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Micro-Continuum Modeling of Mineral Nucleation and Precipitation at Pore-Scale

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Mineral nucleation and precipitation commonly occur in nature and plays an important role in many energy-related applications with reactive flow, especially, at pore-scale. For instance, minerals nucleate and precipitate as scale in the pore structure in unconventional reservoirs and significantly reduce the permeability of the porous media. This phenomenon could lead to a rapid decrease in production and cause significant financial loss. The need to predict the dynamic properties of such systems has resulted in questions about the fundamental mechanisms of reactive flow as well as mineral nucleation and precipitation in pores. Additionally, there is still a discrepancy between laboratory molecular scale findings and large-scale observations. To address this discrepancy, modeling methods at the pore scale started gaining interest recently due to the capability of capturing reactive and nonreactive species transport, effects of pore topology, and interface chemical reaction within the same approach, which typically is difficult to observe directly in experiments.

For some solutions, especially high saturation index solution, the nucleation process could potentially play an important role in the precipitation due to either heterogeneous or homogenous nucleation, which was largely overlooked in most previous numerical models for mineral precipitation. In this study, we coupled the micro-continuum simulation approach based on Darcy-Brinkman-Stokes (DBS) equation with the classic nucleation theory (CNT) to study the stochastic nucleation process in reactive flow. A range of different parameters were studied to understand their impact on the nucleation process and precipitation. It was discovered that such a nucleation process was affected by the Damköhler number and Peclet number as well as other effects. As the precipitation reaction on the crystal surface enhances, the total amount of nucleus formed on the substrate decreases due to the depletion of species in the vicinity of the substrate. In general, the competition between flow/transport of species and precipitation consumption governs the behavior of phase change process and produces different scenarios. The results of this study are expected to shed light on the mechanism of liquid-solid interaction within porous medium.

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