

Finding the Optimum Blend Time Calculation

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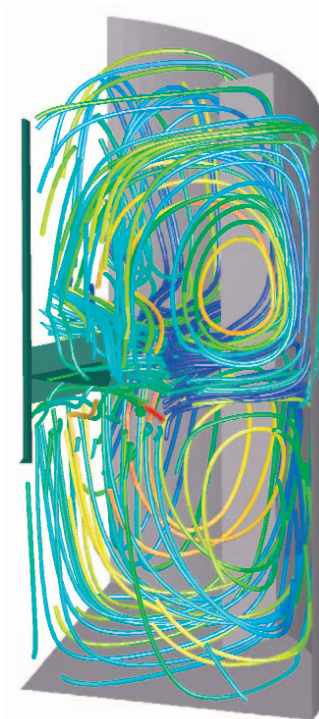
THE MIXING OF SINGLE AND MULTIPHASE FLUIDS in stirred tank reactors is a common operation in many industries, such as chemicals, water treatment, pharmaceuticals, and petroleum. Understanding the fluid flow in these tanks is critical for equipment design, scale-up, process control, and economic factors. CFD is now being used routinely to provide this information, enabling engineers to select the best agitator design to obtain the desired process performance. Blending time evaluation is one of the key objectives of such CFD studies, and there are currently several numerical approaches that can be used for this purpose [1]. The objective of a project recently performed at Fluent France and Fluent India was to compare these different approaches in terms of quantitative results and CPU time.

A cylindrical, flat bottom, stirred tank with 4 baffles and a non-standard, Rushton-type impeller with 4 radial blades was used for the simulations. Owing to the rotational symmetry of the geometry, a 90° sector of the tank was modeled.

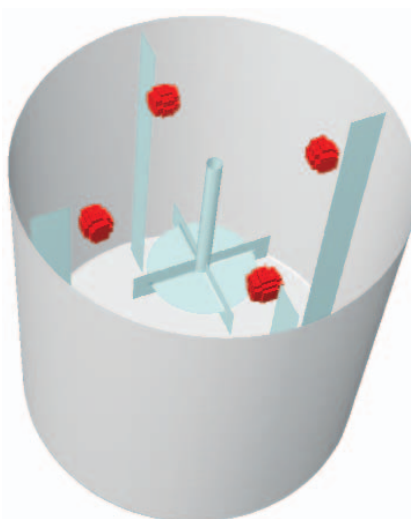
The different approaches studied made use of either the multiple reference frames (MRF) or sliding mesh (SM) model. For the MRF runs, a steady-state flow field was first computed and a transient calculation of a tracer species was performed using the "frozen" flow field. The first such blending calculation was done using the default settings, including the use of relative velocities. A second blending calculation was performed with absolute velocities. For this case, the paddles on the impeller were changed to interior zones, since this setting is more appropriate for walls moving normal to the fluid when absolute velocities are used. The walls exerting shear on the fluid (the impeller disk) were not changed. For the transient sliding mesh calculations, the flow field and tracking of the tracer species were computed simultaneously. Two solver options were used: the iterative time advancement (ITA) scheme and the non-iterative time advancement (NITA) scheme, which was introduced in FLUENT 6.2. The sliding mesh results are the most rigorous, so they served as a standard for comparison with the other methods. A correlation was also used to compare the results.

A steady state, MRF solution for the flow was first obtained. On this frozen flow field solution, the transient species calculation was performed after initializing a volume of tracer in the upper part of the vessel. The MRF flow field was also used as the starting point for the unsteady sliding mesh calculation. Before introducing the species, the sliding mesh calculation was done for a few cycles until periodic behavior was obtained. At this point, the species was introduced in the same location used for the MRF calculations, and the transient calculation of the flow field and species was performed.

