Using Lagrangian coherent structures to understand dynamics in multiphase flows with chemical reactions

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Reactive bubbly flows are essential for many chemical industrial applications, e.g., hydrogenation, oxidation and chlorination reactions in bubble column and loop reactors. The efficiency of these reactors is mostly described by the yield and selectivity of the products and side products, which can be measured and estimated globally by various methods [1]. However, to achieve more reliable estimations it has to be taken into account that yield and selectivity depend sensitively on the coupling of the fluidic and microscopic transport processes and the reaction kinetics [2].

To study the dependency between local hydrodynamics, mass transfer and a chemical reaction at a single gas bubble we use Taylor bubbles which are a helpful simplification. This enables us to obtain quasi steady conditions with well-defined and reproducible flow structures. It also allows us to adjust the hydrodynamics in the bubble wake by changing the hydraulic diameter of the capillary and accordingly the Reynolds number of the flow. Taylor bubbles are elongated gas bubbles in channels, where the gas volume is forced into a bullet shape by the channel geometry and the continuous liquid which wets the glass wall. The rising velocity of Taylor bubbles is independent of the bubble volume and can be predicted by the dimensionless Eötvös number $\mathrm{Eo}_D = (\rho_L - \rho_G) g D_h^2 / \sigma$ of the fluidic system [3], where σ is the interfacial tension, ρ_L and ρ_G are the densities of the liquid and gaseous phases, g is the magnitude of the gravitational acceleration, and D_h is the hydraulic diameter of a channel.

In order to analyse the hydrodynamics in our reactor we calculate the Lagrangian coherent structures (LCS) and the finite-time Lyapunov exponent fields (FTLE-fields) from the measured two-dimensional velocity and concentration fields (PIV-LIF). LCS are defined to be the most repelling, attracting or shearing material lines of the tracer field in finite-time [4]. Here we focus on the so called hyperbolic LCS which correspond to the most attracting and repelling material lines. The LCS give us new insights into the flow topology for the finite time τ: imagine an artificial tracer released at some point in the fluid inside or outside the red repelling LCS in Fig. 1. After a time τ the tracers released inside the red LCS will still largely remain in the vortical structures close to the bubble bottom while tracers released below the red LCS will have been flushed away rapidly. This affects the local residence times of the chemical molecules dramatically. Especially the dissolved gas is thus highly dependent on the local hydrodynamics and thus prone to chemical reactions with longer timescales. This fact can have undesired effects on overall yield and selectivity of the targeted reaction. We find that the local residence times vary strongly for different Reynolds numbers of the flow. We show that these local effects of mixing intensity and residence times should be taken into account for the design and operation of bubbly flows in multiphase reactors. These local effects on residence behaviour analyzed by LCS might also play a role in other multiphase and chemical reactors where wake flow is the main cause for mixing.

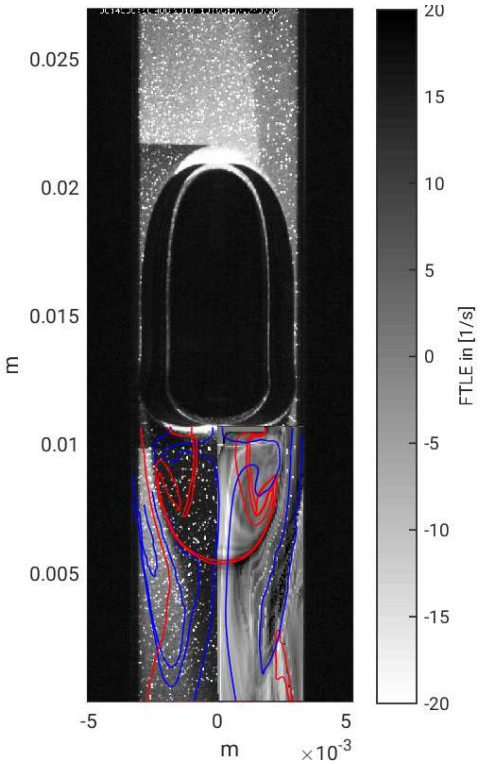

Fig. 1. LCS calculated from the velocity fields derived from Particle Image Velocimetry (PIV) data for a pipe channel diameter of $D = 6$ mm. The mean free velocity (sufficiently ahead of the bubble) is 6 mm/s. The red lines denote the repelling- and the blue lines the attracting LCS. On the right side below the bubble a combination of the forward and the backward FTLE-field $\Lambda_+ - \Lambda_-$ is shown in the background. The liquid is an aqueous solution of fluorescein sodium salt which shows a decrease in fluorescence intensity for higher amounts of dissolved carbon dioxide gas released from the bubble. This decrease is visualized using Laser Induced Fluorescence (LIF) [1].

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