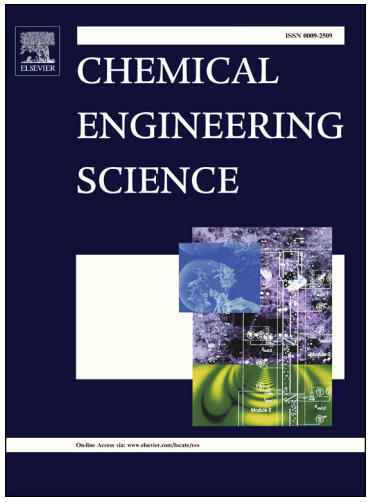

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Simulations and Analysis of Multiphase Transport and Reaction in Segmented Flow Microreactors

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Abstract

We present volume-of-fluid (VOF) based simulations of coupled transport and reaction processes in microscale segmented flow microreactors. The simulations implemented in OpenFOAM accurately capture the circulation patterns and micron-scale wetting film of the segmented flow. The accurate prediction of the interfacial concentration discontinuity is shown to depend on the local Peclet number. The integrated computational fluid dynamics (CFD) and mass transfer simulations provide complete spatial and temporal information about the concentration field within the reactor, which enable quantification of the mass transfer coefficient $k_L a$ as a function of time and operating condition. Mass transport in the segmented flow system is shown to be a two-regime process, dominated first by convection and then by diffusion. Scaling analysis provide a means for estimating mass transfer coefficients and give insights into how to select optimal operating conditions in segmented flow reactors. Finally, we predict mass transfer in segmented flow with reaction, specifically, the mass transfer enhancement as a function of the Damköhler number.

Keywords

Segmented flow microreactor, CFD simulation, mass transfer and reaction simulation, OpenFOAM

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