Geophysical Research Abstracts
Vol. 16, EGU2014-12543-2, 2014
EGU General Assembly 2014

Understanding the variability of crystal surface reactivity - A key to improve the quantitative prediction of diagenetic reactions

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Diagenetic reactions result in complex spatial patterns of reaction products. These patterns reflect the variability of reaction rates. The quantitative predictability of such patterns is still very limited. We discuss two important aspects of the underlying rate variability in greater detail. First, this variability reflects differences of the reaction kinetics of chemically identical systems. Second, it is able to govern the degree of surface inhibition of subsequent diagenetic reactions.

The first aspect is related to an intrinsic variability of crystal surface reactivity. Fischer et al. (2012) have introduced a new concept of rate spectra. These can be used to analyze the variability of actual rates. Rate spectra quantify the frequency of specific contributors to the overall reaction rate. Analysis of these contributors may also help to explain spatial contrasts of diagenetic reactions at the pore scale and, thus, provide the link to upscale reactivity contrasts. In situ observations of reacting mineral surfaces showed the fundamental role of kink sites in mineral dissolution and growth processes. The reaction mechanisms at this scale can be understood using stochastic modeling of reaction kinetics at the molecular level. At larger scales, the reacting framework is superimposed by a multitude of physical discontinuities such as crystal defect structures or domain boundaries. As a result, structures such as grain surfaces in porous networks and at depositional boundaries (facies, bedding, etc.), define the heterogeneity of the system on macroscopic scales. Thus, our ability to integrate molecular scale theory with observations of reacting mineral surfaces constrains any quantitative prediction of “whole rock” reactivity.

The second aspect is related to the dominant role of a particular reaction mechanism, such as the adsorption of inhibitors at specific reactive sites of the crystal surface. The prevalence of a specific reaction pathway among the others predefines subsequent steps of any diagenetic reaction. For example, early-diagenetic grain coats can inhibit cementation, thus governing significantly the diagenetic evolution of sediments. We focus here on the early-diagenetic formation of grain coats, such as clay mineral or iron oxide coats, through adsorption of mineral colloids under common electrostatically unfavorable conditions. Analog experiments with collector surfaces having well-defined variations in surface roughness indicate that submicron-sized surface structures enhance the efficiency of colloidal retention and therefore the initial formation of grain coats.

Here we will discuss the different aspects of intrinsic variability of crystal surface reactivity from experimental and modeling results in light of early diagenetic reactions. Important reaction processes include crystal dissolution and sorption of small particles, i.e. nanoparticles and colloids.

Thus, by considering the surface reactivity contrasts of water-rock interactions in early diagenetic systems we can improve the predictability of the spatial and temporal heterogeneities of diagenesis.

Fischer, C., Arvidson, R.S., Luttge, A. (2012): How predictable are dissolution rates of crystalline material? Geochimica et Cosmochimica Acta 98, 177-185.