Project Number: 55388

Project Title: Stable Isotopic Investigations of In-Situ Bioremediation of Chlorinated Organic Solvents

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Number of graduate students and/or post-doctorates actively involved in the project:
1 graduate student and 2 postdocs (during project).

Specific DOE problems that are being addressed by your project, and potential practical relevance to improved knowledge, techniques, processes, or technology:

The new scientific information generated by this research focuses on the problem of the environmental management of chlorinated solvents. The results of this research have yielded a new tool that will significantly improve the understanding of the fate and transport of chlorinated solvents in ground water aquifers and vadose zones, which can translate into large savings of cleanup costs.

The principal benefits to DOE of the new information generated are that: (1) it will improve site characterization by revealing the nature and extent of natural attenuation processes occurring at a site and can be used in conjunction with hydrologic data to estimate attenuation rates and (2) it can be used to monitor cleanup and to help evaluate the most effective engineered remedial strategy for a given site.

Research Objective:

The research objectives of this program are threefold: to develop methods for measuring stable isotope ratios of carbon and chlorine in chlorinated aliphatic hydrocarbons (CAHs); to apply these methods to experimental determinations of kinetic and equilibrium isotope effects during biological, chemical, and physical transformation of CAHs; and to apply these methods to CAHs extracted from ground water at well-characterized, contaminated aquifer sites. The overall objective is to develop an understanding of the environmental isotopic behavior of CAHs and to apply this understanding to better characterize, monitor, and evaluate natural and engineered bioremediation. This is an important problem because of the magnitude and frequency of ground water contamination by CAHs and the resultant health risks imposed to the population, as well as the enormous costs involved in cleaning up such contamination.

This project is innovative as it represents the first systematic effort of its kind. Since its inception, a number of other scientists have also started research into the stable isotope chemistry of CAHs in both laboratory and field investigations . Complementary experimental and theoretical studies of the equilibrium stabilities and kinetics of CAH degradation by microbial and abiotic mechanisms continue to be a major field of research.

Research Progress and Implications:

This project was completed in September, 1999. This research has advanced our understanding of the isotope effects associated with biological, chemical, and physical transformations of the CAHs. It has advanced our knowledge of the extent to which various processes affect the isotopic composition of chlorinated solvents in ground water aquifers. We have applied our methods to the analysis of CAH in a number of contaminated aquifers having contrasting hydrogeologic characteristics and treatment histories, resulting in valuable insights into the extent and mechanisms of natural and engineered remediation. Additional scientific hurdles include: (1) establishing a larger database of experimentally measured kinetic isotope effects for microbial degradation of chlorinated solvents and (2) integrating isotopic data more fully into conceptual and numerical ground water and vadose zone transport models for chlorinated solvents.

Planned Activities:

N/A (project completed).

Information Access:

Holt B. D., Sturchio N. C., Abrajano T. A., and Heraty L. J, 1997. Conversion of chlorinated organic compounds to carbon dioxide and methyl chloride for isotopic analysis of carbon and chlorine. *Analytical Chemistry* **69**, 2727-2733.

Sturchio N. C., Clausen J. C., Heraty L. J., Huang L., Holt B. D., and Abrajano T., 1998. Stable chlorine isotope investigation of natural attenuation of trichloroethene in an aerobic aquifer. *Environmental Science and Technology* **32**, 3037-3042.

Dayan, H., Abrajano T., Sturchio N. C., and Winsor L., 1999. Carbon isotopic fractionation during reductive dechlorination of chlorinated solvents by metallic iron. *Organic Geochemistry* **30**, 755-763.

Heraty L. J., Fuller M. E., Huang L., Abrajano T., and Sturchio N. C., 1999. Carbon and chlorine isotopic fractionation during microbial degradation of dichloromethane. *Organic Geochemistry* **30**, 793-799.

Huang L., Sturchio N. C., Abrajano T., Heraty L., and Holt B. D., 1999. Carbon and chlorine isotope fractionation of chlorinated aliphatic hydrocarbons by evaporation. *Organic Geochemistry* **30**, 777-785.

Sturchio N. C., Heraty L., Holt B. D., Huang L., Abrajano T., and Smith G., 2000. Stable isotope ratios of chlorinated aliphatic hydrocarbons in contaminated aquifers. *Second International Conference on Remediation of Chlorinated and Recalcitrant Compounds*, Monterey, CA, May 22-25, 2000.

Additional Information:

U. S. Patent # 5,942,439. Ben D. Holt and Neil C. Sturchio. *Method for Isotopic Analysis of Chlorinated Organic Compounds* (issued 8/28/1999).