

## Model-based evaluation of the use of CSIA to detect chemical reduction of chlorinated ethenes in aquifers and in low-permeability zones

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Compound-specific isotope analysis (CSIA) has been successfully employed as a site-assessment tool in monitored natural attenuation (MNA) of chlorinated solvents. MNA is increasingly accepted as a remediation strategy relying mostly on reductive dechlorination as key transformation process. Chemical reduction capable of complete dechlorination may be also significant for MNA, but the lack of clear degradation indicators hampers its consideration for MNA. Indeed, chemical reduction is sometimes confused with stalling reductive dechlorination. For this reason, the potential use of carbon CSIA to detect and quantify chemical reduction will be evaluated by means of reactive transport modeling of hypothetical hydrogeological conditions.

The model was applied both to advective flow conditions in aquifers and to diffusion-controlled transport in low-permeability layers. Back-diffusion from low-permeability layers causes contaminant persistence long after DNAPLs are dissolved or removed, and it increasingly becomes a concern in site remediation work. At some polluted locations, back-diffusion from clays and rock matrices is expected to release contaminants at concentrations above the maximum contaminant levels for decades after DNAPL source removal [1, 2]. Chemical reduction and biodegradation of chloroethenes in low-permeability zones might mitigate pollutants release. The model enables predicting concentration and isotope ratio patterns within and at the surface of the clay layer as well as in the aquifer. Isotope fractionation due to sorption and diffusion is also included in the model. Such fractionation is particularly relevant in modeling the fate of contaminants in low-permeability layers.

We present the model background, as well as different virtual model experiments based on a literature compilation of model parameter values. Initial model results show that impact of physical processes on isotope patterns might interfere with degradation process assessment.

[1] Liu & Ball (2002), *Ground Water*, **40**, 175-184. [2] Parker, Chapman & Guilbeault (2008), *Journal of Contaminant Hydrology*, **102**, 86-104.