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# An Isotope Fractionation - Reactive Transport Model to Assess Natural Attenuation of Chlorinated Solvents

P. Stack (1), T Kuder (2), M Vanderford (3), P Philp (2), and B van Breukelen (1)

(1) VU University, Amsterdam, Department of Hydrology and Geo-Environmental Sciences, Netherlands (p.e.stack@vu.nl), (2) University of Oklahoma, (3) GSI Environmental Inc.

While compound-specific isotope analysis has been used successfully to demonstrate in situ degradation of chlorinated solvents, it suffers from uncertainty resulting from geological heterogeneity and variability in redox conditions. The primary objective of this project was to create an Isotope Fractionation - Reactive Transport Model (IF-RTM) capable of simultaneously simulating multiple isotopes within a complex reaction network, in this case C, Cl and H isotopes during the sequential degradation of chlorinated ethenes, and with heterogeneous environmental conditions. This IF-RTM can then be used as a tool to quantitatively assess contaminant mass destruction through natural attenuation processes, potentially reducing the required monitoring effort, informing remediation or mitigation efforts, and providing insight into the relative impacts of mass attenuation mechanisms. A greater level of model confidence can be obtained by incorporating isotope fractionation into the model output, rather than the usual concentration only approach.

A model code capable of simulating concentration changes and isotope fractionation of multiple isotopes (C, Cl, H) during reductive dechlorination and aerobic degradation has been developed using the biogeochemical speciation and transport modelling programme PHREEQC-2. This model is novel not only because it simulates multiple isotopes, but also because it also incorporates secondary isotope effects in the simulation of chlorine isotope fractionation. Microcosm data, including a dataset representing the first a comprehensive, three-isotope (C, Cl, H) characterisation of the TCE reductive dechlorination sequence will be presented and have been used to calibrate/validate this model. The model was found to be capable of simulating the carbon, chlorine and hydrogen isotope fractionation patterns and change in concentration for TCE and its degradation products throughout the reductive dechlorination process.

In the next stage of this project solute transport capability will be added to the model by modifying it to be used with a reactive multi-component transport model such as PHAST. The final IF-RTM product will have the capability of simulating changes in concentrations of the parent compound (e.g. PCE) and its degradation products (e.g. VC) and the isotope ratios (of C, Cl and H) of each compound in 3D space. This IF-RTM can also be modified to include fractionation resulting from physical processes such as hydrodynamic dispersion. The developed model will be tested on a large dataset collected at a contaminated field site, namely the TCE plume at Hill AFB, UT.