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Towards Digital Twin of Carbonate Precipitation Experiments: An Integrated Physics-based Machine-Learning Framework for Modeling of Reactive Transport Processes

HAONAN PENG[1,2], ASHISH RAJYAGURU[3], ATHANASIOS MOKOS[1], ENZO CURTI[3], DANIEL GROLIMUND[3], SERGEY V. CHURAKOV[1,2] AND NIKOLAOS PRASIANAKIS[1]

[1]Paul Scherrer Institute
[2]University of Bern
[3]Paul Scherrer Institut

Presenting Author: haonan.peng@psi.ch

Formation of secondary mineral precipitates within porous media is a complex process as it involves strong coupling between mineral reactivities (nucleation, precipitation kinetics, solubility) and diffusion of ionic species. To model such systems, pore-scale models based on the Lattice-Boltzmann method and supported by advanced machine learning techniques are being developed, which involve the integration of dynamically derived lab-based experimental observations with numerical simulations.

In this study, a first prototype of the digital twin (increased realism model with the possibility of near real-time calculations) was developed and used to model solute diffusion in a counter-diffusion experiment aiming at studying the in-situ nucleation and growth of $CaCO_3$ polymorphs (vaterite, aragonite, calcite, amorphous $CaCO_3$) in silica-gel. These experiments were conducted using a counter diffusion setup (two reservoirs at bulk conditions connected by a sub-millimetre capillary at confined conditions). Information on nucleation, crystal growth and morphology and ionic diffusion was obtained via coupled chemical imaging (XRF/XRD) at the Swiss Light Source (SLS, Paul Scherrer Institute).

For the modelling, we used the three-dimensional multi-component lattice Boltzmann method (LBM) as the basis framework. We developed a hybrid CUDA-MPI code coupled with a Neural Network-based surrogate model for the geochemical solver, resulting in a significant speed-up of the calculations and overall analysis. At a first level of complexity, diffusion and simplified chemistry were implemented to reproduce the experimental observations of crystal growth. The experimentally observed crystal growth locations were used as seeds for the model. The complementary use of the numerical model along with the experiments allows us to assess the local composition at the crystal-liquid interface during growth at high resolution. Further research is required to explore more complex and advanced methods to incorporate additional physical and chemical processes into our model, such as non-classical nucleation theory and more complex chemistry.