Geostatistical Modeling of Nanoscale Dissolution Dynamics at Mineral–Water Interfaces

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We present a geostatistical framework for analyzing the spatiotemporal dynamics of nanoscale dissolution at mineral–water interfaces. These processes play a fundamental role in a broad range of geochemical phenomena, including chemical weathering, reactive transport in porous media, and mineral–fluid interactions. Recent experimental observations have shown that dissolution rates and surface morphology exhibit pronounced spatial variability, primarily due to the heterogeneous distribution of reactive sites across mineral surfaces. As a result, the evolution of surface topography during dissolution can be interpreted as a stochastic process that varies in both space and time. To address this complexity, we investigate the ability of advanced statistical and geostatistical approaches to model and reconstruct nanoscale surface evolution. In particular, we combine Gaussian Process Regression (GPR), including localized variants supported by Self-Organizing Maps (SOM), with Multiple-Point Statistics (MPS) for pattern-based simulation. These approaches are selected to capture different aspects of the evolving dissolution patterns. GPR provides a flexible probabilistic regression framework for interpolating and predicting local surface behavior, while SOM-assisted localization improves the representation of spatially varying structures. MPS, in contrast, is used to reproduce complex spatial patterns and higher-order dependencies that are often not adequately represented by conventional two-point statistics. Model performance is evaluated through cross-validation and controlled masking experiments designed to test the reconstruction of missing or unobserved surface regions. Reconstruction accuracy is quantified using standard statistical metrics, including Root Mean Squared Error (RMSE) and Mean Absolute Error (MAE). The results demonstrate that regression-based and pattern-based methods offer complementary strengths: GPR-based methods are effective in representing smooth large-scale organization, whereas MPS is particularly well suited to preserving fine-scale heterogeneity and spatial continuity. Overall, the study highlights the value of integrating geostatistical and machine learning approaches for the analysis of complex dissolution dynamics at the nanoscale. The proposed framework provides a flexible basis for modeling spatiotemporal variability in reactive mineral systems and contributes to a more robust quantitative understanding of surface evolution at mineral–water interfaces.