

Hydrogen Isotope Effects in Reactions of Chlorinated Ethenes: Potential Tool for Discrimination of Chlorinated Ethenes Degradation Pathways

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Background/Objectives.

Recent introduction of compound-specific isotope analysis (CSIA) technology for determination of hydrogen isotope ratios of halogenated compounds opened new opportunities for assessment of the sources and the fate of chlorinated ethenes (CEs). Current technology permits determination of hydrogen isotope ratios of trichloroethene (TCE) and other CEs in groundwater samples at concentrations as low as a few $\mu\text{g/L}$ at cost similar to that of the well-established carbon CSIA. A key limitation to widespread implementation of hydrogen isotope data in contaminated sites assessment is the near absence of reference data from controlled studies (e.g., laboratory degradation experiments). In comparison with carbon and chlorine CSIA, where considerable body of reference data has been accumulated over past years, interpretation of hydrogen CSIA data is often uncertain and inconclusive, since field results cannot be compared to (nonexistent) reference data.

In this presentation, we will discuss hydrogen isotope data collected in biodegradation and abiotic degradation experiments. Such data will serve as a benchmark for using hydrogen CSIA data from field samples, for identification of degradation mechanisms and for discrimination of different sources of CEs, for example, in the form of dual-element CSIA combining hydrogen and carbon CSIA data.

Approach/Activities.

This presentation discusses the existing and anticipated results from an ongoing project (SERDP ER-2623). Batch degradation experiments address the following areas: i) abiotic degradation on $\text{Fe}(0)$; ii) anaerobic biodegradation by different dehalogenating cultures, including *Dehalococcoides*; and iii) aerobic cometabolic degradation by cultures utilizing different oxygenases.

Results/Lessons Learned.

Currently, data from anaerobic biodegradation and from biodegradation of TCE by $\text{Fe}(0)$ have been collected, while the aerobic cometabolic biodegradation experiments are in progress. Hydrogen isotope ratios of the degrading parent CE compound (TCE) represent kinetic isotope effects of the degradation process involved, and hydrogen isotope ratios of the degradation product (TCE produced by degradation of PCE and cis-DCE produced by degradation of TCE), mainly represent the isotope effect of hydrogenation of the degradation product. Both parameters are potential lines of evidence on the degradation pathway involved. Similarly, both parameters are potential lines of evidence on the provenance of the CEs present in the groundwater. This study significantly expands the hydrogen isotope effect reference database for chlorinated ethenes, to be used in evaluation of field site data.