Contribution ID: **660** Type: **Poster (+) Presentation**

Global random walk solvers for flow and multi-component reactive transport in heterogeneous porous media

Wednesday, 2 June 2021 10:00 (1 hour)

Flow and multi-component reactive transport in unsaturated/saturated porous media are modeled by ensembles of computational particles moving on regular lattices according to specific random walk rules. The occupation number of the lattice sites is updated with a global random walk (GRW) procedure which simulates the evolution of the ensemble with computational costs comparable to those for a single random walk simulation in sequential procedures. To cope with the nonlinearity and the degeneracy of the Richards equation the GRW flow solver uses linearization techniques similar to the L-scheme developed in finite element/volume approaches. Reactive transport schemes, coupled with the flow solver via numerical solutions for saturation and water flux, are implemented in splitting procedures. Diffusion-advection steps are solved by GRW algorithms using either biased or unbiased random walk rules. Since the number of particles in GRW simulations can be as large as the number of molecules involved in chemical reactions, one avoids the cumbersome problem of rescaling particle densities to approximate concentrations. Reaction steps are therefore formulated in terms of concentrations, as in deterministic approaches. The numerical convergence of the new reactive scheme is demonstrated by comparison with analytical solutions of a model problem for nonlinear bi-molecular reactions. Coupled flow-reactive transport problems of contaminant biodegradation based on a Monod type model are further solved and the influence of flow nonlinearity/degeneracy and of the spatial heterogeneity of the medium is investigated numerically.

Time Block Preference

Time Block A (09:00-12:00 CET)

References

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Student Poster Award

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