

Parametrization of intrinsic surface reactivity in reactive transport models

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Reactive transport investigations of subsurface hydrogeochemical processes have shown that the heterogeneity in dissolution rate observed in numerous experiments cannot be explained by fluid transport effects alone. Instead, this heterogeneity is attributed to intrinsic variability in the surface reactivity of the dissolving material. Therefore, reactive transport models require a parameterization of the surface reactivity for reliable predictions. Here we discuss and propose how to parameterize such varying surface reactivity of pore-scale systems, from the crystal surface to the single crystal geometry, going beyond the previous reactivity parameterization. We compare the results between classically parameterized models, models with new parameterization, and experimental data. We show how this parameterization is able to accurately reproduce the experimental results on a crystal surface with a broad field of view, a large height variability of the topography, and over a long reaction period.

Recently, dissolution rate maps revealed the existence of rhythmic pulses of the material flux from the crystal surface. Until now, the dominant factor underlying this behavior has not been understood, and both surface- and transport-controlled conditions have been discussed to govern the pulsating reaction kinetics in the system. Numerical investigations with the new parameterization presented above now allow the conclusion that the self-organization of various reactive surface building blocks causes the pulsating resolution. This is a fundamental factor in crystal dissolution and deserves to be considered for an in-depth understanding and improved upscaling of dissolution kinetics.