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Upscaling of mixing-limited chemical reactions in a laminar flow through a pore channel

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Quantifying mixing accurately in aquifers is of primary importance when assessing attenuation of pollutants. Fluid mixing plays a fundamental role in groundwater chemistry as it is often a controling factor in driving chemical reactions that are fast compared to mass transfer processes. Chemical reactions are local phenomena that fluctuate at the pore scale but predictions are often upscaled to much larger scales. Due to the inherent heterogeneities of aquifers at all scales, complex concentration distributions of reactants are created by flow variabilities which enhance or reduce mixing and thus chemical reactions. Determination of the impact of flow variability at pore scale is key to understand the behavior of mixing-driven chemical reactions at larger scales.

We study a bimolecular irreversible chemical reaction $A + B \rightarrow C$ in a laminar Poiseuille flow reactor to analyse and quantify the impacts of flow heterogeneity in a single pore. We use a reactive random walk particle tracking method which represents the reactants by particles. We observe three different time regimes characterized by different behaviours of the product formation. Mixing is dominated by diffusion at times smaller than the advective time (τ_V), time in which the solute covers the same distance by diffusion and by advective transport with the mean flow velocity. For times larger than τ_V, where advection inhomogeneity begins to dominate over diffusion, we find enhanced reaction efficiency due to flow variability. Finally, for times larger than the characteristic time of diffusion mixing is represented by the Taylor dispersion coefficient. We characterize mixing in the reaction by introducing a dispersive lamella model based on the effective dispersion coefficient, which captures the features of stretching, compression and coalescence of the mixing front in the reaction and accurately predicts the total mass of product C. We compare our effective model prediction of product mass to other predictions using traditional approaches such as the apparent dispersion coefficient, and the stretched lamellae theory which measures mixing through diffusive flux in a stretching interface. We find that the use of the apparent dispersion coefficient, or the stretched lamellae theory overestimate the width of the mixing zone, and thus the chemical reaction, when flow heterogeneity dominates over diffusion. While our dispersive lamella model is able to describe the impact of flow heterogeneity on mixing-driven reactions at pore scale.