Geophysical Research Abstracts
Vol. 21, EGU2019-16463, 2019
EGU General Assembly 2019

Multilevel pore-scale reactive-coupled transport model for dissolution and precipitation reactions on a rough fracture surface

Anna Varzina (1,2), Janez Perko (2), Li Yu (2), and Diederik Jacques (2)

(1) KU Leuven, Civil Engineering Department, Heverlee, Belgium (anna.varzina@kuleuven.be), (2) Belgian Nuclear Research Centre, Engineered and Geosystems Analysis, Institute for Environment, Health and Safety, Belgium (anna.varzina@sckcen.be, janez.perko@sckcen.be, li.yu@sckcen.be, diederik.jacques@sckcen.be)

Natural fractures in porous media exhibit typically an irregular surface with multiple peaks or pits of variable heights. The irregular surface influences flow and transport processes and also geochemical reactions including precipitation and dissolution. We present a new concept for precipitation and dissolution modelling at the pore-scale. In our particular implementation, we used the lattice-Boltzmann method to solve the governing transport equations using YANTRA (Patel et al., 2014). The solver is coupled with PHREEQC (Parkhurst et al., 2013) for geochemical calculations including precipitation and dissolution. The pore-scale model allows for representing the details of the surface roughness obtained with e.g. micro-profilometry measurements at a resolution of 1 μm in horizontal dimension and 0.01 μm in the vertical dimension.

In a pore scale model, nodes are often described as either solid or pores. However, at the micrometer scale used to represent the surface roughness, a precipitating phase does not always fill the complete pore space, some residual pore space may remain in a precipitated layer covering the rock material. Consequently, mass exchange between the fluids in the pores and the underlying rock material is still possible. Within a multilevel pore-scale model, both resolved pores (solid/pore nodes explicitly represented in the model) and unresolved pores (porous system within a computational node) are present which enables to account for the incomplete filling of nodes during precipitation. Similarly, it is used for nodes in which the solid phase is dissolving or to represent gel pores (size much smaller than the resolution of the pore-scale model).

The last aspect of our concept is the mechanism to control the amount of precipitation in a node. The solubility of solid phases increases with decreasing pore radius. Thus, precipitation will stop before all (unresolved) pores are filled and complete clogging of a node is avoided. The concept of the pore-size dependent solubility will control the residual pore space in a precipitating layer.

The presentation will illustrate these concepts for the simulation of precipitation and dissolution in a rough fracture using a pore-scale model.

Parkhurst, D.L. and Appelo, C.A.J. (2013) Description of Input and Examples for PHREEQC Version 3 — A Computer Program for Speciation , Batch-Reaction , One-Dimensional Transport , and Inverse Geochemical Calculations Chapter 43 of Section A, Groundwater Book 6, Modeling Techniques.

Patel, R.A., Perko, J., Jacques, D., De Schutter, G., Van Breugel, K. and Ye, G. (2014) A versatile pore-scale multicomponent reactive transport approach based on lattice Boltzmann method: Application to portlandite dissolution. Physics and Chemistry of the Earth 70-71, 127-137.