Quantitative Modeling and Characterization of Hydrodynamics and Transport in Multiphase Microreactors

by

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Abstract

On-chip flow chemistry synthesis has advanced rapidly in recent years as a fast and effective means to discover and screen suitable reaction candidates for continuous production. Among the many chemical reactions, multiphase reactions constitute a major category with important industrial applications, and microreactors have been shown to effectively enhance the efficiency of such reactions. However, compared to single-phase flow chemistry systems, many unknowns remain in the design, optimization and scale-up of multiphase microreactors – primarily due to the complex nature of the multiphase flow. Therefore, this work aims to obtain fundamental knowledge of the hydrodynamics, transport and reactions in multiphase microreactors through a combination of computation, theory and characterization.

Specifically, I studied five typical multiphase flow chemistry modules: the segmented flow microreactor, the post microreactor, the tube-in-tube microreactor, the capillary microseparator and the membrane microseparator. A series of C++ solvers that simultaneously model multiphase hydrodynamics, transport and reactions on the microscale were developed and validated. Parallel computation with up to 128 cores were performed to accelerate simulation. Laser-induced fluorescence visualization combined with image analysis was used to systematically quantify key features such as interfacial area and phase holdup. A variety of analytic models were also developed to provide guidelines for enhanced reactor design. The integrated strategy elucidated the complex hydrodynamics and transport in microreactors with full physical details. The enhanced physical insight into multiphase microreactors would be crucial to predicting reactor performance, reducing experimental cost, and achieving reactor scale-up.

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