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Estimating prior distributions of TCE transformation rate constants from literature data

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Stochastic modeling of contaminant reactions requires the definition of prior distributions for the respective rate constants. We use data from several experiments reported in the literature to better understand the distribution of pseudo-first-order rate constants of abiotic TCE reduction in different sediments. These distributions can be used to choose informed priors for these parameters in reactive-transport models.

Groundwater contamination with trichloroethylene (TCE) persists at many hazardous waste sites due to back diffusion from low-permeability zones such as clay lenses. In recent years, the abiotic reduction of TCE by reduced iron minerals has gained attention as a natural attenuation process, but there is uncertainty as to whether the process is fast enough to be effective. Pseudo-first-order rate constants have been determined in laboratory experiments and are reported in the literature for various sediments and rocks, as well as for individual reactive minerals. However, rate constants can vary between sites and aquifer materials. Reported values range over several orders of magnitude.

To assess the uncertainty and variability of pseudo-first-order rate constants, we compiled data reported in several studies. We built a statistical model based on a hierarchical Bayesian approach to predict probability distributions of rate constants at new sites based on this data set. We then investigated whether additional information about the sediment composition at a site could reduce the uncertainty. We tested two sets of predictors: reactive mineral content or the extractable Fe(II) content. Knowing the reactive mineral content reduced the uncertainty only slightly. In contrast, knowing the Fe(II) content greatly reduced the uncertainty because the relationship between Fe(II) content and rate constants is approximately log-log-linear. Using a simple example of diffusion-controlled transport in a contaminated aquitard, we show how the uncertainty in the predicted rate constants affects the predicted remediation times.