Reactive transport modeling using heterogeneous flow field data based on positron emission tomography

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Discrepancies between experimental and RTM results are often attributed to flow field heterogeneities. Positron emission tomography (PET) provides direct and quantitative insight into flow fields in complex media, such as barrier materials or porous rocks [1, 2].

Adsorption and transport of the herbicide 2-methyl-4-chlorophenoxyacetic acid (MCPA) in a homogeneous sand-goethite system were investigated as a function of pH. Interaction of MCPA with the solid surface was geochemically modeled using the charge distribution multisite complexation (CD-MUSIC) approach [3, 4]. Based on this calibrated surface complexation model, retardation of MCPA in transport experiments was significantly underestimated by 1D simulations with hydrodynamic parameter values obtained from a fit to the breakthrough of HTO as a conservative tracer.

On the basis of flow field data derived from PET measurements, heterogeneous flow observed for $^{18}F^{-}$ as a tracer was reproduced in 2D simulations (with flow velocities controlled by the pressure gradient field according to Darcy's law) assuming a peripheral zone with increased porosity and permeability. Using this flow model, the predicted breakthrough of MCPA was significantly more realistic compared to 1D simulations with the same chemical parameter values. Thus, this study demonstrates quantitatively that inconsistencies between static (batch) and dynamic (column) systems can be caused by heterogeneities in fluid flow, i.e., not necessarily by non-equilibrium conditions. This in turn highlights the need to consider real flow fields in predictive transport models.

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