# Development of algorithms for mixing prediction


**Reliable prediction tools and accurate measurement techniques are essential elements for an innovative and lean product development cycle. For mixing applications, commercially available simulation tools fail to provide the required speed and accuracy. Therefore, Sulzer engineers developed an in-house tool for reliable prediction of mixing quality.**

Mixing occurs constantly all around us – on the earth where we live, within our atmosphere and oceans and even in our bodies. Reducing inhomogeneity by mixing different materials is also an essential part of many processes in the chemical, pharmaceutical, construction, food or general industries. Novel mixing solutions are required for the efficient use of two-component or multicomponent materials. Developing techniques and mechanisms to induce, control and optimize mixing is an important part of the expertise at Sulzer Applicator Systems.

The emergence of new materials in many markets and industries over the last few decades requires novel production or application techniques. Therefore, during the same time period, the application of multicomponent filling, sealing and bonding solutions has grown significantly. Today, numerous customers use the highly efficient mixing and dispensing solutions offered by Sulzer to mix and apply various sealants and adhesives. The products cover a wide range of applications from healthcare to construction, from do-it-yourself to large-scale industrial manufacturing.

Due to the ever-expanding use of two-component materials, the quest for more-effective and more-reliable applicator systems continues. Along the process chain, the mixing system remains a crucial element in the successful use of multicomponent materials. In high-end applications, the mixing performance and quality can influence product reliability and, therefore, has to be extremely precise.

## Laminar mixing processes

Sulzer offers various static mixer designs for laminar mixing processes (Fig. 1 and 2). These miniature mixers are cost-efficient and easy to use. However, they might depict suboptimal performance when components have different material properties, such as viscosity. The same applies to cases where there is a lot more of one component in use than of the other. For such demanding applications, dynamic mixers (Fig. 3) are often the preferred choice. In these mixers, fast rotating blades induce high shear forces and enable precise mixing and dispensing. The moving parts of these mixers rotate up to 1'500 rpm. Within the mixer, the axial velocity of the material can be as low as a few cm/s. Sulzer offers various dynamic mixers to overcome the most challenging mixing problems encountered in different areas of life – from a car repair shop to a dentist's office.

Fig. 1 Static mixer for construction purposes.

Fig. 2 Static mixer for dental applications.

Fig. 3 Dynamic mixer used in dental applications.

## Product optimization using simulation techniques

When Sulzer customers require new mixing solutions adapted to their specific requirements, the development engineers have to keep the development cycles as short as possible. At Sulzer, computational fluid dynamics (CFD) is one of the commonly used tools. CFD is a numerical simulation of fluid state and motion. It has advanced to account for increasingly complex phenomena such as multiphase interaction, phase conversion, fluid-solid interaction, etc. Thanks to the increase of computational resources and advancements in numerical techniques, development engineers increasingly use simulations for design and optimization in various fields.

Using state-of-the-art cluster computers, the CFD calculation time for a static mixer takes 48 – 72 hours. The capacity of a cluster computer equals the capacity of 150 – 200 personal computers. This gives us an idea how complex the calculations are and how many computational resources are needed for such applications. Despite the advances in calculation possible by using commercial software, the laminar mixing process cannot be predicted accurately. The process of laminar mixing depends on the generation, division and stretching layers of material inside the mixer (Fig. 4). These layers are increasingly refined and mixed over the mixing length.

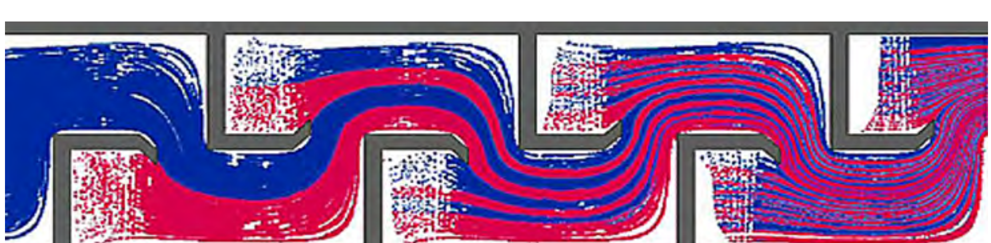


Fig. 4 Schematics of layer generation and mixing within laminar static mixers.

