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How probabilistic nucleation controls spatiotemporal dynamics and dimensionality of mineral growth in porous media?

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Precipitation and growth of solid phases during a reactive fluid flow and solute transport are critical in many natural and industrial systems. Mineral nucleation and growth is a prime example where (geo)chemical reactions give rise to geometry evolution in porous media. The precipitation reactions can reduce the amount of void space, alter pore space connectivity and morphology, modify tortuosity, deteriorate permeability, and change the fluid flow and solute transport. Additionally, precipitation events reshape the available surface area for growth, leading to changes in reactivity, reaction progress, and reaction rates. The target is to ideally limit the mineral growth in many applications, such as avoiding damage to reservoir permeability due to solid precipitation near CO₂ injection wells. In other cases, maximizing mineral growth in porous media can be highly favorable, such as sealing fractured caprocks or increasing mineral trapping in the sequestration sites. Understanding, controlling, and predicting this reactive transport phenomenon is challenging because it requires coupling flow, transport, and chemical processes often characterized by different temporal and spatial resolutions. Nucleation is the pre-growth process that controls the primary position of any mineral precipitation and subsequent growth dynamics. Mineral nucleation is a probabilistic process where crystals might nucleate anywhere given similar conditions, such as surface properties, supersaturation, and temperature. It is imperative to use a probabilistic approach or an upscaled physically sound representation to understand the effect of mineral precipitation on porous medium hydrodynamics. Motivated by the importance of incorporating stochastic dynamics of nucleation and growth kinetics in studying various multiphase and multi-scale processes occurring in geo-environmental and geo-energy systems, this paper provides numerical and experimental insights into the recently proposed probabilistic nucleation model. We present laboratory experiments (microfluidic and flow-through column reactor) and pore-scale reactive Lattice Boltzmann Method (LBM) numerical simulations. As variations in the properties of the porous medium are intimately linked to the spatial distribution of the precipitation events, we quantify the evolution of experimental and numerical modeled systems at different physiochemical conditions by mapping the disorder of the system (Shannon's entropy) induced by the spatial mineral distributions across time. We use experimental and numerical results to show the importance of the spatial and temporal location and distribution of nucleation and growth events, particularly when the interplay among several determining parameters is inevitable. The results show that probabilistic nucleation contributes to broad stochastic distributions in both amounts and locations of crystals in temporal and spatial domains.

Participation

In-Person

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