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On the Challenges of Pore Scale Models to Capture Minerals Precipitation and Dissolution in microfluidic setups: A Combined Computational-Lab-on-a-Chip Approach

Tuesday, 31 May 2022 17:30 (15 minutes)

Minerals precipitation and dissolution dominate and control a large number of geochemical processes in porous media. The precipitation/dissolution reactions alter the pore space and its connectivity in a way that has a complex feedback on the solutes transport. Pore-scale reactive transport models provide the numerical framework to understand and predict such interactions. While incorporation of minerals dissolution into pore-scale reactive transport models has been extensively studied in the past[1], incorporation of minerals precipitation is still scarce and lacks experimental validation[2]. This can be explained by the fact that precipitation is more fundamentally complex process compared to dissolution. Precipitation involves creation of a new mineral phase via nucleation, which is a purely molecular phenomenon occurring at a scale much smaller than the pore-level resolution. This in turn represents a challenge for pore scale models to accurately predict minerals precipitation, and more investigations are still needed.

In this work, we investigate mineral precipitation processes by combining lab-on-a-chip experimental investigations with pore-scale modeling. The experiments are a set of microfluidics in which Celestine mineral precipitate[3]. The computational model is a pore-scale multi-component model incorporating fluid flow, solutes transport, aqueous speciation, nucleation modelled at a sub-voxel level, and crystals growth and dissolution. In the developed model, the Lattice Boltzmann Method (LBM) was used to model fluid flow and solute transport, while the nucleation effects are incorporated using the classical nucleation theory, and chemical reactions were modeled using the Law of Mass Action (LMA). Coupling between the chemical reactions and solutes transport is done using a sequential non-iterative approach (SNIA). Reactive transport simulations were accelerated using machine learning techniques [4]. During the experiments, the spatiotemporal evolution of the precipitating/dissolving crystals were monitored using optical microscopy. This allowed direct comparison between the modeling and the experimental results in the following aspects: induction time, location of the first crystallite, crystal shape, crystal orientation, and crystal growth/dissolution rates.

Our results highlight that computational and experimental microfluidics is a promising tool to unravel the coupled physiochemical processes occurring in geological porous media. Several experimental observations were successfully reproduced such as the flow and concentration fields, precipitation induction times, and reaction rate at crystal-fluid interfaces. However, it still remains challenging to predict the exact location of the first crystallite and the number of critical nuclei which will form into crystals.

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References

[1] Molins, Sergi, et al. “Simulation of mineral dissolution at the pore scale with evolving fluid-solid interfaces: Review of approaches and benchmark problem set.” Computational Geosciences (2020): 1-34.
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[3] Poonoosamy, Jenna, et al. “A microfluidic experiment and pore scale modelling diagnostics for assessing mineral precipitation and dissolution in confined spaces.” Chemical geology 528 (2019): 119264.
[4] Prasianakis, Nikolaos I., et al. “Neural network based process coupling and parameter upscaling in reactive transport simulations.” Geochimica et Cosmochimica Acta 291 (2020): 126-143.

Time Block Preference

Time Block B (14:00-17:00 CET)

Participation

Unsure

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