466c Continuous-Phase Mixing in Reactive Bubble Swarms with Fully Resolved Dynamic Interfaces

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In many industrial applications, where reactants are initially available in different phases (i.e. gas and liquid), sparging bubbles is often the scheme of choice for bringing these phases in contact. An additional, secondary role, often played by the gas bubbles is that of providing local continuous-phase mixing. Even when global, reactor-scale stirring is supplied (for example, by means of an impeller), local mixing shows a strong correlation to the medium and small scale hydrodynamics of the bubbly flows. Since for many fast reactions, it is the local mixing, which has the strongest impact on yields and selectivities, gas-liquid flow hydrodynamics and their influence on transport need to be studied in detail.

In our work, we performed Direct Numerical Simulations of reactive bubble swarms with continuously evolving dynamic interfaces. The obtained flow fields were then used to quantify the mixing in different bubbly flows. Since, at the Reynolds numbers considered, the flow is still predominantly laminar, the study of mixing focused on identifying regimes characterized by chaotic passive transport and computing the corresponding stretching fields. Detailed parameter studies, including number of bubbles, bubble size distribution, as well as a variety of system properties were carried out in order to provide the basis for a statistical examination of the correlation between hydrodynamics and continuous phase mixing.

Due to the complexity of the phenomena and the multitude of time and length scales involved, knowledge of the Lagrangian mixing characteristics of a flow is not always sufficient to gauge their impact on chemical reactions. In order to obtain a predictive relation, a reactive species conservation model has been added to the simulations. The phenomena described by the model include gas-liquid interfacial mass transfer (based on first principles), continuous phase transport and chemical reactions. Different reaction networks have been considered.