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Towards a rigorous mesoscale modeling of reactive flow and transport in an evolving porous medium and its applications to soil science

Nadja Ray, Andreas Rupp, and Peter Knabner
Department of Mathematics, University of Erlangen-Nürnberg, Erlangen, Germany (ray@math.fau.de)

Soil is arguably the most prominent example of a natural porous medium that is composed of a porous matrix and a pore space. Within this framework and in terms of soil's heterogeneity, we first consider transport and fluid flow at the pore scale. From there, we develop a mechanistic model and upscale it mathematically to transfer our model from the small scale to that of the mesoscale (laboratory scale). The mathematical framework of (periodic) homogenization (in principal) rigorously facilitates such processes by exactly computing the effective coefficients/parameters by means of the pore geometry and processes.
In our model, various small-scale soil processes may be taken into account: molecular diffusion, convection, drift emerging from electric forces, and homogeneous reactions of chemical species in a solvent. Additionally, our model may consider heterogeneous reactions at the porous matrix, thus altering both the porosity and the matrix. Moreover, our model may additionally address biophysical processes, such as the growth of biofilms and how this affects the shape of the pore space. Both of the latter processes result in an intrinsically variable soil structure in space and time.
Upscaling such models under the assumption of a locally periodic setting must be performed meticulously to preserve information regarding the complex coupling of processes in the evolving heterogeneous medium. Generally, a micro-macro model emerges that is then comprised of several levels of couplings: Macroscopic equations that describe the transport and fluid flow at the scale of the porous medium (mesoscale) include 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.
Numerical computations using mixed finite elements and potentially random initial data, e.g. that of porosity, complement our theoretical results. Our investigations contribute to the theoretical understanding of the link between soil formation and soil functions. This general framework may be applied to various problems in soil science for a range of scales, such as the formation and turnover of microaggregates or soil remediation.