless way to validate a complex flow simulation. In addition, with the aid of FLUENT simulations, process scale-up can be facilitated without expensive work on an intermediate scale in a pilot plant. The question of whether to construct a pilot plant or not depends on whether engineers are in control of all the major variables for the process. Using FLUENT, a small-scale reactor can be modeled to accurately predict its residence time distribution. Various potential large-scale reactor designs can also be modeled in the same manner, and the residence times predicted to verify that upon scale-up, the large-scale reactor controls the major variables for the process in the same way that the small-scale reactor does. ■
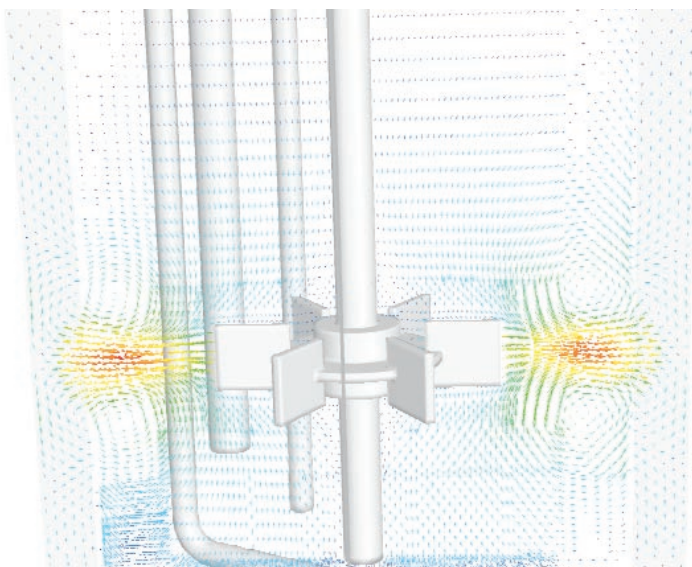
Fluid flow simulation of a 1.4 liter baffled stirred tank operating with a Rushton impeller
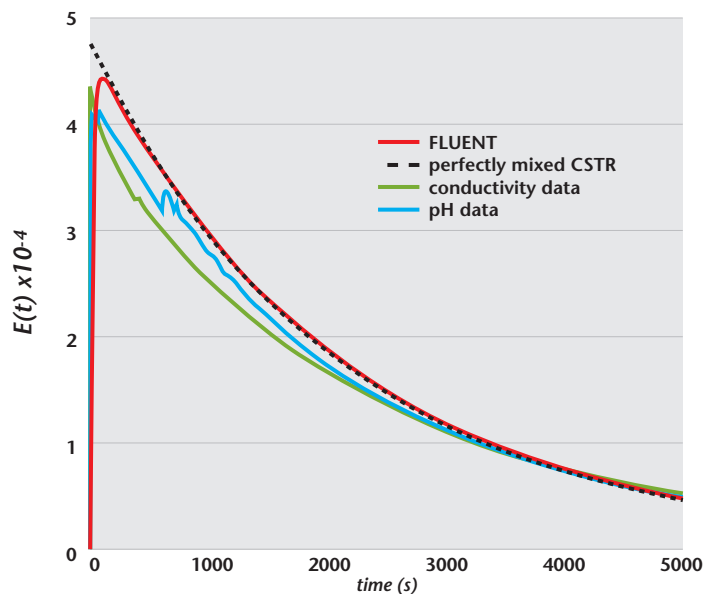
Comparison of experimental and calculated residence time distribution function, E(t), for a CSTR; operating conditions are 200 rpm, 40 ml/min