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Modelling field-scale dispersion in heterogeneous groundwater systems with multi-component reactions

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Many environmental problems require assessment of non-linear, multi-component reactions within natural subsurface flow systems exhibiting large physical and biogeochemical heterogeneity. Commonly, spatial variability in groundwater flow is a major contributor to physical field scale solute dispersion, which often is accounted for by use of a large dispersion coefficient in Eulerian reactive-transport models. However, this approach may imply unrealistic mixing, thereby introducing artificial effects on chemical reactions and impair model results. Alternatively, a LaSAR (Lagrangian Stochastic Advection-Reaction) approach, which is based on the conceptual model of a flow field resolved into streamtubes, each characterized by a water travel time, can be used [e.g. 1].

In this study, we assess the spreading of acid mine drainage in the surroundings of a mill tailings deposit, as one environmentally relevant example of a multi-component reaction system with relatively high solute concentrations, and compare results from the two different model approaches. In the LaSAR-PHREEQC approach [2], we use PHREEQC [3] to quantify the geochemical processes along an individual streamtube. We interpret time dependent concentrations at different positions along the streamtube as representing streamtubes of different travel times, and calculate field scale concentrations by integrating over the distribution of travel times that represents field scale physical dispersion. In the Eulerian approach, we let PHREEQC handle both reactions and advective-dispersive transport, using a large dispersion coefficient that corresponds to the dispersion implied by the travel time distribution.

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Geochemical coupled transport code for variably saturated flow conditions: Metal leaching in a podzol

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To model multicomponent transport during transient variably-saturated flow in the vadose zone, complex models are needed. Ideally such models should incorporate simultaneous solutions for the water flow equations in variably-saturated porous media, solute transport and equilibrium or kinetically homogeneous and heterogeneous geochemical reactions. A new coupled model, presented here, combines two comprehensive exisiting models: HYDRUS-1D [1] and PHREEQC [2]. HYDRUS-1D is an one-dimensional finite element model simulating the movement of water, heat and multiple solutes in variably-saturated heterogeneous or layered soils subject to a variety of atmospheric and other boundary conditions. PHREEQC is a computer program simulating the behavior of complex chemical systems including a wide variety of homogeneous and heterogeneous reactions. These reactions include aqueous speciation and complexation, ion exchange, surface complexation, and mineral dissolution/precipitation. This coupled code provides thus a strong tool to interpret and analyse all kind of reactive transport experiments under different flow conditions, especially those including interaction between the solution and the mineral surfaces.

Different verification examples including several interrelated processes and pathways are compared with an independent model (CRUNCH [3]) for steady state flow conditions. A hypothetical problem illustrates the possibility of the new code by simulating heavy metal transport in a podzol and simulating the long term behaviour of these heavy metal under natural (rainfall and evaporation) flow conditions. Transport of Cd, some other heavy metals (Cu, Pb, Zn) and major cations (Mg, Ca, Na, K) is modelled and simulations are compared with measured outflow concentrations from an acid sandy podzol soil.

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