A New Tool for CFD Simulation of Laminar Flow in Mixers

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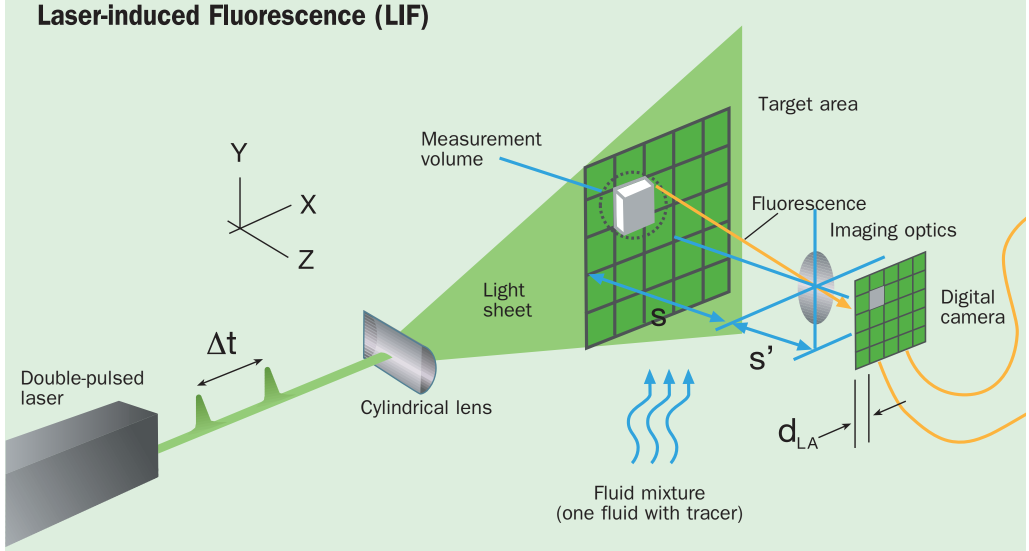
Standard CFD solvers are suitable for the calculation of velocity and pressure fields. In static mixing, however, concentration distributions are essential for the prediction of homogeneity and therefore, simulations of this process are much more challenging. In collaboration with Sulzer Chemtech, Sulzer Innotec developed a numerical method that allows predicting the effect of molecular diffusion—which is essential for laminar-flow mixing—while avoiding artificial numerical diffusion. Measurements of homogeneity and diffusion coefficients with the laser-induced fluorescence method (LIF) were performed at Sulzer Chemtech in order to validate the calculations. This effort led to an understanding of the processes in static mixers that would not have been possible with other methods.

Generally, mixing has the goal to minimize concentration or temperature deviations in a liquid in order to secure desired product quality. In fluid dynamics, turbulent flow is characterized by a mean flow with superimposed intense transient fluctuations of the velocity. These fluctuations strongly increase the momentum exchange and consequently support the mixing processes. In a laminar flow regime, on the other hand, the fluid moves along parallel streamlines without any transversal movement, with molecular diffusion being the main transport mechanism that drives the equalization of concentration. In order to generate convective motion in the direction normal to the main flow, bars and walls are used as elements in static mixers. In such devices, mixing is achieved by repeated division, transposition, and recombination of liquid flowing around mixing elements. The components to be mixed are spread into many fine layers. More mixing elements lead to finer layers and the finer the layers, the better becomes the homogeneity of the mixture (Fig. 1).

Improving Standard CFD

The flow field in static mixers for highly viscous laminar flow can be calculated with standard CFD

Laser-induced Fluorescence (LIF)

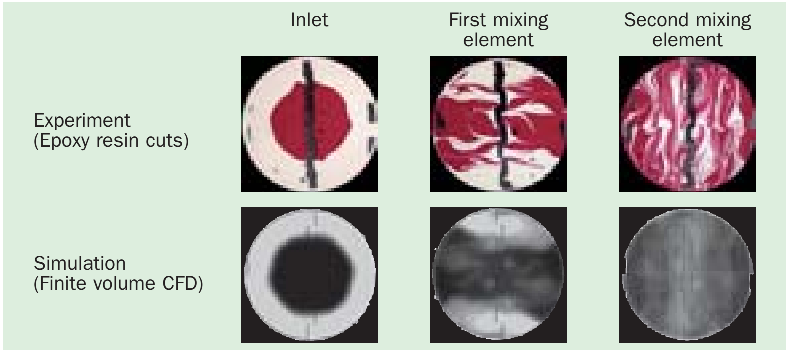


A LIF measurement does not disturb the flow. The measurement area, however, has to be optically accessible from 2 directions.

