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Cross-scale tracking and quantification of surface reactivity and fluid transport in geomaterials

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The analysis of reactive transport processes has an integrated basis of analytical and numerical approaches. Two dynamics and their interplay are crucial: (i) changes in local flow paths and (ii) variability in surface reactivity. The resulting interactions at the interface determine the evolution of the studied system, with consequences for a wide range of applications. Here we focus on two aspects: First, analyzing the variability of solid surface reactivity is a challenge with implications for the analysis of reaction kinetics. Here we discuss recent results in addressing this problem in reactive transport models. The quantitative basis for this is provided by surface-sensitive analytical techniques that allow conclusions to be drawn about the range of variability and possible steady state evolution. In this overview, we discuss scale-crossing surface analysis from the nm to the dm scale and combine it with several numerical approaches to cover a similar length scale range. Second, the flow path evolution in porous materials is usually predicted by simulation results based on the pore network geometry. There are few validation options for this, although the question of the sufficiency of the geometry models used urgently requires such, and we discuss possibilities here. The materials studied range from low permeability mesoporous argillaceous rocks to sandy reservoir rocks and fractured porous host rocks. The resulting residence time contrasts largely determine the thermodynamic framework of fluid-rock interactions. Understanding the feedback between reactivity and transport defines the quality of our predictive capability for important application areas.