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A stochastic assessment of the relevance of electrostatic effects during contaminant transport in heterogeneous groundwater systems

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The presence of aquitards, such as clays and clay-rich low permeability zones, can significantly impact the fate, transport, and remediation of subsurface contaminant plumes. These low-conductivity regions embedded in more permeable groundwater flow systems can effectively trap the contaminants and/or act as long-term secondary pollution sources. Besides the low hydraulic conductivity, the electrostatic properties of clay mineral surfaces exert key controls on the persistence, retention, and migration of charged solutes, major ions, and contaminants. Despite increasing efforts to investigate contaminant transport in low-permeability settings in recent decades, the understanding of charge induced electrostatic processes during field-scale contaminant transport in complex, heterogeneous subsurface systems containing both low and high permeability zones is still limited.

In this study [1], we present a stochastic assessment of the impact and relevance of microscale electrostatic effects on macroscopic, field-scale contaminant transport in heterogeneous groundwater systems involving spatially distributed clay zones. The investigation involves Monte Carlo simulations in ensembles of two-dimensional heterogeneous fields, comprising heterogeneous distributions of physical (i.e., hydraulic conductivity, porosity, tortuosity) and electrostatic (i.e., surface charge) properties, and compares scenarios with different combination and extent of physical and electrostatic processes. The simulations were performed with the multi-continua based reactive transport code, MMIT-Clay [2], considering a Nernst-Planck formulation of solute fluxes and an explicit treatment of the diffuse layer processes [3]. The results reveal that the microscopic electrostatic mechanisms within clay's diffuse layer can significantly accelerate or retard a particular contaminant depending on its charge, leading to considerably different solute breakthroughs and mass loading/release behaviors in low permeability inclusions. Furthermore, we show that such variations in the macroscale transport behavior, solely driven by charge interactions, are statistically significant over the ensembles of Monte Carlo realizations. The simulations also demonstrate that the omission of electrostatic processes, which is still a common practice in subsurface hydrology, can lead to substantial over- or underestimation of contaminant migration.

References:

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