Modeling multicomponent ionic transport in groundwater with IPhreeqc coupling: Electrostatic interactions and geochemical reactions in homogeneous and heterogeneous domains - DTU Orbit (23/12/2018)

Modeling multicomponent ionic transport in groundwater with IPhreeqc coupling: Electrostatic interactions and geochemical reactions in homogeneous and heterogeneous domains

The key role of small-scale processes like molecular diffusion and electrochemical migration has been increasingly recognized in multicomponent reactive transport in saturated porous media. In this study, we propose a two-dimensional multicomponent reactive transport model taking into account the electrostatic interactions during transport of charged ions in physically and chemically heterogeneous porous media. The modeling approach is based on the local charge balance and on the description of compound-specific and spatially variable diffusive/dispersive fluxes. The multicomponent ionic transport code is coupled with the geochemical code PHREEQC-3 by utilizing the IPhreeqc module, thus enabling to perform the geochemical calculations included in the PHREEQC's reaction package. The multicomponent reactive transport code is benchmarked with different 1-D and 2-D transport problems. Successively, conservative and reactive transport examples are presented to demonstrate the capability of the proposed model to simulate transport of charged species in heterogeneous porous media with spatially variable physical and chemical properties. The results reveal that the Coulombic cross-coupling between dispersive fluxes can significantly influence conservative as well as reactive transport of charged species both at the laboratory and at the field scale.

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