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The significance of isotope specific diffusion coefficients in reaction-transport models describing microbial sulfur isotope fractionation in porous sediments

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Modeling isotopic signatures in systems affected by diffusion, advection, and a reaction which modifies the isotopic abundance of a given species, is a discipline in its infancy. Traditionally, much emphasis has been placed on kinetic isotope effects during biochemical reactions, while isotope effects caused by isotope specific diffusion coefficients have been neglected. A recent study suggested that transport related isotope effects may be of similar magnitude as microbially mediated isotope effects. Although it was later shown that the assumed differences in the isotope specific diffusion coefficients were probably overstated by one or two orders of magnitude this study raises several important issues: 1) Is it possible to directly calculate isotopic enrichment factors from measured concentration data without modeling the respective system? 2) Do changes in porosity and advection velocity modulate the influence of isotope specific diffusion coefficients on the fractionation factor alpha 3) If one has no a priori knowledge whether diffusion coefficients are isotope specific or not, what is the nature and magnitude of the error introduced by either assumption? Here we argue A) That the direct substitution of measured data into a differential equation is problematic and cannot be used as a replacement for a reaction-transport model; B) That the transport related fractionation scales linearly with the difference between the respective diffusion coefficients of a given isotope system, but depends in a complex non-linear way on the interplay between advection velocity, and downcore changes of temperature and porosity. Last but not least, we argue that the influence of isotope specific diffusion coefficients on microbially mediated sulfate reduction in typical marine sediments is considerably smaller than the error associated with the determination of the fractionation factor.