PORE-SCALE MODELLING OF MULTIPHASE REACTIVE FLOW

Cyprien Soulaine, Sophie Roman and Julien Maes

Keywords: Pore-scale, dissolution, immiscible flow, microfluidics.

In this talk, we discuss the recent progress in the modelling of multiphase reactive transport at the pore-scale. The dynamics modelling of reactive flow phenomena in reactive environment is complex because it involves the tracking of multiple interfaces that evolve as a function of the details of the reactive transport: on the one hand, the fluid/fluid interface is subject to surface tension forces, on the other hand, the fluid/solid interface moves with chemical reaction at the mineral surface. The approach developed here employs an extended Darcy–Brinkman–Stokes formulation that accounts for the interfacial tension between the two immiscible fluid phases and the moving contact line at the mineral surface [1]. The mass transfer across fluid/fluid interfaces is modeled using an improved Continuous Species Transfer technique that will be described [2, 3]. The simulation framework is validated using an experimental microfluidic device that provides time-lapse images of the dissolution dynamics. The set-up involves a single-calcite crystal and the subsequent generation of CO_2 bubbles in the domain. The experimental dataset can be used to verify other numerical codes along the lines of the recent benchmark on single-phase dissolution at the pore-scale [4].

References

[1] C. Soulaine, S. Roman, A. Kovscek, and H.A. Tchelepi, *Pore-scale modelling of multiphase reactive flow. Application to mineral dissolution with production of CO_2*, Journal of Fluid Mechanics, 855, pp. 616-645, 2018.

[2] J. Maes and C. Soulaine, *A new compressive scheme to simulate species transfer across fluid interfaces using the Volume-Of-Fluid method*, Chemical Engineering Science, 190, pp. 405-418, 2018.

[3] J. Maes and C. Soulaine, *A unified single-field Volume-of-Fluid-based formulation for multi-component interfacial transfer with local volume changes*, Journal of Computational Physics, 2019

[4] S. Molins, C. Soulaine, N.I. Prasianakis, A. Abbasi, P. Poncet, A.J.C Ladd, V. Starchenko, S. Roman, D. Trebotich, H.A. Tchelepi and C.I. Steefel *Simulation of mineral dissolution at the pore scale with evolving fluid-solid interfaces: Review of approaches and benchmark problem set*, Computational Geosciences, 2019

C. Soulaine
Earth Sciences Institute of Orleans
cyprien.soulaine@cnrs-orleans.fr

S. Roman
Earth Sciences Institute of Orleans
sophie.roman@univ-orleans.fr

J. Maes
Heriot-Watt University
j.maes@hw.ac.uk