It is quite difficult to represent these layers with conventional CFD grids. The prognosis of a mixing pattern is challenging for any CFD tool because of excessive numerical diffusion. This numerical diffusion results in an overestimation of the mixing quality and a blurred appearance of the mixing patterns (Fig. 6). This stands in contrast to the measurement where the distinct borders between the two materials are still recognizable (Fig. 5).

## Diffusion-free particle tracking

Sulzer engineers aimed to overcome these limitations in the past years to speed up the development process for mixers and obtain accurate mixing performance.

A well-known approach to overcoming the problem is to assess the mixing pattern and concentration field by using discrete particles colored by concentration. The red and blue colors in Fig. 8 represent different concentrations. The particles are used to calculate how materials with different concentrations move through the mixer. This allows high-resolution mapping in static mixers. This method and implementation has been already developed and used in the past for static mixers. Fig. 5 shows a mixing pattern obtained in measurements. In Fig. 6, you see the calculated mixing result of commercial CFD, and in Fig. 7, the result of the in-house tool.

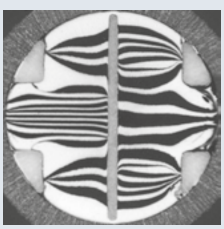


Fig. 5
Observed mixing pattern within the static mixer.

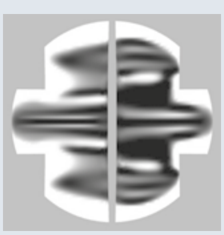


Fig. 6
Blurred fields are the result of numerical diffusion in classical CFD methods.

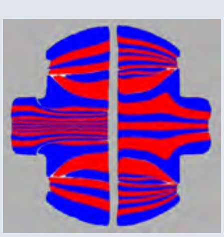


Fig. 7
Simulated mixing pattern with the in-house tool.