Homogeneity measurements are essential for characterizing the performance of static mixers. Common methods for the determination of the mixing quality include conductivity measurements across the diameter or freezing the mixture along the mixer length by using epoxy resins. The conductivity method aims to produce a measurable value for the homogeneity, e.g., the coefficient of variation (CoV), which describes the ratio of standard deviation and mean value of a quantity. The epoxy-resin method gives good visual understanding of the mixing behavior, however does not necessarily produce quantitative results.

LIF is a nonintrusive measurement technology that is related to other light-sheet based laser methods like particle image velocimetry (PIV). It uses a fluorescent tracer in one of the two components to be mixed. A sheet of laser light illuminates a plane in the outlet section of the mixer and initiates the fluorescence of the tracer according to its concentration in the mixture, whereas the unseeded fluid does not react. A digital camera captures the distribution of the light intensity. The image is processed electronically to determine a concentration distribution at the measurement cross section of the static mixer. It comprises data of the whole cross section and enables direct measurement of the CoV and therefore combines the advantages of both traditional methods mentioned above.

1 In static mixers, like this Sulzer SMX™, fixed internals cause the mixing of fluid streams. Sulzer Innotec has developed a method to simulate the process of laminar mixing with high accuracy for Sulzer Chemtech.



2 Numerical diffusion is the mixing of scalar quantities caused by the influence of the calculation grid. The scalar values are passed from node to node in the calculation. If the direction of flow differs from the main direction of the grid, numerical diffusion occurs.

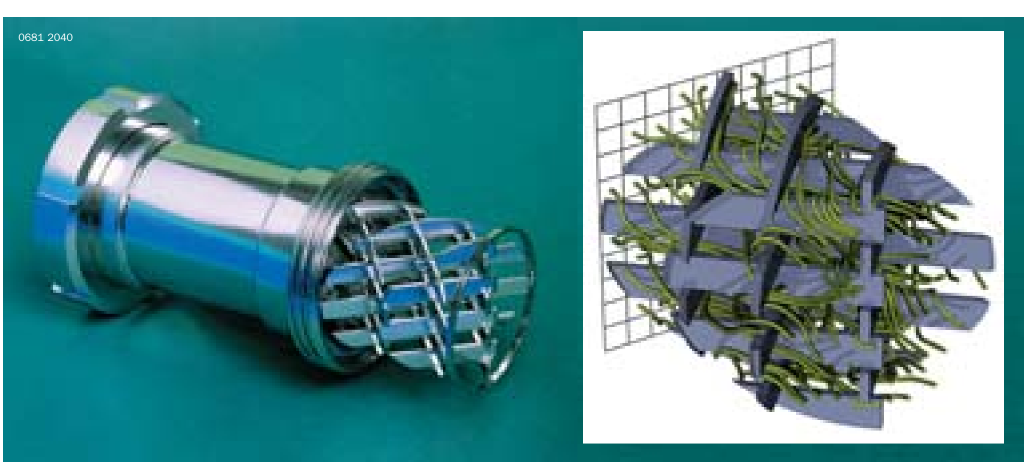
solvers. If the two components to be mixed have similar rheological properties and the resolution of the calculation grid is fine, the solvers can predict the velocity and pressure fields with high accuracy. It is also possible to handle complex fluids with temperature and shear-rate dependent viscosities without additional effort. However, concentration distributions within static mixers for laminar flow are much more difficult to predict than velocity fields. Since molecular diffusion is a very slow process, sharp concentration gradients remain present in the laminar flow through static mixers. Resolving these gradients exactly by standard cell-based simulation programs is hardly possible today. Simulations using standard CFD schemes for the prediction of concentration distributions within mixers intrinsically overestimate the mixing efficiency due to numerical diffusion, an effect of insufficient grid resolution. The comparison of a simulation using a finite-volume based CFD solver with epoxy-resin cuts taken at the inlet, after 1, and after 2 mixing elements of a Sulzer SMX™ mixer clearly shows this effect (Fig. 2). With current standard CFD codes, it is not possible to accurately predict concentration distributions and to characterize mixing quality without ambiguities.

Tailor-made Code

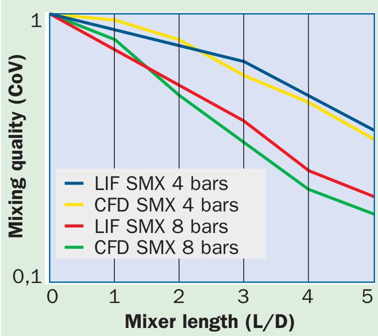
Without molecular diffusion, the concentration would be constant along each streamline. The concentration distribution in the outlet plane could then be calculated by following streamlines through the mixer (Fig. 3). This procedure allows to predict the development of concentration distributions in static mixers by suppressing all effects of numerical diffusion. However, it also suppresses the natural molecular diffusion.

