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A new probabilistic nucleation model to predict crystal growth in porous medium

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Nucleation is the first step of any mineral precipitation and crystal growth process. It is often overlooked in studying the reactive transport phenomena. Nucleation controls the location and timing of crystal formation in a porous structure. The spatial distribution of stable secondary nuclei is crucial to predict hydrodynamics of the porous medium after mineral precipitation precisely. To better understand the nucleation process, we developed a new probabilistic nucleation approach in which the induction time is considered a random variable. The random induction time statistically spreads around the measured or reported induction time, either obtained from experiments or approximated by the exponential nucleation rate equation suggested by the classical nucleation theory. In this work, we utilized inputs from the classical nucleation theory. In our model, both location and time of nucleation are probabilistic, affecting transport properties in different time- and length-scales. We developed a pore-scale Lattice Boltzmann reactive transport model and implemented the new probabilistic nucleation model to investigate the effect of nucleation rate and reaction rate on the extent, distribution, and precipitation pattern of the solid phases. The simulation domain is a 2D substrate with an infinite source of the supersaturated solution. We use Shannon entropy to measure the disorder of the spatial mineral distributions. The results of the simulations show that all the reactions follow similar random behavior with different Gauss-Laplace distributions. The simulation scenarios start from a fully ordered system with no solid precipitation on the substrate (entropy of 0). Entropy starts to increase as the secondary phase precipitates and grows on the surface until it reaches its maximum value (entropy of 1). Afterward, the overall disorder declines as more surface areas are getting covered, and eventually, entropy approaches a constant value. The research results indicate that the slower reactions have longer windows of the probabilistic regime before entering the deterministic regime. The outcomes provide the basis for implementing mineral nucleation and growth for reactive transport modeling across time-scales and length-scales.

Time Block Preference

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

References

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Primary authors: MASOUDI, Mohammad (University of Oslo, Department of Geosciences); Dr NOORAIEPOUR, Mohammad (University of Oslo (UiO)); Dr BERNTSEN, Andreas (SINTEF Industry, Trondheim, Norway); HELLEVANG, Helge (University of Oslo)

Presenter: MASOUDI, Mohammad (University of Oslo, Department of Geosciences)

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