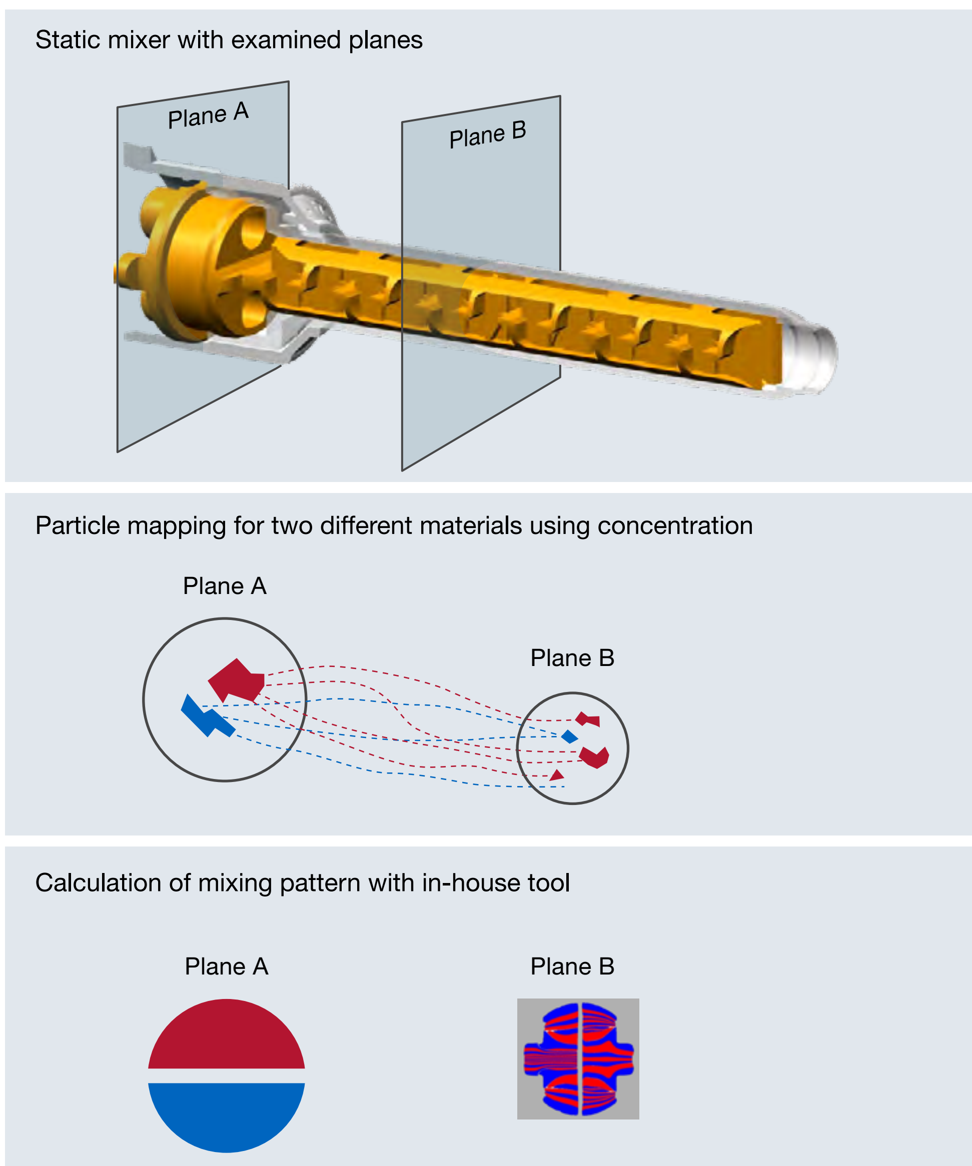



Fig. 8 Prediction of mixing pattern of a static mixer with the Sulzer in-house tool.

## Particle tracking for dynamic mixers

Unlike in static mixing tips, in dynamic mixing tips, the flow field within the mixer varies over time. Therefore, the previous approach of offline tracking of a limited number of particles based on steady-state flow field is no longer applicable. In addition to an unsteady flow field, the multiscale nature of the problem poses further practical challenges. The moving part of these mixers rotates with up to 1'500 rpm. The axial velocity of the flow within these mixers, on the other hand, can be as low as a few centimeters per second. Covering the simulation time required for filling the mixers and capturing the rotation with sufficient accuracy proves to be a challenge.

Video 1
Click here to see a video of a simulation calculated with conventional CFD.

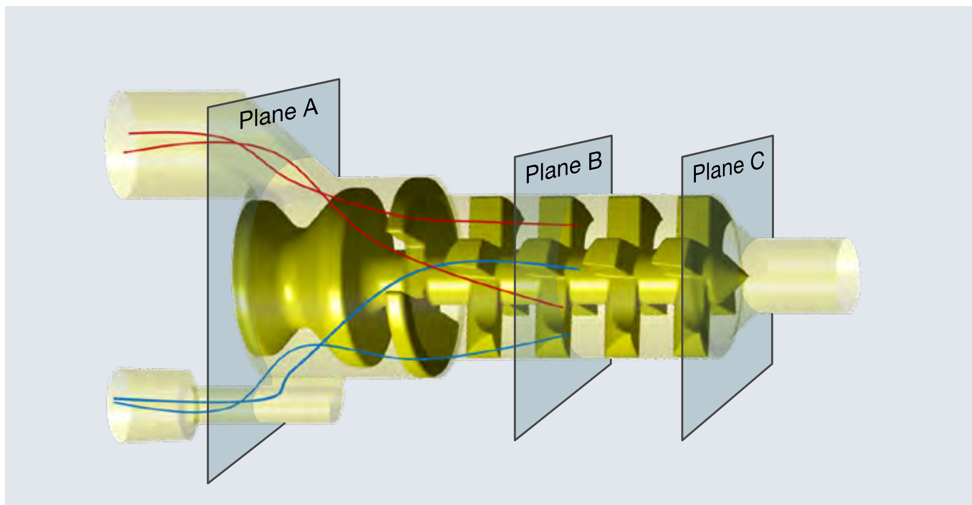



Fig. 9 Dynamic mixer – blue and red lines symbolize the particle tracking.

Video 2
Click here to see a video showing real mixing results.

