Contribution ID: **314** Type: **Oral Presentation**

Pore-scale modeling of the dynamics of interface-coupled dissolution-precipitation

Tuesday, 31 May 2022 11:00 (15 minutes)

In interface coupled dissolution-precipitation (ICDP) systems, pore structures change following the dissolution of the primary mineral and the precipitation of the secondary mineral. In order to predict the dynamics of the mineral-fluid interface, it is important to understand the interplay between macroscopic flow regimes and microscopic reaction mechanisms (e.g., nucleation and crystal growth pathways). In this study, we use a micro-continuum pore-scale reactive transport model to investigate ICDP processes with explicit consideration of surface passivation and the diffusion process through the precipitating layer. Our model results highlight that the drastically different coating behaviors at the macroscopic scale and their dependence on solution supersaturation observed in previous column experiments are primarily controlled by the interplay between mineral reaction rates, advective flow, and diffusion through the dynamically forming coating layer. Furthermore, in order to examine the controls on the textures of precipitates that will largely dictate the diffusion properties of the coating layer, we developed a probabilistic nucleation module building upon the classical nucleation theory. This new capability allowed us to consider saturation-dependent nucleation rate and the stochastic nature of the nucleation process, and the results highlight the complex dependence of precipitates'texture on solution chemistry and substrate properties. The modeling observations also underscore the necessity of further investigations to better characterize the properties of the coating layer and to improve modeling descriptions of the nucleation processes.

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References

Deng, H., Poonoosamy, J., Molins, S., 2022. A reactive transport modeling perspective on the dynamics of interface-coupled dissolution-precipitation. Applied Geochemistry, 105207, https://doi.org/10.1016/j.apgeochem.2022.105207.

Time Block Preference

Time Block A (09:00-12:00 CET)

Participation

Unsure

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