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Diffusive-dispersive C and Cl Isotope Fractionation in Flow-through Porous Media: A Study from Pore to Field Scale

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Diffusive isotope fractionation in aqueous systems has been documented with different approaches for a number of elements and species, including major cations and anions [1-2], dissolved gases [3], and dissolved organic compounds [4]. The propagation of such effects in subsurface flow-through systems is still under investigation and debate.

In this work, we assess the effect of diffusion-induced isotope fractionation on carbon and chlorine isotope signals during transport of chlorinated ethenes. We consider the diffusive isotope fractionation determined in previous experimental and molecular dynamics simulation studies [5-6] and we investigate its impact in flow-through porous media. We perform a multiscale study from the small pore scale to the large field scale. We investigate the propagation of isotope fractionation using pore-scale simulations, high-resolution flow-through experiments, and detailed numerical field-scale modeling in a heterogeneous aquifer. We consider *cis*-dichloroethene (*cis*-DCE) as model contaminant in the lab-scale setup. For the numerical simulations, we use C and Cl isotopologues of *cis*-DCE and trichloroethene (TCE) to study the lateral displacement of diffusive-dispersive fronts in porous media over a wide range of seepage velocities (0.1-10 m/day). The transverse concentration profiles and isotope signatures are evaluated to quantify diffusion-induced isotope fractionation.

The results reveal the importance of diffusion in isotope fractionation of chlorinated ethenes not only at the small pore scale but also at larger macroscopic scales. These findings are relevant for the interpretation of isotope signatures of organic contaminants in groundwater, as well as for the general understanding of diffusive isotope fractionation in subsurface flow-through systems.

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