

Interpretation of hydrocarbon plume biodegradation in 2-D bench-scale tank experiments by reactive transport modelling

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Abstract High resolution reactive transport modelling was applied as a tool for a model-based interpretation of detailed laboratory experiments on the interplay of transverse mixing and aerobic and anaerobic hydrocarbon biodegradation. As a typical groundwater contaminant, ethylbenzene (as a mixture of unlabelled and fully deuterium-labelled isotopologues) was continuously injected into a 2-D bench-scale flow-through tank through a central inlet port, generating a hydrocarbon plume along the whole length of the tank. During the first phase of the experiment, where the tank was recharged with water containing oxygen as the major dissolved electron acceptor, the aerobic strain *Pseudomonas putida* F1 was inoculated in order to initiate aerobic biodegradation of the ethylbenzene. Later, nitrate was added as an additional electron acceptor and the denitrifying strain *Aromatoleum aromaticum* EbN1 was inoculated to study competitive degradation under aerobic / anaerobic conditions. The spatial distribution of anaerobic degradation was investigated using measurements of compound-specific stable isotope fractionation along a vertical profile at the tank outlet. The numerical model was calibrated to fit the measured concentration profiles of these compounds at the outlet ports. Simulated and measured ethylbenzene and oxygen concentrations showed a good agreement for the aerobic degradation phase of the experiment, while the evaluation of the aerobic/anaerobic phase with competitive biodegradation was ambiguous due to uncertainties regarding the actual stoichiometry of the specific denitrification reaction. The model results, calibrated on the stable isotope signatures, showed that for the case of aerobic/anaerobic degradation the observed isotopic pattern strongly depends on the assumed initial distribution of microbial biomass.

Key words hydrocarbon biodegradation; isotope fractionation; numerical modelling; transverse dispersion