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Process-based, mechanistic modeling of dynamic structures at the pore scale

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Although advanced imaging techniques now allow snapshots even down to the nanoscale, the evolution of elemental distributions, different liquid phases and dynamic microbial processes still cannot always be assessed experimentally. Consequently mechanistic models operating at the pore scale facilitate the study and understanding of such phenomena.

We present a versatile hybrid discrete continuum modeling approach combining cellular automata and partial differential equations which integrates the complex coupling of biological, chemical, and physical processes. Dynamic liquid and gas phases, diffusive processes for solutes, mobile bacteria transforming into immobile biomass, and ions are prescribed by means of partial differential equations. Furthermore the solid phase is dynamic, e.g. through aggregation of soil particles, growth of biofilms or the distribution of particulate organic matter in the system [1, 2, 3, 4].

Finally mathematical homogenization techniques are used to show a way to incorporate information as the diffusivity from the pore scale to macroscale models [1,5].

Applications include structure formation of clay minerals [4], the interplay of liquid phase connectivity, substrate supply and organic matter turnover [3], or the quantification of the effective diffusivity by upscaling on 3D geometries from CT scans of a loamy and a sandy soil.

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