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Pore-scale numerical study of coupled dissolution and precipitation processes and their implication in subsurface carbon mineralization

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The dynamic interplay between dissolution and precipitation processes at the pore scale plays an important role in the subsurface sequestration of carbon dioxide via mineralization. This study utilizes a pore-scale model integrating the lattice Boltzmann method (LBM) and fluid-solid interface tracking to simulate diffusion-reaction phenomena encompassing dissolution and precipitation.

Our simulations explored various kinetics of dissolution-precipitation reactions, examining how the precipitation of a secondary solid phase influences the dissolution of a primary phase. These effects were scrutinized under different conditions, such as reaction kinetics, molar volumes of primary and secondary phases, powder size, surface roughness, and nucleation and crystal growth mechanisms. The model predicted distinct morphologies of precipitates and delineated four types of coupled dissolution-precipitation processes based on their interaction extent.

The results reveal that precipitation can either facilitate dissolution by consuming its products or inhibit it by forming a barrier over the reactive surface. Specifically, scenarios were identified where the formation of a secondary mineral phase expedites the dissolution of the primary phase, underscoring a potentially favorable effect for enhanced mineral trapping of carbon dioxide. Conversely, in instances where precipitates envelop the primary mineral, the process retards, signaling a detrimental impact on sequestration. Through extensive parametric studies, the simulation outcomes underscore the significance of accurate pore-scale models for predicting the behavior of subsurface sequestration of carbon dioxide via mineralization.

The study's insights into the pore-scale mechanisms of coupled dissolution and precipitation demonstrate the intricate nature of these coupled processes and provide a foundation for improving the predictive models used to assess the efficiency and long-term stability of subsurface carbon sequestration strategies.