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Seven years of research on process-based, mechanistic modeling of aggregation and its drivers

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Advanced imaging techniques now allow to take snapshots of soils even down to the nanoscale. Nevertheless, assessing the temporal evolution of elemental distributions, distinguishing different liquid phases and identifying dynamic microbial processes is experimentally still challenging. Consequently mechanistic models operating at the pore scale facilitate the study and understanding of phenomena shaping soil structures as, e.g., carbon turnover, and vice versa.

We present an overview of 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 gaseous 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, the addition and decomposition of particulate organic matter, or the mechanical influence of roots and their exudates. The virtual soil structures rely on micro-CT images or particle libraries derived from dynamic image analysis of water-stable aggregates.

Applications include structure formation of clay minerals, the interplay between soil structural dynamics and organic matter turnover, or the impact/importance of liquid phase connectivity and substrate supply. Finally the mathematical homogenization technique is used to show a way how to incorporate information from the pore scale to macroscale models, e.g. by coupling microscale carbon turnover to profile-scale CO2 transport.