

Monte Carlo modelling of surface speciation and dissolution kinetics of carbonate minerals in the presence of electrolytes

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The interplay between dissolution and growth kinetics of carbonate minerals controls the behavior of complex carbonate-fluid systems across the scales at a variety of natural and man-made environments.

The chemical composition of the reacting fluid, acidity, and ionic strength significantly influence dissolution and growth kinetics, as it is supported by extensive experimental evidence. The exact mechanisms controlling the reactive behavior of carbonate surfaces are not well-understood. A major obstacle is the fundamental problem in relating kinematics of reactive surface features (e.g., atomic steps and etch pits) at the nano/microscopic scale and macroscopic phenomena [1]. We overcome this problem by using Kinetic Monte Carlo (KMC) simulation techniques of the reactive events at the mineral-fluid interface to evaluate surface topographies and reactive site distributions [2]. We utilize KMC method as a tool to test hypotheses regarding rate controlling mechanisms via generating a large number of computational experiments. The controls of water chemistry (pH and electrolyte concentrations) are incorporated by using a complementary Grand Canonical Monte Carlo (GCMC) simulation technique, allowing us to obtain distributions of charged and adsorbed species at the calcite-water interface [3]. We discuss how the simulated surface speciation and reaction mechanisms at the nano/microscopic scale can be upscaled and related to the macroscopically observed rates.

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