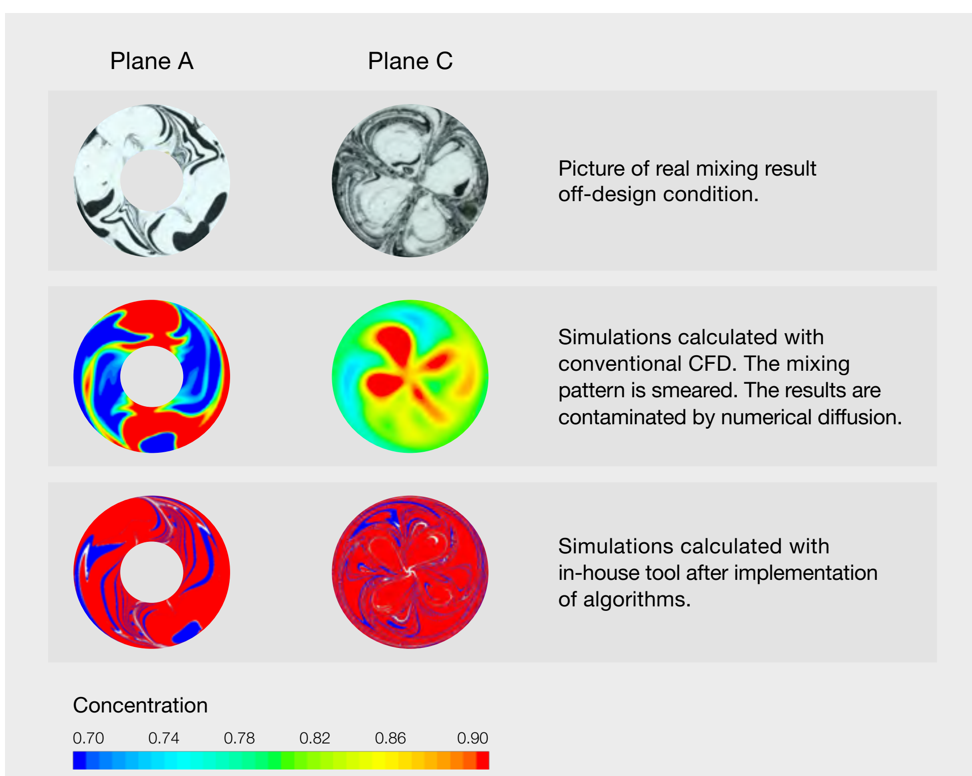
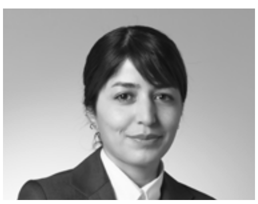



Fig. 10 Comparison of real mixing results with conventional CFD and in-house tool for dynamic mixers.

## Methodology and algorithms

In earlier attempts, the Sulzer engineers tried to couple the particle tracking online with the flow field in the dynamic mixer. The approach, which is theoretically sound, fails due to the limitations of computational resources. Such simulations require computational time and memory beyond the practical limits. Therefore, Sulzer engineers examined further alternative approaches for the offline coupling of particles similar to those used in static mixers. However, the challenge is the unsteady nature of the flow in dynamic mixers. This limitation has been overcome using the periodic nature of the flow.

This allows the engineers to construct the solution for any length of time using the solution obtained from one rotation. The periodic essence of the solution enables the engineers to perform offline particle tracking for dynamic mixers with a rather limited number of particles. For the calculation, the particles are released at plane B and tracked backward to the inlet (plane A) to obtain the concentration.



Dr. Samira Jafari,
Haag, Switzerland

## Verification and validation

Prior to their use in product development, all in-house numerical tools are carefully verified and validated by the Sulzer engineers. Both measurement and computational setups should be carefully constructed in order to achieve the ultimate reliable comparison. The predicted mixing quality is compared to optically assessed mixing patterns in measurements. The blue and red lines in Fig. 8 symbolize the particle tracking inside the dynamic mixer. A mixing simulation inside a dynamic mixer – obtained with a conventional CFD program – is shown in video 1. The validation study confirms the applicability and accuracy of the method (Fig. 9 and video 2).

Joachim Schoeck,
Haag, Switzerland

## Fast and lean mixer development

After numerous tests and measurements, the Sulzer engineers were able to develop a reliable in-house tool that they trust. The newly developed and implemented algorithms enable the engineers to assess the mixing quality in dynamic mixers with increased accuracy. Furthermore, these calculations can be realized within the practical limits of available computational resources. The tool is used to accelerate the design and optimization cycle for new and existing products. It enables our engineers to realize innovative designs and solutions for the ever-expanding application of two-component materials in all aspects of our modern life.