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Calibration of a subsurface reactive transport model to assess long-term efficiency of a Permeable Reactive Barrier

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Fe0 permeable reactive barriers (PRBs) are used to remediate groundwater pollution, especially in the case of VOCs (volatile organic compounds) contamination. These systems are installed in the subsurface where the naturally present hydraulic gradient makes the contaminated groundwater flow through the barrier. Inside the barrier the contaminants are removed by complex abiotic and biotic reactions. Precipitation of carbonate minerals reduces the barrier reactivity and permeability, hampering its long term efficiency.
To assess the long-term efficiency of a field-scale PRB installation, two column tests that replicate the field conditions were performed and a multi-component reactive transport model based on PHAST was developed to simulate the measured concentrations along the columns. The model employs kinetic formulations for the degradation of contaminants and for the precipitation of minerals. The model parameters were estimated using the nonlinear regression program PEST.
The statistics generated by PEST were used to adapt the model structure and identify insensitive and correlated parameters. Furthermore, confidence intervals at the optimal parameter set provide an estimation of parameter uncertainty and composite sensitivities for observation groups were valuable indicators of the information content of the measurements.
Long-term efficiency of the PRB under field conditions was estimated by forcing the calibrated model with a representative groundwater flow velocity, which is 300 times smaller than the inflow rate used in the lab experiments. Predictions with two different iron deactivation models are compared.