

## Interacting Surface Features - Data Analysis of Calcite Dissolution Rate Spectra

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Connecting small-scale processes at dissolving mineral surfaces is a challenging task that is nevertheless necessary to gain an improved understanding of the overall behavior of a rock (reservoir) in its specific environment. In this study, we examine ways to extract data from kinetic Monte Carlo (kMC) simulations [e.g., 1,2] and to process them in ways that make them useful as parametrization input for simulation methods operating at larger scales. Our examined system involves reactive transport processes in a Rotliegend sandstone cemented with calcite. We focus on calcite dissolution kinetics, as this carbonate is the fastest dissolving main mineral and its content largely determines the porosity of this rock. Since reactive transport models have to operate at continuum scale, the raw output kMC calculations can not directly be used in another model. Rather, key parameters that still reflect the heterogeneity of rates have to be extracted. Specifically, we tested several approaches to deconvolve and analyze rate spectra [3] gained with kMC simulations, and to interpret them physically in relation to the surface processes. Far-from-equilibrium calcite dissolution at a cleavage surface is driven by steps moving over the surface [4], interpreted by the stepwave model [5]. As such steps are generated at defects, we simulated dissolution at different defect densities and defect distributions.

Results show that while rate contributors are easily identified in the earliest stage of dissolution of an initially flat surface with pre-defined defect positions, the behavior of rate spectra soon becomes very complex when different etch pits and other surface features form and begin to interact with each other. We were also able to demonstrate the effect of defect clustering on the evolution of etch pit depths, and ultimately the rate spectrum.

[1] Meakin & Rosso (2008) *J. Chem. Phys.* **129**, 204106. [2] Kurganskaya *et al.* (2016) *J. Phys. Chem. C* **120**, 6482-6492. [3] Fischer *et al.* (2012), *GCA* **98**, 177-185. [4] Hillner *et al.* (1992) *Ultramicroscopy* **42-44** (2), 1387-1393. [5] Lasaga & Luttge (2001) *Science* **291**, 2400-2404.