Compound-specific isotope fractionation of dispersion and diffusion at natural isotopic abundance in sediment flow-through tanks

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Many dissolved organic compounds in groundwater have an adverse effect on human health and are regarded as micropollutants due to their presence at low concentration levels. Carbon and nitrogen isotope fractionation of these compounds at their natural isotopic abundance can provide a concentration-independent line of evidence of their biodegradation in natural subsurface environments and improve our understanding of their fate and transport. Nevertheless, isotope fractionation in reactive aqueous environments may potentially also result from physical processes such as diffusion [1] or transverse dispersion, as recently suggested based on experiments with isotopically labelled compounds [2,3].

To investigate this possibility with organic micropollutants at their natural isotopic abundance, the present study investigated (i) diffusive fractionation of the pesticide metabolite 2,6-dichlorobenzamide (BAM) in aqueous solutions using gel diffusion tubes and (ii) effects of transverse dispersion in a 2D sediment tank with narrowly spaced inlet (and outlet) ports mimicking a homogeneous sandy aquifer [2,3]. For the first time, we generated a consistent dataset (a) comprising data on pure diffusion as well as transverse dispersion, (b) working at natural abundance, (c) targeting isotopes of more than one element ($^{15}N/^{14}N$ and $^{13}C/^{12}C$) and (d) performing experiments at several flow velocities to allow an improved characterization of the terms contributing to transverse dispersion.

A sophisticated 2D numerical model was developed for the simulation of the fate and the transport of the contaminant inside the experimental systems above and to determine the isotope fractionation effects due to each individual process.

[1] Jin *et al*. (2014) *Environ. Sci. Technol*. **48**(11), 6141-50. [2] Bauer *et al*. (2008) *J. Contam. Hydrol*. **96**, 150-68. [3] Rolle *et al*. (2015) *Environ. Sci. Technol*. **44**(16), 6167-73.