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Micro-macro models for reactive two-mineral systems

Wednesday, 1 June 2022 11:00 (15 minutes)

Porous media naturally exhibit a heterogeneous structure including two different spatial scales: The pore/micro-scale is the fundamental scale, on which flow and reactive transport processes take place whereas the macro-scale, i.e. the scale of the porous medium itself, is of practical relevance for many geoscientific applications. (Periodic) homogenization has been successfully applied for several decades to bridge these scales and to arrive at macroscopic (upscaled) models, which only keep the microscopic information by means of a de-coupled computation of 'effective'parameters on a so-called unit cell. However, the situation becomes more intertwined, if competing minerals dissolve and precipitate and consequently dynamically alter the porous medium's structure and its bulk properties.

In this talk, we discuss the formal upscaling and numerical investigation in such a situation. We start from a pore-scale model for reactive flow and transport in an evolving porous medium being composed of two distinct minerals. We derive an effective micro-macro model by formal two-scale asymptotic expansion in a level-set framework. For such a micro-macro model, the macroscopic equations (reactive flow and transport equations) and the equations posed at the unit cell are fully coupled: At each macroscopic point a unit cell is attached and the solution to the equations on the unit cell depends on the macroscopic solution at that point. This is due to the fact that the macroscopic concentration triggers mineral reactions, which alter the unit cells' geometrical structure. On the other hand, the macroscopic solution depends on the microscopic solutions by means of 'effective'hydrodynamic parameters such as porosity, reactive surface, diffusion, and permeability.

Finally, we present numerical simulations of the fully coupled micro-macro problem with application to dissolution of calcite and dolomite. Our results can be found in [1-3].

[1] S. Gärttner S., P. Frolkovič, P. Knabner, N. Ray. "Efficiency of micro-macro models for reactive two-mineral systems."accepted in SIAM Journal of Multiscale modeling and Simulation, 2021

[2] S. Gärttner, P. Frolkovič, P. Knabner, and N.Ray. "Efficiency and Accuracy of Micro-Macro Models for Mineral Dissolution/Precipitation."Water Resources Research 56(8), 2020.

[3] N.Ray, J. Oberlander, and P. Frolkovič. "Numerical investigation of a fully coupled micro-macro model for mineral dissolution and precipitation."Computational Geosciences 23, 2018.

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References

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Participation

Unsure

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