

### PICTURES

*Single-phase microfluidics: continuous mixing of two liquids in a split-and-recombine micromixer: concentration profile (1) and pressure drop (2); exothermal reaction in a micro-shaped T-crossing: temperature distribution (3).*

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## COMPUTATIONAL FLUID DYNAMICS (CFD)

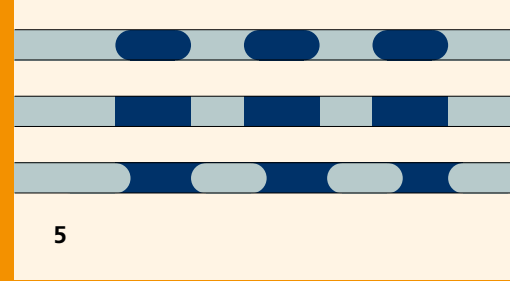
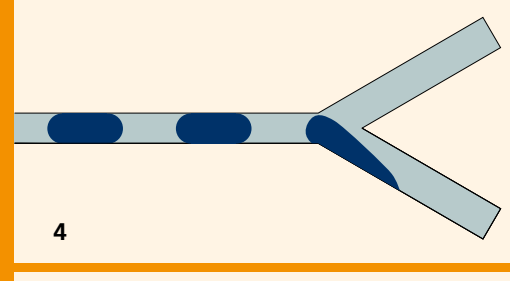
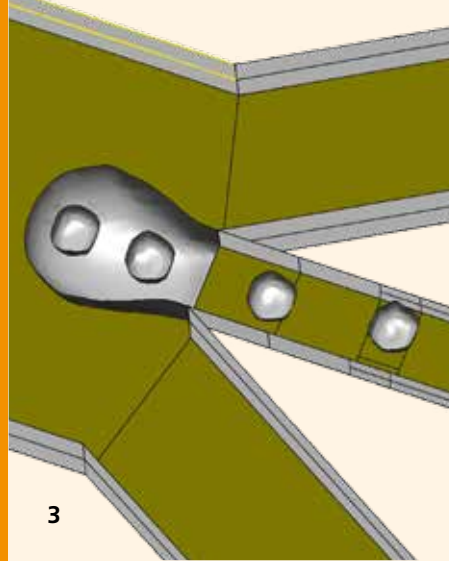
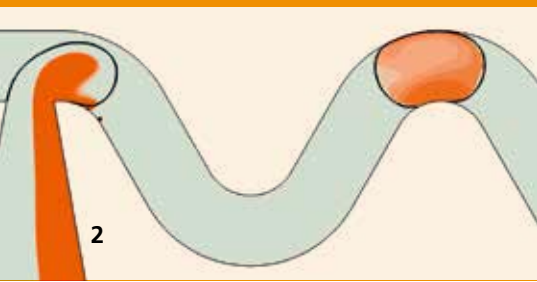
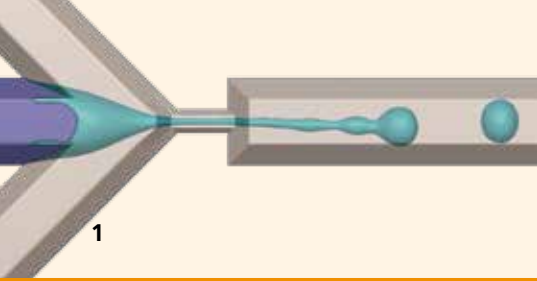
### DESIGN AND OPTIMIZATION OF CHEMICAL PLANTS AND PROCESSES

Numerical modeling using CFD is increasingly applied as a tool for the development of new chemical processes and plants in addition to or instead of extensive experimental testing. The approximate calculation of flow conditions and related parameters such as mass and heat transfer, mixing quality, residence time and pressure drop allows the prediction of performance and effects within chemical plants and processes before or during the process development.

For this reason, CFD modeling can help to reduce the expensive and time-consuming prototyping often needed for the design and optimization of new or already existing plants and processes, for example by performing systematic parameter studies.

Apart from calculating characteristic process data, modern CFD tools allow comprehensive visualization of flow and transport phenomena. Especially in complex geometries, where conventional experimental testing is restricted by spatial or temporary limits, CFD simulations provide information about almost all existing chemical or physical effects and conditions, without any restrictions in space or time.

The resulting improved understanding of the chemical and hydrodynamic phenomena enables faster and more reliable development and optimization of chemical plants and processes.



## CFD at the Fraunhofer ICT

Reliable and representative numerical calculations require comprehensive knowledge of numerical methods and CFD software as well as chemical and physical phenomena within plants and processes. CFD simulations are therefore performed by a team of experts in both numerical simulation and technical fields (e. g. chemistry, engineering, physics), depending on the process to be simulated.

In addition to modeling fluid dynamics, numerical calculations are performed concerning a variety of physical-chemical phenomena associated with fluid flows, e.g.:

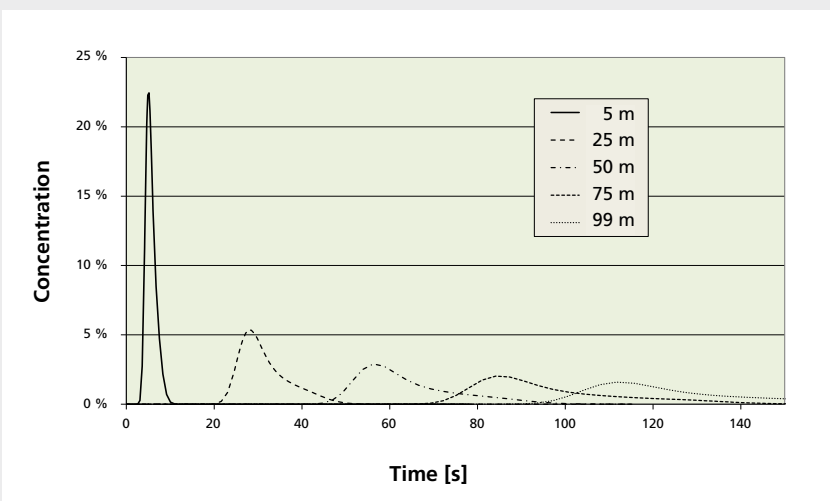
- Heat and mass transfer
- Mixing / residence time distribution
- Multiphase simulation (VOF)
- Turbulent flows
- Microfluidics considering microstructure-specific effects (e. g. surface tension and wetting phenomena)

## Our offer

Our services in the field of CFD calculations before or accompanying the design and development of chemical plants and processes include:

- Feasibility studies
- Virtual prototyping in addition to or accompanying experimental testing for shorter development cycles
- Systematic parameter studies for the optimization of chemical plants and processes
- Visualization of physical and chemical phenomena
- Determination of characteristic process parameters (including mixing quality, yield and residence time) and their relationship with process variables (e.g. geometry, flow rate, temperature, concentration) and material characteristics (e.g. viscosity, surface tension, heat transfer coefficient)
- Failure analysis
- Experimental evaluation

### Simulation of dispersion in turbulent tube flow ( $\varnothing$ 0.4 m): residence time.



## PICTURES

*Multi-phase simulation: 1 Droplet formation in a microreactor (flow focusing). 2 Advective mixing in a microreactor. 3 Formation of a multiple emulsion. 4 Separation of a two-phase mixture in microchannels with different wetting properties. 5 Wetting behavior in a microchannel depending on varied contact angle.*