

Barite Particle Precipitation Kinetics and Trace Metal Uptake

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Removal of hazardous metals and radionuclides from industrial wastewaters via co-precipitation with barite requires an understanding of the precipitation of solid solutions. Solid solutions are controlled thermodynamically by the solubilities of the pure endmembers (BaSO_4 , SrSO_4 , BaHAsO_4 , etc.). Variation in the kinetics of precipitation can also affect the quantities of the co-precipitates within the solid solution. Solution chemistry conditions such as salinity, saturation, and cation/anion ratio have been shown to change the rates of nucleation and growth. Because the endmembers have different solubilities and surface free energies, classical nucleation theory predicts their rates of nucleation will be affected differently by changes in solution chemistry. The number and size distribution of the particles formed will also vary with solution conditions, often with important implications for trace element uptake.

Previous findings by our group using nanoscale resolution X-ray fluorescence (XRF) show the importance of particle growth dynamics on trace element incorporation into barite. Low solid-phase concentrations of the co-precipitating ions HAsO_4^{2-} and Sr^{2+} were observed within barite particles precipitated at low salinity. At high salinity (>1.0 M NaCl), zoned particles were observed with regions of higher As or Sr content emerging over time. We developed thermodynamic models for these systems, but they fail to explain the observations, underscoring the importance of kinetic considerations in describing solid solution co-precipitation. In this study, we combine laboratory UV-Vis measurements of particle formation with a particle population balance model. This model enabled investigation of the effect of solution chemistry on the rates of different particle growth mechanisms. The population balance model tracks individual particles as they nucleate, grow, aggregate and settle. We calibrated the model to UV-Vis measurements to explore how salinity, saturation, and cation/anion ratio affect the rates of barite-celestine nucleation, growth, aggregation, and settling.