Goldschmidt 2026 Abstract
https://doi.org/10.46427/gold2026.35538

Reactive transport modeling of rare earth elements in groundwaters: Fate and transport of emerging contaminants in groundwater flow systems

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The rare earth elements (REE) have been referred to as the "seeds of technology" because of their importance to the functioning of modern technologies [1]. However, their increasing use in high-tech industries suggests they are likely to become emerging environmental contaminants during the 21st century. Here, we examine the fate and transport of the REE neodymium (Nd) in shallow groundwater systems because Nd is a key ingredient for permanent magnets used in a wide variety of miniature electronics. We develop 1-D reactive transport models (RTM) that simulate advective- dispersive flow, mineral dissolution/precipitation, aqueous complexation, and sorption/desorption of Nd along a modeled flow path. Sorption/desorption is achieved by coupling surface complexation models (SCM) to the RTMs for goethite and HFO. Simulations employing SCMs are compared to the linear isotherm approach, which is still in common use. All models assume an imbibition phase where Nd-polluted water (1 mmol kg^{-1}) infiltrates the aquifer. Subsequently, the aquifer is flushed with Nd-free water to evaluate the time required to remediate the aquifer. Simulations that employ SCMs produce similar results with sharp adsorption fronts and nearly saturated sorption sites (e.g., 91% of Nd sorbed for goethite SCM). In contrast, the desorption front is highly attenuated with a long tail. Consequently, Nd required more than 30 pore volumes of "clean" water to be flushed through the aquifer before Nd concentrations in the effluent approached values reported in uncontaminated aquifers. For the linear isotherm, the adsorption and desorption fronts are symmetrical and mimic conservative Br^-, although the advective front for Nd trails that of Br^-. The K_d approach under predicts the persistence of the tailing desorption front by more than an order of magnitude compared to the goethite SCM. Finally, simulations with or without dissolved inorganic carbon (DIC) at both pH 7 and pH 8.3, are strongly affected by the presence or absence of DIC. This is because DIC favors the formation of aqueous carbonate complexes, which inhibits Nd sorption compared to simulations without DIC, where the chief aqueous species is the highly surface reactive, free metal ion, Nd^{3+}.

[1] Martinez-Gomez et al. (2016) Inorg. Chem. 55, 10,083-10,089.