Discrete-continuum multiscale model for microaggregates in soils

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Microaggregates are the fundamental building blocks of soils and thus important for their structure, properties, and functions. Although there has been much research investigating the dynamics, stability, and structure of soil microaggregates, there is still a substantial lack in quantifying the relationships between the major driving forces. The major driving forces are known to be soil fauna, microorganisms, roots, inorganics, and physical processes. Mathematically based modeling can facilitate the understanding of self-organization, formation, build-up, composition, properties and stability of microaggregates, provided that these major driving forces are taken into account. We assess the complex coupling of biological, chemical and physical processes with the help of a mechanistic modeling approach in order to create a process-based tool to study
the interplay of relevant mechanisms in silico and consequently gain a model-based understanding of the microaggregate dynamics in soils.

In our framework, dynamic wetting (fluid) and non-wetting (gas) phases are included, in which the diffusion of mobile bacteria, possibly transforming into immobile biomass, sticky agent (EPS), nutrients, and ions are prescribed by means of partial differential equations. In particular a kinetic Langmuir isotherm for heterogeneous surface reactions and a Henry condition for the transfer from/into the gas phase are applied. The model further includes the development of the biomass phase and structural changes in the solid phase originating from stabilizing sticky agents or electrostatic attraction/repulsion. Arbitrary shapes for the potentially charged solid building units (e.g., spherical, needle-like, or platy particles), and also their compositions are incorporated into the model. The interplay between and within the different phases results in a structural self-organization of the respective phases which defines the time-dependent composition of the computational domain. It is realized in a cellular automaton framework while the partial differential equations are discretized by a fully implicit local discontinuous Galerkin method.

The operational, comprehensive model allows to study structure formation as a function of the size and shape of the solid particles. Moreover, the effect of attraction and repulsion by charges
is thoroughly discussed. Another main objective of this research is to examine the strong interplay between functional properties and geometric structure. To that end standard homogenization results are used to compute the soil's characteristic properties such as porosity or effective diffusion tensors for the resulting complex and time-dependent geometries.