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Stochastic modeling of calcite dissolution rates from microscale observations

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We illustrate an original stochastic approach grounded on the use of Gaussian mixtures to characterize heterogeneous distributions of rock dissolution reaction rates. The latter are evaluated from *in-situ* and real-time Atomic Force Microscopy (AFM) imaging of a calcite sample subject to dissolution in far-from-equilibrium conditions. Accurate characterization of these reactive phenomena is critical to a variety of scenarios of environmental concern including, e.g., geological sequestration of CO_2, contamination of subsurface environments, or nuclear waste disposal. Advanced high-resolution imaging techniques such as Vertical Scanning Interferometry (VSI) or AFM enable direct inspection of reacting surfaces and have recently contributed to enhance our knowledge of the detailed mechanisms involved in the reaction at fluid-solid interfaces at the nanoscale. Experimental observations of this kind document that several elements contribute to the overall reaction kinetics. These are associated with the uneven distribution of surface energy arising from discontinuities at the mineral lattice level, which ultimately yields a markedly heterogeneous distribution of reaction rates. This, in turn, weakens the viability of relying on descriptions of the reaction kinetics relying solely on average values. In this context, a stochastic approach is key to capture the intrinsic variability of rates. Our modeling framework rests on Gaussian Mixtures, each mode being associated with a given mechanism governing the reaction. We show that temporal trends of model parameters are strongly linked to the dynamics of the evolution of the pattern of the mineral surface, thus providing insights on the effects of the processes driving the reaction.