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Combining a microcosm biodegradation concept with reactive transport modelling of phenol attenuation for a field case

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Biodegradation is a key factor contributing to the fate of many organic contaminants in groundwater. A biodegradation concept was developed by detailed modelling of a 3-years laboratory microcosm experiment, and then has been transferred from laboratory scale to the implementation into a field scale reactive transport model. Two-dimensional and three-dimensional simulations were performed for this non-linear multicomponent reactive transport system, and compared to existing field data, especially multi-level samplers. At the plume fringes a high degree of refinement was required to improve the conceptual understanding of the plume processes. Computations were based on the partial differential equation toolbox, UG (Unstructured Grids), which offers advanced numerical tools including adaptive remeshing, parallel processing, and multigrid solvers.

The use of a two-step kinetic biodegradation concept with separate fermentation and respiration steps, and with hydrogen and acetate as an intermediate species, allowed for good reproduction of detailed discrete field data after adjusting the degradation rates to the field conditions. Important processes identified are the long term microbial acclimatization to the contaminant matrix, differential toxicity effects between fermentation and respiration affecting hydrogen distribution, the availability of FeOOH mineral electron acceptor decreasing with time, and sorption of microbially produced Fe(II) as surface complexation reactions.

The results suggest that plume core processes are at least as important as plume fringe processes based on a 47 year cumulative mass balance. The effects of using a heterogeneous flow field in two-dimensional and a spatially variable source zone in three-dimensional are that more mass is degraded, but still mainly in the plume core. Notably, the biogeochemical modelling concept used was the most important factor in representing the plume biodegradation.

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Stable isotope and SEM study of recent calcite precipitation related to microbial oxidation of natural gas in soils

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A methanotrophic microbial community metabolizes large volumes of natural gas (>99 vol. % CH_4) in sandy soils near leaking resource wells in Western Canada. Regular monitoring at two research sites near wells drilled in 1986 indicates that natural gas concentrations at the water table (~2 m depth) fall from 100 vol. % close to the well bore to <10 ppm/v 4 m away, and to <1000 ppm/v at 20 cm depth near the well bore. The presence of a microbial community is also evident from the high concentration (10-20 vol. %) of low $\delta^{13}C$ (-76 ‰) soil CO_2, and the low $\delta^{13}C$ of bulk soil carbonate (-57 ‰) and bulk soil organic matter (-43 ‰) near the well bore. The $\delta^{13}C$ of soil carbonate and SOM vary laterally in the soil profile reaching background values of -11 ‰ and -30 ‰ respectively 4 m away from the well bore. Significant correlations between soil temperature and $\delta^{13}C$ of CO_2 and CH_4 - C_4H_{10} gases indicate a strong seasonal effect on bacterial oxidation (soil temperature at 1 m depth varies from -2ºC in March to +17ºC in August).To determine the role of microorganisms in carbonate precipitation soil samples were studied by SEM and EDS. SEM imaging and EDS analyses showed that soil carbonate is porous microgranular calcite that coats and/or cements mineral particles. A thriving community of microorganisms of diverse morphologies (e.g., rod-shaped, coccoid, filamentous) lives on the surface and in the pores of the calcite cement. Incipient calcite precipitation as small (<100 nm) rounded to filamentous aggregates indicative of bacterial replacement is evidence for the active involvement of the microorganisms in calcite precipitation [1]. Subsequent mineral growth transforms the small aggregates into larger (>1 um) grains with distinct crystalline shapes.

Preliminary estimates of carbonate formation temperatures indicate that soil calcite away from the well bore precipitated at +10 to +17ºC. In contrast, low $\delta^{13}C$ calcite from a zone of active methane oxidation yields lower formation temperature (+2 to +5ºC) possibly reflecting seasonal effects on the microbial metabolism in a high P_{CO2} environment.

Soil carbonate precipitation mediated by microorganisms capable of oxidizing high concentrations of CH_4 may have acted as a carbon sink during periods when atmospheric methane concentrations were significantly higher than today.

Reference

[1] Castanier. S., *et al.* (1999) *Chemical Geology* **126**, 9-26.