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Kinetics of microbial degradation of deicing chemicals in percolated porous media – the modeling perspective

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A quantitative knowledge of the fate of deicing chemicals in the subsurface can be provided by analysis of laboratory and field experiments with numerical simulation models. In the present study, experimental data of microbial degradation of the deicing chemical propylene glycol (PG) under flow conditions in soil columns and field lysimeters were simulated to analyze the process conditions of degradation and to obtain the according parameters.

Results from the column experiment were evaluated applying different scenarios of an advection-dispersion model using HYDRUS-1D. To reconstruct the data, different competing degradation models were included, i.e. zero order, first order and inclusion of a growing and decaying biomass. The general breakthrough behavior of propylene glycol in soil columns can be simulated well using a coupled model of solute transport and degradation with growth and decay of biomass. The susceptibility of the model to non-unique solutions was investigated using systematical forward and inverse simulations. We found that the model tends to equifinal solutions under certain conditions. Complex experimental boundary conditions can help to avoid this.

Under field conditions, the situation is far more complex than in the laboratory. Studying the fate of PG with undisturbed lysimeters we found that aerobic and anaerobic degradation occurs simultaneously. We attribute this to the physical structure and the aggregated nature of the undisturbed soil material . This results in the presence of spatially disjoint oxidative and reductive regions of microbial activity and requires, but is not fully reflected by a dual porosity model. Currently, the numerical simulation of this system is in progress, considering several flow and transport models. A stochastic global search algorithm (DREAM-ZS) is used in conjuction with HYDRUS-1D to avoid local minima in the inverse simulations. The study shows the current limitations and potentials of modeling degradation in an aggregated and structured system under flow conditions.