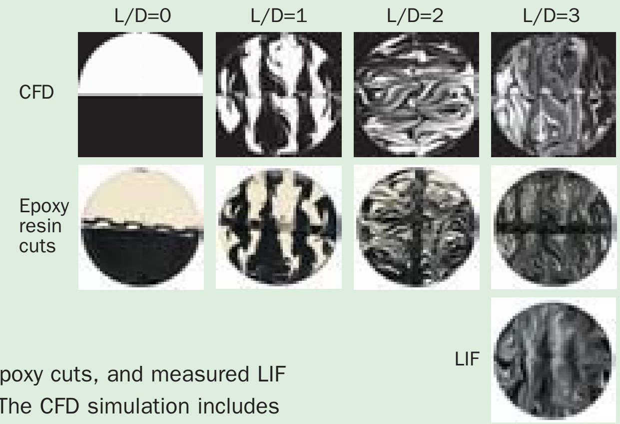
Steep concentration gradients exist at the interfaces between the thin fluid sheets of constant concentration in a static mixer under laminar flow regime. Steep gradients drive molecular diffusion and this effect cannot be neglected in laminar flow mixing. In order to include the effect of molecular diffusion in the concentration distribution analysis, the developers at Sulzer Innotec evaluated several numerical approaches. In the model that was finally applied, the effect of the Brownian motions is approximated by varying the end points of the streamlines, using a statistical distribution around the point obtained with streamline integration without random walk effect. The amount of diffusion depends on the residence time of the fluid in the mixer. Based on measurements, the correct diffusion coefficient for the laminar flow mix-

3 By assigning the same concentration value to the streamline end points in the outlet plane as to their start points in the inlet plane, it is possible to calculate the distribution of concentration without numerical diffusion.



ing was determined and the numerical scheme has been calibrated with these values. The newly developed trajectory scheme for the evaluation of concentration distributions in static mixers with natural molecular diffusion has been implemented in an in-house code at Sulzer, which has since been used successfully for the prediction of mixing properties of different mixer geometries.





5 Comparison of CFD simulations, epoxy cuts, and measured LIF homogeneity for Sulzer SMX mixers. The CFD simulation includes the tailor-made module for the calculation of molecular diffusion.

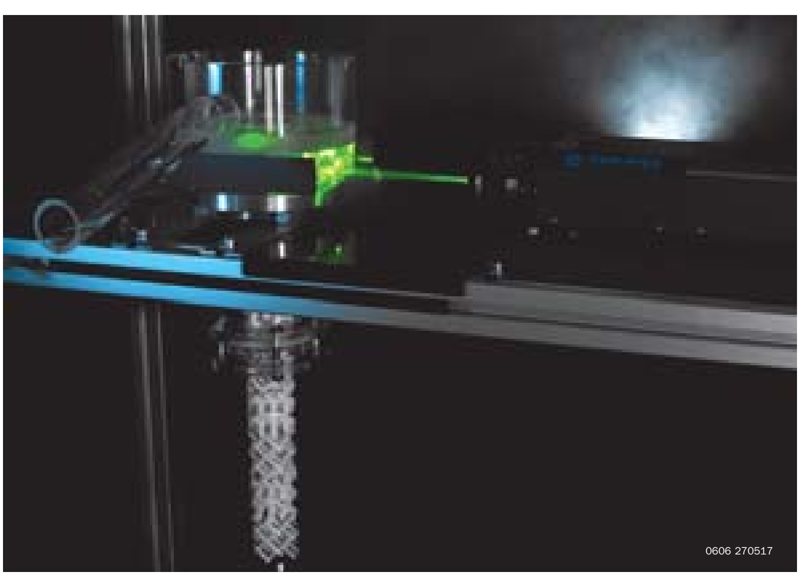
Calculations Validated

The calculations have been validated through measurements using laser-induced fluorescence (LIF) (Fig. 4 and box) and through conventional epoxy cuts. The comparison between simulated and LIF-measured homogeneity shows good agreement in the measurement planes. Epoxy cuts are produced by pressing two differently colored epoxy resins through the mixer and solidifying the mixture held therein. The mixer is then cut into slices. Epoxy cuts do not deliver values for the fluid concentration. The comparison with CFD is therefore performed on a qualitative basis, and again shows excellent agreement with measurements (Fig. 5).

Flow Analysis Now Possible

Diffusion coefficients can be derived through LIF measurements. Sulzer Chemtech is therefore able to validate the CFD code for homogeneity simulations. Once the new CFD tool is validated for essential test cases, it can be applied to other load cases with sufficient reliability. This tool is able to analyze the laminar flow in mixers even at locations and conditions where LIF measurements are not possible. ◄

4 The LIF measurements on Sulzer Chemtech's mixer test facility in Switzerland verified the calculation results.



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