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A mechanistic investigation of oscillatory zoning using reactive transport modeling

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Solid solutions are widely studied because their formation is ubiquitous in natural and anthropogenic systems. Co-precipitation in rock matrix can result in oscillatory zonation phenomena with solid solutions exhibiting compositional variations (e.g., plagioclase). The principle of co-precipitation of sulphate solid solution is relevant for wastewater treatment of produced waters from hydraulic fracturing and oil/gas extraction, for removing contaminant in uranium mines etc. For nuclear waste disposal, the formation of solid solutions is considered as an important retention mechanism for 226Ra. Despite the widespread occurrence of solid solutions and well-established thermodynamic models, their formation in rock matrix and the effects of transport and kinetics are poorly understood. Previous microfluidic experiments of diffusion-controlled precipitation showed patterns of oscillatory zoning of solid solution crystals of (Ba,Sr)SO4 [1]. In this study, reactive transport modeling is performed to provide a mechanistic understanding of the oscillatory zoning behavior. A micro-continuum approach based reactive transport model that considers probabilistic nucleation was used to simulate the precipitation of (Ba,Sr)SO4 solid solutions following the experimental geometry and setup [2]. It enabled us to compare the contributions of physical-chemical processes that include species-specific diffusion at the solid-fluid interface, solubilities, nucleation kinetics and crystal growth. The models have highlighted that reaction kinetics, rather than transport, are more important in shaping the oscillatory zoning phenomena.

1. Poonoosamy, J., et al., A lab-on-a-chip approach integrating in-situ characterization and reactive transport modelling diagnostics to unravel (Ba,Sr)SO4 oscillatory zoning. Scientific Reports, 2021. 11(1): p. 23678.

2. Deng, H., J. Poonoosamy, and S. Molins, A reactive transport modeling perspective on the dynamics of interface-coupled dissolution-precipitation. Applied Geochemistry, 2022. 137: p. 105207.

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