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Modelling reactive transport of chlorinated hydrocarbons in groundwater under spatially varying redox conditions

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Abstract Chlorinated ethene degradation in groundwater has proven to be highly dependent on environmental conditions. Nevertheless, literature dealing with the interaction between chlorinated ethene degradation and inorganic electron acceptors such as nitrate is scarce. A study area located in Braunschweig (Germany), where redox conditions vary from nitrate-reducing to iron(III)-reducing conditions, is utilised for validation of a reactive transport model. A groundwater model using conventional 1st-order degradation kinetics, which was additionally optimised via sequential Monte-Carlo simulations, could not satisfactorily describe the pollutant distribution of the site. Thus, laboratory experiments considering the influence of inorganic electron acceptors were used to formulate enhanced inhibition kinetics that were implemented into the field scale model. The results yield a better accordance of simulated and measured concentration data than applying the previous 1st-order kinetics.

Key words DNAPL pollution; modelling; reactive transport