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Hybrid discrete-continuum modeling for transport, biofilm development and solid restructuring including electrostatic effects

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We want to present an approach for the mathematical, mechanistic modeling and numerical treatment of processes leading to the formation, stability, and turnover of soil micro-aggregates. This aims at deterministic aggregation models including detailed mechanistic pore-scale descriptions to account for the interplay of geochemistry and microbiology, and the link to soil functions as, e.g., the porosity.

We therefore consider processes at the pore scale and the mesoscale (laboratory scale). At the pore scale transport by diffusion, advection, and drift emerging from electric forces can be taken into account, in addition to homogeneous and heterogeneous reactions of species. In the context of soil micro-aggregates the growth of biofilms or other glueing substances as EPS (extracellular polymeric substances) is important and affects the structure of the pore space in space and time. This model is upscaled mathematically in the framework of (periodic) homogenization to transfer it to the mesoscale resulting in effective coefficients/parameters there. This micro-macro model thus couples macroscopic equations that describe the transport and fluid flow at the scale of the porous medium (mesoscale) with averaged time- and space-dependent coefficient functions. These functions may be explicitly computed by means of auxiliary cell problems (microscale). Finally, the pore space in which the cell problems are defined is time and space dependent and its geometry inherits information from the transport equation's solutions. The microscale problems rely on versatile combinations of cellular automata and discontiuous Galerkin methods while on the mesoscale mixed finite elements are used. The numerical simulations allow to study the interplay between these processes.