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Using Positive Matrix Factorization to Investigate Microbial Dehalogenation of Contaminants in Groundwater

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Background/Objectives. Chlorinated ethenes, chlorinated benzenes, and halomethanes are common groundwater contaminants in the United States, and demonstrating whether they undergo degradation in the subsurface is important in determining the best remedy for this contamination. The purpose of this work was to use a new approach to investigate degradation pathways in the subsurface. Positive matrix factorization (PMF) was applied to historical groundwater monitoring data at a contaminated site in New Jersey. The goals of this work are to: a) determine whether the groundwater monitoring data can be successfully analyzed by PMF; b) determine whether PMF can give useful information of microbial dehalogenation processes in groundwater; c) if so, to investigate where and when microbial dehalogenation of each organohalide contaminant class occurred in the subsurface at the site; and d) investigate correlations between PMF outputs related to microbial dehalogenation and ancillary parameters such as redox indicators, alkalinity and nutrients in order to understand which conditions favor microbial dehalogenation.

Approach/Activities.
1.) Apply PMF analysis on groundwater monitoring data for aqueous concentrations of chlorinated benzenes, chlorinated ethenes, and halomethanes.
2.) Examine temporal and spatial trends of PMF model output for each organohalide contaminant class.
3.) Investigate correlations between PMF outputs related to microbial dehalogenation and ancillary parameters such as geochemical and field data.
4.) Indicate any practical approaches that the operators of the site could use to enhance the natural dehalogenation.
5.) Make recommendations about how data collection and management should be conducted in the future to aid data mining efforts.

Results/Lessons Learned. PMF analysis is useful in interpreting groundwater data. For all data sets, the PMF analysis did converge on a stable solution that provided insights into the processes occurring in the subsurface. Analysis also provided enough data on ancillary parameters that are indicative of redox conditions in the subsurface, correlating the PMF output with those parameters can suggest the conditions that are conducive to dehalogenation. PMF was also capable of the conditions that are conducive to dehalogenation of chlorinated benzenes and chlorinated ethenes. Specifically, advanced dehalogenation regimes were correlated with methanogenic conditions indicating that advanced dehalogenation is most prevalent in highly reducing environments. Finally, this data mining approach works best with a relatively cohesive dataset. For future work we recommend the following regarding data collection and management: a) measure all possible degradation products, b) report all quality assurance criteria including field and laboratory surrogate recoveries, c) measure analytes using the same analytical methods and d) measure all the contaminants and redox indicators in the same sample at the same time.