Simulation of Mass Transfer in a Microfluidic Experiment Using the Moving Mesh Method

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Abstract

Introduction: Two phase liquid-liquid systems are used extensively in chemical processes involving reaction engineering and separations. Recently, microreactors are being developed to exploit the very high mass transfer rates that accompany flow on the sub-millimeter scale. Simulation through multiphysical models is helpful for designing these systems. Before a model may be used as a predictive tool, validation with experimental results is needed. This paper describes modeling of the Burns-Ramshaw experiments that involve extraction of acetic acid from kerosene into an aqueous phase where it is neutralized.

Use of COMSOL Multiphysics®: Owing to the limitations of the Level Set and Phase Field formulations (to be described in the presentation and paper), the Moving Mesh method was utilized to model the experiment in a COMSOL Multiphysics® simulation. While this method cannot represent the formation of slugs, it provides a discrete boundary between phases without leakage where boundary conditions may be implemented. The following physics was included in the model: convective and diffusive transport in each phase, interfacial tension and contact angles through the Navier Slip condition, partition coefficient of acetic acid at the boundary between phases and reaction kinetics within the aqueous phase. Both 2-D and 3-D models were created.

Results: To solve the convection-diffusion equations, computations were performed in two steps. First, the steady-state flow field was generated by simulating three slugs with a symmetry plane splitting the center of the slugs (Figure 1). In the second step, mass transfer between phases is modeled with a periodic boundary splitting the organic phase (Figure 2). Figure 3 illustrates the potassium hydroxide concentration in the aqueous phase. (In the presentation, movies of both the acetic acid and KOH concentrations will be presented for both 2-D and 3-D models.) Conversion rates are predicted to go through a minimum at intermediate contact angles (Figure 4).

Conclusions: The moving mesh method can be effectively applied to model hydrodynamics and mass transfer behavior in complex systems. System variables may be explored, such as contact angle, to predict changes in conversion rates. While model sensitivities may be explored in 2-D, a full 3-D model is needed to capture conversion rates that were observed in the experiment.

Reference

1. M. N. Kashid, a. Renken, et.al., Gas-Liquid and Liquid-Liquid Mass Transfer in Microstructured Reactors, Chem. Engr. Science, 66, 3876-3897 (2011).

2. J. R. Burns, C. Ramshaw, The Intensification of Rapid Reactions in Multiphase Systems Using Slug Flow in Capillaries, Lab on A Chip, 1, 10-15 (2001).

3. P. Yue, C. Zhou et. al., Spontaneous Shrinkage of Drops and Mass Conservation in Phase-Field Simulations, J. Comp. Physics, 223, 1-9 (2007).

Figures used in the abstract

Figure 1: Configuration of the flow field where slug hydrodynamics is developed; note slugs leading and following a middle slug where flow behavior is captured for mass transport modeling. Colors indicate flow velocity.

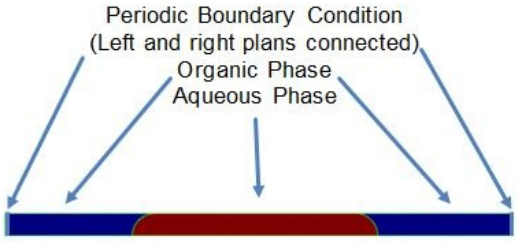

Figure 2: Mass transfer configuration of the central slug with periodic boundary conditions splitting the organic phase.

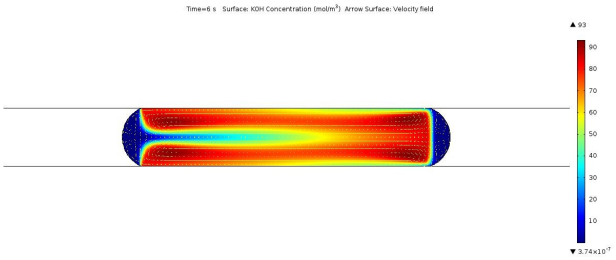

Figure 3: Aqueous phase KOH concentration showing acetic acid flow distribution; 2.8 mm/sec, contact angle 7π/8 after 6 seconds.

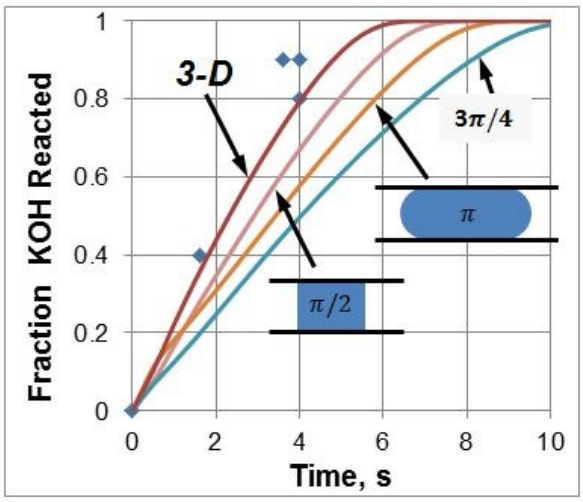

Figure 4: Impact of contact angle upon fraction KOH reacted, all curves for 2-D model except for one noted as 3-D model.