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A BENCHMARK FOR THE NUMERICAL SIMULATION OF PORE-SCALE MINERAL DISSOLUTION WITH FLUID-SOLID INTERFACE EVOLUTION

P. Poncet, S. Molins, C. Soulaine, N. I. Prasianalis, A. Abbasi, A. J. C. Ladd, V. Starchenko, S. Roman, D. Trebotich, H. Tchelepi, C. I. Steefel

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This talk presents a benchmark problem for the simulation of single-phase flow, reactive transport and solid geometry evolution at the pore scale [1]. The problem is organized in three parts that focus on specific aspects: flow and reactive transport, dissolution-driven geometry evolution in two dimensions, and a three-dimensional dissolution-driven geometry evolution including an experimental validation.

Five codes are used to obtain the solution to this benchmark problem, including Chombo-Crunch, OpenFOAM-DBS, a lattice Boltzman code, Vortex method, and dissolFoam. These codes cover a good portion of the wide range of approaches typically employed for solving pore-scale problems in the literature, including discretization methods, characterization of the fluid-solid interfaces, and methods to move these interfaces as a result of fluid-solid reactions. Among the discretization methods, one can find finite volumes, Lagrangian methods, grid based methods (stochastic and deterministic).

Results from the simulations performed by the five codes show remarkable agreement both quantitatively based on upscaled parameters such as surface area, solid volume and effective reaction rate and qualitatively based on comparisons of shape evolution. This outcome is especially notable given the disparity of approaches used by the codes.

References

[1] 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*, to appear in Computational Geosciences, 2019.

P. Poncet LMAP, UMR CNRS 5142, E2S-UPPA, France philippe.poncet@univ-pau.fr

S. Molins, D. Trebotich, C. I. Steefel Lawrence Berkeley National Laboratory, USA

N. Prasianakis, A. Abbasi Paul Scherrer Institute, Zürich, Switzerland

V. Starchenko Oak Ridge National Laboratory, USA C. Soulaine, S. Roman Institute of Earth Sciences of Orleans, UMR CNRS 7327

A. J. C. Ladd University of Florida, USA

H. Tchelepi Stanford University, USA