Hydrothermal experiments and data-driven approaches for water-rock reactions

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The Earth’ s crust is mainly composed of rocks and fluids, and there are various water-rock reactions from deep crusts to surface environments, including metamorphism, metasomatism, mineralization, hydrothermal alteration as well as weathering. In spite of difference in pressure, temperature and water-to-rock ratios among these reaction systems, these are several similarities as follows: (1) the water-rock interaction is essentially heterogeneous reactions in multiphase and multicomponent systems, which involves many kinds of minerals and aqueous species, (2) the systems commonly do not reach fully equilibrium states, meaning that the extent of reactions are commonly change with time and space, and (3) the data, we can get, is sparse and noisy; in some cases, we got only the spatial variation of reactant and product minerals in the rocks, and the other cases, we can get temporal evolution of fluid chemistry in the limited sampling points. For understanding reaction paths, mass transfer, and rates from the limited data, we need to develop the data-driven approaches suitable for the types of observable data. Since natural systems are too complicated, as a first step, we have conducted several series of hydrothermal experiments on water-rock interactions. In this talk, we summary our recent experiments and data analyses on silica-water interaction (nucleation of silica particles and diagenesis following the Ostwald step rule), formation of reaction zone associated with serpentinization (spatial variation of the minerals), and basalt-water interactions in flow-through system (PCA for the evolution of solution chemistry).

Keywords: water-rock interaction, hydrothermal experiments, temporal and spatial variation

