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Modelling the Hydrodynamics and Transport in Multiphase Microreactors LU YANG, Department of Chemical Engineering, MIT, YANXIANG SHI, BASF Corporation, MILAD ABOLHASANI, KLAVS JENSEN, Department of Chemical Engineering, MIT — Multiphase flow is prevalent in a variety of industrial applications, but the extent of these processes is often limited by the innate mass transfer resistance across phase boundaries. Microscale multiphase systems, owing to their reduced characteristic length scales, increase specific interfacial areas and unique hydrodynamic patterns, can significantly enhance the rate of mass transfer, thereby improving the efficiency of multiphase processes. However, many uncertainties still remain in the prediction of multiphase hydrodynamics and scalar transport on the microscale, primarily due to the complex nature of the multiphase flow. In this work, to elucidate the mechanism of mass transfer enhancement in microscale multiphase flows, a computational fluid dynamic (CFD) model using the volume-of-fluid (VOF) method is developed, and the method is validated with experiments. By introducing a scalar transport equation with sink/source terms using the one-fluid formulation, we enable the simultaneous capturing of multi-phase hydrodynamics, mass transfer and reactions. In tandem with the numerical simulations, we also perform mass transfer analysis of multiphase flows based on the penetration theory and a two-stage theory, which further examines the mechanism of mixing enhancement in multiphase flow, and reveals a two-fold increase in mass transfer coefficients in the microreactors compared to conventional multiphase contactors.

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