

A semi-Lagrangian numerical method for the simulation of precipitation/crystallization at the pore scale of porous media.

Sarah Perez¹, Jean-Matthieu Etancelin¹ and Philippe Poncet¹

¹ Université de Pau et des Pays de l'Adour, E2S UPPA, CNRS, LMAP, Pau, France.

e-mail address: philippe.poncet@univ-pau.fr

This talk presents advances in numerical methods for the simulation of single-phase flow, reactive transport and solid geometry evolution at the pore scale, involving dissolution, precipitation and crystallization, and will be structured in three parts.

Firstly, we will present the semi-Lagrangian approach of the problem and the related models [1], involving particle/Lagrangian treatment of the transport phenomena and reactions, and underlying grids for the diffusion and flow computation. Frequent remeshing procedure is required in order to keep particles on a regular network, in order to avoid holes of information and particle accumulation. This remeshing technique is either high order but can generate sign changes, which is unacceptable in chemistry, or low order but leads to spurious diffusion. An a posteriori kernel selection will be provided in order to deal with this difficulty.

Secondly, we will describe the validation of the method by a dissolution process of 2D and 3D calcite cores (including experimental validation) with a benchmark approach [2]. Five codes are used to obtain the solution to this benchmark problem, including Chombo-Crunch, OpenFOAM-DBS, a lattice Boltzmann code, the present semi-Lagrangian 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. 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.

Thirdly, we will focus on the simulations of precipitation and crystallization. This last aspect can include either the rheology of precipitation [3] or the crystal growth, and the ability to manage the divergence of the velocity induced by the reaction and its related evolution of the global volumic mass. Indeed, in this context, a fast change of state from liquid to solid means incompressible but non-divergence-free flows.

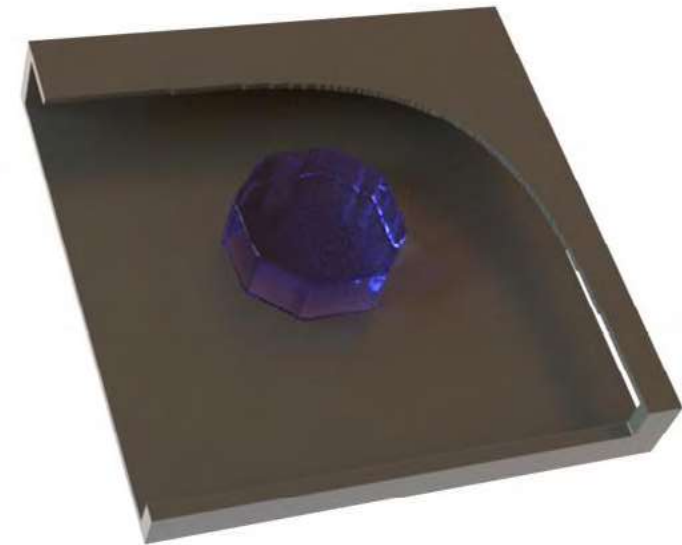


FIG. 1. Rendering of the grain as used for dissolution simulations and experiments.

Open-access references

[1] R. Chatelin and P. Poncet, A hybrid grid-particle method for moving bodies in 3D Stokes flow with variable viscosity, *SIAM J. Sci. Comp.* 35(4), B925–B949 (2013). DOI: 10.1137/120892921

[2] S. Molins, C. Soullain, N. I. Prismanakis, A. Abbasi, P. Poncet, A. J. C. Ladd, V. Starchenko, S. Roman, D. Trebotich, H. A. Tehelepi, and C. I. Steefel, Simulation of mineral dissolution at the pore scale with evolving fluid-solid interfaces: Review of approaches and benchmark problem set, *Comput. Geosci.* (2020). DOI: 10.1007/s10596-019-09903-x

[3] D. Sanchez, L. Hume, R. Chatelin, P. Poncet, Analysis of non-linear Stokes problem coupled to transport-diffusion for shear-thinning heterogeneous microscale flows, applications to digital rock physics and mucociliary clearance,