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Impact of Compound-Specific Transverse Mixing on Conservative and Reactive Transport: Pore-Scale Modeling and Darcy-Scale Experiments

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Transverse mixing is critical for reactions in porous media. Using multi-tracer bench-scale experiments and pore-scale simulations across a range of relevant groundwater flow velocities, we demonstrate that to characterize such mixing at the Darcy scale a nonlinear compound-specific parameterization of transverse dispersion is necessary. Next, we investigate the impact of compound-specific diffusivity on reactive transport at the pore scale with modeling and compare the results to those of laboratory experiments. The objective is to analyze the effectiveness of using linear and nonlinear parameterizations of transverse dispersion in continuum models in order to predict mixing-limited reactive transport. For both product mass flux and reactant plume extents, the nonlinear parameterization of transverse dispersion consistently provides a very good prediction of both indicators of interest across two orders of magnitude of mean flow conditions. On the other hand, the classic linear parameterization of transverse dispersion, assuming dispersivity as a property of the porous medium, could not consistently predict either indicator with great accuracy. Furthermore, a linear parameterization of transverse dispersion predicts an asymptotic (constant) plume length with increasing velocity while the nonlinear parameterization indicates that the plume length increases with the square root of the velocity. Both the pore-scale model simulations and the laboratory experiments of mixing-limited reactive transport show the latter relationship.