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Pore-scale reactive transport modeling for heterogenous in-situ carbon mineralization in partially-saturated vesicular basalts

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A comprehensive understanding of crystallization mechanisms at the pore scale is necessary to accurately predict the kinetics of in-situ carbon mineralization in basalt formations. In this study, we use a finite-volume pore-scale Reactive Transport Model (RTM) augmented by CFD-based CO2/brine phase distribution and experimentally-informed geochemistry kinetics to understand the dynamic precipitation process of various carbonate phases at the Wallula Basalt Injection Project, where 1000 MT of dry supercritical CO2 was injected over a 25-day period followed by a 2-year shut-in period. Petrographic data (e.g., optical microscopy, SEM, micro-CT) from post-injection sidewall cores collected from three permeable flow-top regions indicate that in-situ carbon mineralization primarily proceeds through heterogeneous nucleation inside geometrically-isolated vesicles, resulting in a variety of chemical-zoned carbonate nodules with different geometries and surface-area-to-volume ratio. However, as the detailed pore-scale processes are not yet well understood, the time series of these processes remain insufficiently constrained by the bulk site monitoring data (e.g., well logs, produced water chemistry) from the Wallula site, hindering reliable predictions for in-situ mineralization inside basaltic formations.

Specifically, we focus on recreating a diffusive- and surface-tension-dominated transport regime inside isolated vesicle systems in the flow top zones over a 2-year post-injection period. Informed by further pore-size analysis (e.g., NMR and BET) and elemental & crystallographic analysis (e.g., EDX, XRF, XRD, TEM), our preliminary analysis of pore-scale carbonate chemistry and morphologies revealed that: 1) inter-vesicle advection of CO2 and diffusion of major cations (Fe2+, Mn2+, and Ca2+) is negligible over the 2-year post-injection period, and 2) pore-lining clays serve as the primary cation source during the early stages of post-injection geochemical processes. Therefore, these isolated vesicles were treated as natural batch reactors in the pore-scale RTM simulation with closed boundaries and a self-sufficient cation source during the post-injection period.

Starting from the two-phase brine/sc-CO2 distribution caused by initial pressure-driven flushing during injection, we explored how dissolution and diffusion of carbonate species control pH and supersaturation distributions within partially saturated vesicles. Lab-scale titration experiments informed the mass transfer rates of cations from pore-lining clays, driven by local Eh-pH conditions. Using a transition-state-theory-based equation, we modeled carbonate growth dynamics to predict the final 3D morphologies of carbonate nodules. Dynamic properties include carbonate surface-area-to-volume ratios, brine/CO2 and brine/mineral interfacial area, and local pH distribution as a function of saturation state, precipitation rate (Da#), and time-lapse inside isolated basalt vesicles.

Our reconstructions of these dynamic geochemical processes were compared with produced water chemistry from the Wallula site to validate our predictions. Going forward, we are looking into how these pore-scale dynamic processes may be upscaled into gridblock-based reservoir simulators (e.g., STOMP-CO2, PFLOTRAN) through continuum-scale variables such as pH and water saturation. We posit that this proposed simulation workflow provides a comprehensive understanding of pore-scale processes that complements current observations and supports more reliable predictions of in-situ carbon mineralization.

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References

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