A Mean Electrostatic Model for Non-Fickian Transport through Heterogeneous Clay

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Short Abstract (within 80 words)

We present here a new model, CrunchShale, that simulates non-Fickian diffusion of ions through clay and clay-rock by taking into account the charge and transport characteristics of the electrical double layer (EDL).

Full version

We present here a new model, CrunchShale, that simulates non-Fickian diffusion of ions through clay and clay-rock by taking into account the charge and transport characteristics of the electrical double layer (EDL). The model makes use of a set of newly developed routines that calculate accurately fluxes between adjacent grid cells with differing charge properties (e.g., bulk water and charged clay). In addition, the model is able to consider time-dependent EDL lengths (or volumes) resulting from salinity changes. The model is based on a global implicit solve of the reaction-diffusion equation with explicit consideration of a bulk water continuum and an EDL continuum in which electrostatic effects are treated. The global implicit approach, while requiring additional exertions and care on the part of the model developer, offers the advantage of improved computational efficiency over operator split treatments of the diffusion-reaction equation, mostly due to the ability to use larger time steps. The model is applied to a set of benchmarks in which adjacent domains have very different charge characteristics (e.g., bulk water adjacent to clay) and to a 2-D heterogeneous clay rock. In addition, the model is applied to an *in-situ* field experiment conducted in the Opalinus Clay in which anions, cations, and uncharged species diffuse out of a borehole at differing rates.