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Mineral surface reactivity: mechanisms and concepts

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Diagenetic reactions in sediments and sedimentary rocks are controlled by both fluid transport and surface reactivity. In this chapter, the major focus is on the effect of crystal surface reactivity and its variability. The “energetic landscape” of the solid material in contact with the fluid exerts control on reaction type, kinetics, and products. Critical surface processes include sorption, catalysis, dissolution, and precipitation. For diagenetic reactions, the sequence of processes and thus the potential inhibition of subsequent reactions due to surface modifications is of great interest. Consequently, the evolution of porosity and permeability is governed by the chronological sequence of surface reactions during the diagenetic history. This provides feedback to the fluid transport behaviour in the complex porous material. Because of this coupling, numerical approaches address the problem appropriately by the use of reactive transport codes. Pore scale treatment follows mechanisms at the scale of crystal surfaces that form the pore walls of the sedimentary rock. Such surface-chemical exercises require a parametrization that includes mechanistic understanding and connection to first-principles treatment. At larger scales, so-called continuum scale simulation treats fluid transport and fluid-solid reactions in a more generalized quantitative way. While such field-scale treatment is required and applied for multiple challenges, the small-scale mechanistic understanding is still a crucial part of geochemical research. The observed heterogeneity of surface reactivity requires specific upscaling strategies that are not yet reflected in large-scale analysis and predictions.