Coupled modeling of biogeochemical and isotope fractionation processes at a BTEX/PAH contaminated site

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A high-resolution data set documenting carbon and sulfur isotope fractionation at a tar oil contaminated, sulfate-reducing field site was analyzed with a reactive transport model. Within a comprehensive quantitative framework the study can link the observed, distinct isotope signatures (depth profiles) with the degradation of various monoaromatic and polycyclic aromatic hydrocarbon compounds (BTEX/PAHs) under sulfate-reducing conditions.

In the site-specific reaction network microbial dynamics were simulated explicitly and isotope fractionation was directly linked to the differential microbial uptake of lighter and heavier carbon isotopes during microbial growth.

Measured depth profiles from a high-resolution multi level sampling well (HR-MLW) served as key constraints for the parameterization of the model simulations. The simulations illustrate particularly well the evolution of the isotope signature of the most rapidly degrading compound toluene, which is also the most important reductant of the contaminant mixture.

The detailed depth profiles at the HR-MLW are characterized by the distinct differences between the small isotopic enrichment in the contaminant plume core and the much stronger enrichment of up to 3.3‰ at the plume fringes.

The profiles of both the simulated and observed sulfur isotope signature exhibit a maximum enrichment of about 30‰. In contrast to the carbon isotopes, the maximum ^{34}S enrichment occurs approximately in the plume's centre. The study highlights the complexity of isotope enrichment patterns created by a mixture of physical (transport) and chemical controls of biodegradation processes.

Phenanthrene sorption to particle size fractions of a Eutric Cambisol from Ultuna, Sweden related to specific surface area and organic matter properties

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Sorption of hydrophobic organic chemicals like polycyclic aromatic hydrocarbons (PAH) to soil particles depends on the characteristics of the organic matter and surfaces present. However, the mechanisms responsible for this process are not yet clear. We intend to investigate the sorption behaviour of phenanthrene to a Eutric Cambisol and relate this to the properties of the organic matter and surface characteristics of the soil. The soil was divided into particle size fractions which were analysed for C and N content and specific surface area (SSA) using BET-N_2 and ethylene glycol monoethyl ether (EGME) retention. Contrary to N_2-physisorption, EGME can access interlayer surfaces of clay minerals and enter organic material leading to increased measured SSA. Phenanthrene sorption was measured using batch incubations according to OECD guideline for the testing of chemicals. 1 g of soil was added to 75 ml of 0.01M $CaCl_2$ solution spiked with phenanthrene and incubated for 24 hours. Experiments were preformed to the bulk soil and to particle size fractions to investigate the relative contribution of different fractions to phenanthrene sorption and to study the effect of changing SSA and organic matter properties on phenanthrene sorption. The organic matter content of the bulk soil was relatively low (15 g C kg-1^{-1}). For the particle size fractions, it increased with decreasing particle size to a maximum of 3 g C kg^{-1} for the fine clay fraction (< 2 µm). The measured SSA increased with decreasing particle size from 1.6 m^2 g^{-1} to 78 m^2 g^{-1} for BET-N_2 and from 8.4 m^2 g^{-1} to 334 m^2 g^{-1} for EGME. The BET-N_2 and EGME SSA measurements were linearly correlated indicating that the changing organic matter content of the particle size fractions had no influence on the EGME SSA measurement. The phenanthrene adsorption isotherm of the bulk soil shows that nonlinear sorption took place. The calculated Freundlich isotherm coefficient is comparable to literature values. The relation between surface properties, organic matter characteristics and phenanthrene sorption can give insight into the mechanisms behind the sorption of PAH to soil.