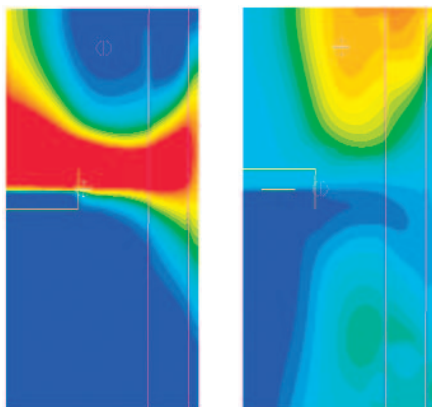
Results were analyzed globally in terms of the blending time, t_{99} , or time required to achieve 99% uniformity in the tank. A published correlation for t_{99} for a six-bladed Rushton turbine was used for comparison [2]. The blend time predicted by the Rushton correlation was found to be longer than that predicted by the CFD methods, a result that is due to the fact that the paddles on the impeller used have more surface area than a standard Rushton. In addition, the tracer species introduced from one location in the 90° model was equivalent to it being introduced from four locations in a 360° vessel.



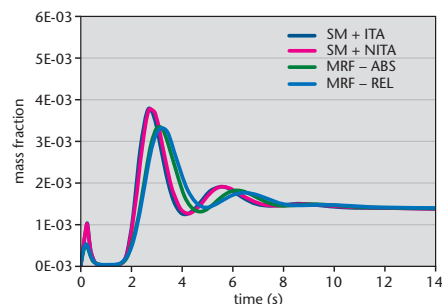
Pathlines illustrate the two circulation loops in the vessel



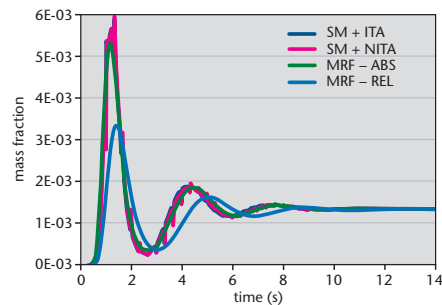
The tracer species initial locations at $t=0$



The tracer distribution after 1.5 (left) and 3.0 (right) seconds for the MRF simulation



Mass fraction of the tracer species computed by the SM and MRF methods, recorded at points near the top of the vessel (top) and near the impeller (bottom)



The correlation assumes that the species is introduced from one location, usually at the surface of the liquid. Comparison of the CFD methods revealed that the MRF model predicted longer mixing times than the sliding mesh model. The two MRF approaches predicted similar blend times, as did the two SM approaches.

	Correlation for 6-bladed Rushton turbine	MRF with relative velocities (default)	MRF with absolute velocities	Sliding Mesh with ITA scheme	Sliding Mesh with NITA scheme
Blending time(s): t_{99}	19.0 (+/- 6)	15.8 (+/- 4)	15.3 (+/- 4)	14.8 (+/- 3)	14.9 (+/- 3)

The various approaches were also compared by monitoring the CPU time required to reach t_{99} . It was found that the sliding mesh model using the new NITA scheme takes about 4 times less CPU time than the sliding mesh model using the ITA scheme. The steady-state MRF solutions are much quicker, requiring about 2.5 times less CPU time than the sliding mesh model with the NITA scheme.

The results were also analyzed locally by monitoring the mass fraction of the tracer species at several sensor locations. Two locations in particular are of interest: near the tip of the blade and near the top of the tank. Near the impeller, the sliding mesh case picked up the blade passing frequency, and in addition, a low frequency oscillation of greater amplitude that was also observed for the MRF approaches. This low frequency oscillation was also picked up at the top of the tank by the sliding mesh and MRF approaches, although the blade passing frequency was not (for the former). The low frequency oscillation is indicative of a macroscopic exchange of the tracer material between the upper and lower regions of the vessel. This type of result is not uncommon when a radial impeller is used and distinct circulation patterns develop above and below the impeller.

Overall, the MRF model is an economic approach for delivering sufficient blending time information. If, however, an accurate representation of the transient dispersion of a tracer is required – for reacting flows, for example – the sliding mesh approach is necessary, and the NITA scheme in FLUENT now makes sliding mesh calculations much more affordable. ■

References:

- 1 Marshall, E.M. and Bakker, A.: Computational Fluid Mixing. In: The Handbook of Industrial Mixing, Ch. 5. Paul, E., Atiemo-Obeng, V. and Kresta, S., Editors, John Wiley, 2004.
- 2 Fasano, J.B., Bakker, A. and Penney, W.R.: Advanced Impeller Geometry Boosts Liquid Agitation. Chemical Engineering, August 1994.



Iso-surfaces of tracer mass fraction show the polarized species distribution in the vessel, even after the liquids are well mixed