Contribution ID: **272** Type: **Oral Presentation**

Experimental basis and numerical modeling for a statistical characterization of multimodal spatial heterogeneity of nanoscale calcite dissolution rates

Monday, 30 May 2022 14:40 (15 minutes)

Dissolution/precipitation of minerals are key reactions in various scenarios (e.g., contaminants transport in subsurface environments or sequestration of CO2). Challenges in the assessment of the reaction kinetics arise from the high spatial heterogeneity characterizing precipitation/dissolution processes, typically resulting in a broad range of reaction rate values. High-resolution imaging of the mineral surface with techniques such as the Atomic Force Microscopy (AFM) enhance our ability to assess the mechanisms taking place at the nanoscale at the solid-fluid interface. Here, we rely on experimental results depicting highly heterogeneous patterns and couple these with kinetic Monte Carlo (kMC) numerical simulations to support the origin of such heterogeneous behavior to local inhomogeneities and defects in the crystal lattice. We then rely on a stochastic approach grounded on the use of Gaussian mixtures to view the spatial heterogeneity of reaction rates evaluated (a) from in situ and real-time AFM imaging of the topography of a calcite sample subject to dissolution at far-from-equilibrium conditions and (b) from kMC simulations. Experimental data and results from kMC simulations are clustered into categories with an imaging semantic segmentation technique, each cluster being associated with a component of the mixture. Analysis of the temporal behavior of the parameters associated with our mixture model leads to a quantitative appraisal of the dynamics of the mechanisms driving the reaction.

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Time Block Preference

Time Block A (09:00-12:00 CET)

Participation

Online

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