Quantifying the Impact of Viscosity Variations Induced by a Chemical Reaction on Mixing Efficiency in Porous Media

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The extent of mixing-induced reactions at the pore scale can play a key role in predictive modeling of reactive transport in porous media. Expanding interest in enhanced subsurface natural resource recovery, environmental remediation, and carbon sequestration motivates altering the fluid properties induced by chemical reactions under flowing conditions in porous media. In this study, we evaluate the impact of viscosity variations due to a bimolecular chemical reaction on mixing efficiency in porous media using a pore-scale finite element numerical model. Two solutions containing each reactant are injected separately, the bimolecular chemical reaction is induced by transverse mixing along the centerline of the system, and product is formed. A simple model of product concentration-dependent viscosity is used to account for viscosity variations due to chemical reaction. The model was verified against previous work in the literature involving no viscosity variation in several different pore geometries. The extent of mixing efficiency due to viscosity variations is evaluated in two different arrays of cylinders at different Peclet and Damkohler numbers. The loosely packed array is a hexagonal packing with a higher porosity (0.556), while the closely packed array is a square packing with a lower porosity (0.434).

When the product increases the fluid viscosity (i.e., viscosity thickening), the flow velocity is reduced along the centerline and higher amount of product is formed due to increased diffusion time, compared to the constant viscosity case. Conversely, reduced fluid viscosity leads to flow focusing with greater fluid velocity along the centerline, resulting in lower amount of product formation. The transverse dispersion is also increased in the closely packed array compared to the loosely packed array, due to the decreased pore spacing and corresponding increased interfacial contact area between the reactants in the closely spaced array. As the Peclet number increases, the width of mixing zone decreases. In particular, for high Peclet (>100) and Damkohler numbers, viscous thinning case shows a very thin band of high concentration of product, that is, possibly unstable due to viscosity variations and enhanced mixing. Analysis of the calculated values of transverse dispersion coefficient also confirms these observations. Aside from the viscosity behavior, the scaling shows the fundamental parameters to be the Damkohler number, Peclet number, and porosity. Progress on upscaling pore-scale models for reactive transport are discussed, and are being applied to engineering of systems for efficient solution delivery.

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