

## **MICRO-MACRO MODELS : THE NEXT GENERATION MODELS FOR REACTIVE FLOW AND TRANSPORT PROBLEMS IN POROUS MEDIA?**

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*Keywords:* Upscaling, multiscale modeling, micro- macro model, evolving porous medium, dissolution/precipitation.

In porous media and other complex media with different length scales, (periodic) homogenization has been successfully applied for several decades to arrive at macroscopic, upscaled models, which only keep the microscopic information by means of a decoupled computation of "effective" parameters on a reference cell. The derivation of Darcy's law for flow in porous media is a prominent example. Numerical methods for this kind of macroscopic models have been intensively discussed and in general are considered to be favourable compared to a direct microscale computation. On the other hand, if the interplay of processes becomes too complex, e.g. the scale separation does not act in a proper way, the porous medium itself is evolving, ..., the upscaled models obtained may be micro-macro models in the sense, that the coupling of the macroscopic equations and the equations at the reference cell is both ways, i.e. at each macroscopic point a reference cell is attached and the solution in the reference cell depends on the macroscopic solution (at that point) and the macroscopic solution depends on the microscopic solutions in the reference cells. At the first glance such models seem to be numerically infeasible due to their enormous complexity (in  $d + d$  spatial variables). If on the other hand this barrier can be overcome, micro-macro models are no longer a burden but a chance by allowing more general interaction of processes (evolving porous media, multiphase flow, general chemical reactions, ...), where the microscopic processes "compute" the constitutive laws, which need longer be assumed (similar to the concept of heterogeneous homogenization). We will discuss various examples and in particular numerical approaches to keep the numerical complexity in the range of pure macroscopic models.

### **References**

- [1] S. Molins and P. Knabner, *Multiscale Approaches in Reactive Transport Modeling*, Reviews in Mineralogy & Geochemistry 85, pp. 27-48, 2019.
- [2] N. Ray, J. Oberlander and P. Frolkovic, *Numerical investigation of a fully coupled micro-macro model for mineral dissolution and precipitation*, Comput. Geosci., 2019.
- [3] A. Rupp, KU. Totsche, A. Prechtel and N. Ray, *Discrete-Continuum Multiphase Model for Structure Formation in Soils Including Electrostatic Effects*, Front. Environ. Sci. 6, Art.Nr. 96, 2018.

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