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How to bridge between different time and length scales using a new probabilistic approach for mineral nucleation and growth

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The reactive transport field lies at the cross-road of several disciplines such as geochemistry, hydrology, geology, and fluid mechanics featuring multi-scale systems and processes in time and length, ranging from nanoseconds to millions of years in time and nano-meter to planetary scales in size. The broad spatiotemporal domain represents systems with ultra-slow to extremely fast evolution. Therefore, it is crucial to implement up/down-scaling workflows and representative models to connect different time and length scales within a system. In the mineral precipitation process, nucleation event, which is a probabilistic process by nature, determines system dynamics via controlling the location and timing of crystal formation in a porous structure. The spatial distribution of secondary nuclei is crucial to precisely predict the changes in hydrodynamics of porous medium after mineral precipitation. We developed a new probabilistic nucleation model and implemented it into a pore-scale Lattice Boltzmann reactive transport model. In the proposed model, both location and time of nucleation are probabilistic, and induction time is considered a random variable that is statistically spread around the measured or reported induction time. We investigated the effect of nucleation and reaction rate on the extent, distribution, and precipitation pattern of the solid phases. We quantified the degree of disorder of the modeled systems using the entropy of the spatial mineral distributions. The results show that different systems take comparable evolution pathways but at different time-scales. Each evolution path starts with an ordered system. When mineral nucleation and growth start, the system goes toward a maximum disorder (entropy of 1). The degree of disorder decreases until all the surface is covered with solid precipitates. All the systems follow a Gauss-Laplace probability distribution. We label this path the "probabilistic domain" because a system can go down this path in countless ways. After the probabilistic domain, the evolved system eventually enters the deterministic domain. The results indicate that the slow reactions have an extended window of the probabilistic domain before entering the deterministic domain. The outcomes provide the basis for implementing mineral nucleation and growth for reactive transport modeling across time-scales and length-scales.