Geophysical Research Abstracts
Vol. 14, EGU2012-10139, 2012
EGU General Assembly 2012

Estimating the Contribution of Individual Degradation Pathways to Overall Biodegradation in Aquifers Based on Compound-Specific Stable Isotope Analysis

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In order to design optimal remediation strategies at field sites contaminated with organic contaminants, the identification of microbial degradation pathways contributing most to overall biodegradation is highly desirable. This task can be difficult if redox conditions vary along an aquifer, leading to different pathways contributing to degradation at distinct locations along groundwater travel paths. In order to provide an estimate for the contribution of individual degradation pathways to overall biodegradation under such conditions, we evaluate the potential of compound-specific stable isotope analysis, which has been established as a viable tool for detecting in situ biodegradation as well as for the identification of single dominant degradation pathways. Based on the stable isotope signatures of two elements, we mathematically derive an estimate for the local and total share of two pathways on overall biodegradation. For the total share, lower and upper limits are provided by assuming that both pathways are either simultaneously active along the flow path in constant ratio, or that both pathways are active in a strictly consecutive manner. To validate the method and assess its applicability under field conditions, the derived concept is applied to simulated data obtained from reactive transport simulations using GeoSysBRNS in zero, one, and two spatial dimensions. A generic benzene plume/degradation scenario is considered with aerobic and anaerobic degradation as exemplary degradation pathways and implementing the concurrent fractionation with respect to carbon and hydrogen. Estimates are very accurate for the zero- and one-dimensional simulations. In the two-dimensional case, estimates for pathway specific contributions to overall biodegradation are most accurate along the center of the plume, but loose accuracy towards the fringe, where transversal mixing processes are shown not only to affect contaminant concentration but also associated stable isotope signatures. Total estimates can be significantly improved if additional observation points are available along the flow path. The novel method complements current stable isotope based assessment methods to quantify and identify biodegradation by a means to attribute biodegradation to distinct degradation pathways at field sites with varying redox condition.