Geophysical Research Abstracts
Vol. 12, EGU2010-10696, 2010
EGU General Assembly 2010

Analysis of Carbon and Hydrogen Isotope Signals obtained by Reactive Transport Simulations of a Benzene Biodegradation Scenario

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Compound-specific stable isotope analysis (CSIA) has been established as a viable tool for the evaluation of *in situ* biodegradation. Isotope signatures can be interpreted by means of the Rayleigh equation to quantify microbially mediated processes leading to the degradation of organic contaminants. Beyond quantification, isotope data from more than one element can be combined to identify and distinguish distinct biodegradation pathways. The Rayleigh approach, however, was originally developed for closed systems. This assumption does not necessarily hold true for field sites at which not only biodegradation, but also abiotic non-destructive processes like diffusion, dispersion, volatilization, and sorption can lead to a decrease in contaminant concentration. This makes the interpretation of isotope signals from field sites challenging. In order to evaluate the explanatory power of the Rayleigh approach, we analyze isotope fractionation data obtained from a multi-dimensional reactive transport simulation. We employ the versatile reactive transport simulator GeoSysBRNS to simulate the simultaneous fractionation of carbon and hydrogen isotopes in a hypothetical benzene plume scenario in a two-dimensional aquifer. Biodegradation of benzene occurs via an aerobic and an anaerobic degradation pathway, which results in a typical redox zonation within the aquifer. With benzene concentrations and isotope signals for carbon and hydrogen available at every location of the simulation domain, the explanatory power of one and two-dimensional isotope data analysis can be thoroughly assessed. The influence of abiotic processes affecting contaminant concentration in the aquifer as well as the effect of vertical mixing in measuring wells on the isotope signal and its interpretation are investigated.