Trajectory-based optimization of SMART reactors

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Abstract

For the design and operation of multiphase reactors, usually temporally and spatially averaged data is used, such as dispersion coefficients, residence time distributions or energy dissipation rates. With this assumption of a homogeneous mixed system, inhomogeneities, as they usually occur in multiphase reactors, are not captured. Nevertheless, these inhomogeneities are important from the point of view of a reacting species, such as a cell or a catalytic particle, as they are exposed to changing conditions in such inhomogeneities on their trajectory through the reactor. In cell culture, for example, each individual cell in the vicinity of a stirrer is exposed to a higher shear stress for a certain period of time that might influence the metabolism. New experimental methods such as 4D Particle Tracking Velocimetry or measurements with Lagrangian Sensor Particles as well as new numerical methods using Lagrangian Coherent Structure Analysis open new possibilities to track reactive species in multiphase reactors on their individual paths. These trajectory-based methods provide deep insights into reactor performance and enable new optimisation strategies. In the lecture, the new possibilities will be presented and discussed with regard to their use in SMART reactors for future process engineering.

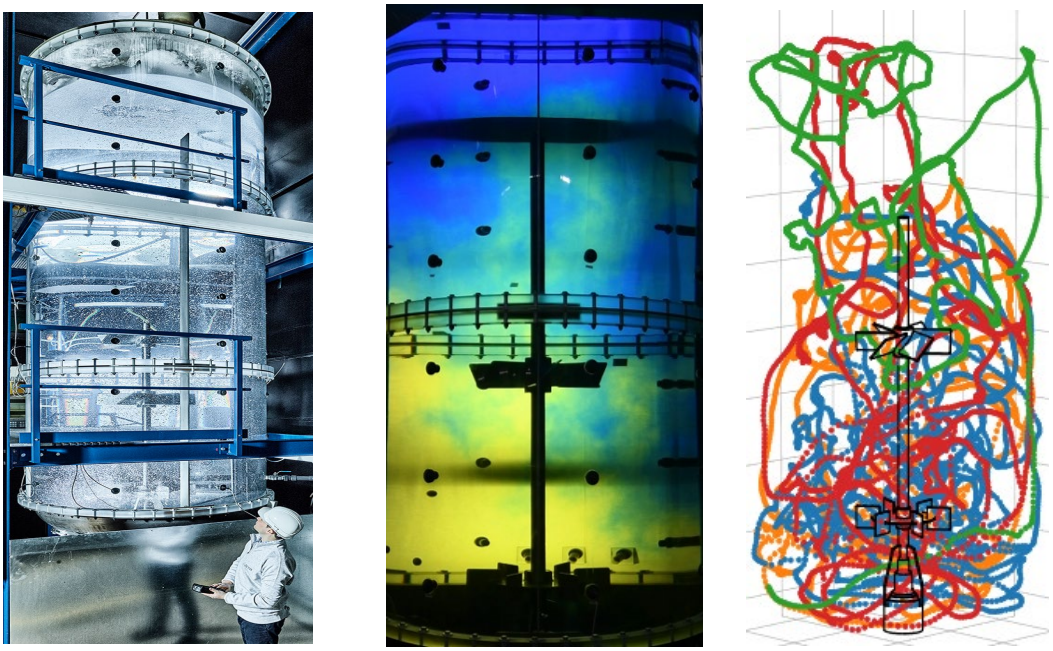

Figure 1: 15000 L acrylic glass stirred tank reactor (left) with visualization of mixing time distribution (middle) and calculated Lagrangian trajectories by means of LBM-LES simulations (right).