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Quantitative assessment of stable isotope fractionation during diffusive transport and biogeochemical transformations

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Compound-specific stable isotope analysis (CSIA) has been established as reliable tool for the detection of biogeochemical transformations in the subsurface. For a quantitative assessment of stable-isotope signatures in no-transport systems or systems with advection-dominated transport standard approaches are based on the well-known Rayleigh equation. However, for systems with diffusion-dominated transport such quantitative assessment is challenged not only by the different diffusivities of the isotopologues but also as the Rayleigh-equation is not applicable and alternative approaches are lacking. This limits the applicability of CSIA for the assessment of e.g., the degradation of organic chemicals in the vapor phase of water-unsaturated porous media such as soils where gas-phase diffusion is the governing transport processes, or of biochemically reactive compounds in aquatic sediments with aquatic diffusion as governing transport process.

The present study introduces a new modified version of the Rayleigh-equation approach applicable to biogeochemical (or other reactive) transformations in diffusion-dominated transport systems (1). This analytically derived approach is making use of some simplifying yet reasonable assumptions. To test this approach and its potential limitations theoretical predictions are compared to data from a laboratory experiment on biodegradation of a volatile organic compound (VOC) along a diffusive transport path in an unsaturated porous medium (2) and to results of numerical reactive transport simulations. Results show that in spite of the used simplifications the proposed quantification approach provides good estimates of stable isotope fractionation factors and suggest its applicability for other systems with similar settings. This widens the range of CSIA being not only a qualitative but also a quantitative assessment tool for biogeochemical transformations in diffusion-dominated systems. Reactive transport modeling can support the interpretation of such data and can determine the limits of theoretical assessment schemes.

References:

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