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Simulation of reactive flows on 3D pore-scale geometries using particle methods, and their impact on macroscopic properties: applications to dissolution, precipitation and crystallization.

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SUMMARY

The study of reactive flows within a porous medium is an essential step in the comprehension and management of the geochemical effects arising in CO2 capture and storage.

While the continuum approach at the Darcy scale finds its effectiveness in modeling the behaviour of natural reservoirs, simulations on pore-scale geometries provide significant insights into the fluid-mineral interfaces and the monitoring of their evolutions due to complex chemical reactions. Through homogenization theory and numerical modeling, we are able to simulate the effects of reactive processes occurring at this pore-scale and predict the impact on the medium main effective properties at the macroscale. The wide range of pore-scale modeling approaches includes, among others, discretization methods, pore network models, lattice Boltzmann method, and particle methods.

This talk will focus on the latter category, and present the advances in the semi-Lagrangian method involving a particle treatment of the chemical species transport coupled with underlying grids for the hydrodynamic [1]. The numerical method developed shows remarkable agreement with the others pore-scale modeling methodologies but also with experimental results, providing cross-validation in a calcite dissolution benchmark [2].

We will also present simulations of precipitation and crystallization in 3D porous media with a two-scale porosity. It includes nucleation of the dissolved chemical species and crystal growth due to their interactions with the solid interfaces. A Particle-Strength-Exchange method [3] is dedicated to the approximation of Archie's law term with heterogeneous diffusion coefficients, and the numerical method is extended to GPU-CPU computing using HySoP HPC platform developed at UPPA-LJK-CNAM.

Keywords: Pore-scale modeling, reactive flow, Darcy-Brinkman, porous media

AMS Classification: 76-10, 76S05, 65M22

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