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Thermodynamic view of trace element retention in mineral “sorption continuum”

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Driven by reactive transport, the minor- or trace element (Tr) retention process in time and space can be seen as interplay of uptake and release processes in a “*sorption continuum*”. *Uptake* embraces Tr surface complexation, surface entrapment and solid solution incorporation. *Release* involves mineral recrystallization, replacement, Tr desorption, and dissolution mechanisms. Various thermodynamic, structural, kinetic and transport controls apply to each Tr + host mineral case, clarified in detailed studies. Structural factors and thermodynamics of solid solution and sorption systems are key in confirming possible Tr retention pathways and in usability of available computer tools, thermodynamic and kinetic approaches for simulation and interpretation of systems.

Structural factors determine the most stable Tr incorporation into the host mineral toward the aqueous (Aq) - solid solution (SS) equilibrium where non-ideal mixing directly affects Rd(Tr) values. The uptake process starts from adsorption of Tr and host elements. On persistent host mineral surface (goethite, quartz), the main retention mechanism is surface complexation. If the host mineral is relatively soluble and has a labile surface (calcite) then Rd(Tr) values may depend on the growth rate via the *surface entrapment* - a tradeoff between Tr adsorption and solid solution, the lower the growth rate the closer to Aq-SS equilibrium. Some Aq-SS systems (barite – trace radium) can slowly recrystallize with Tr uptake enhanced over time. Fluid transport may drive mineral transformations with preferential release of Tr and its re-sorption on other mineral surfaces. Complexity further increases in *sublattice* SS, where Tr can access different structural sites (apatite, LDH, C-S-H).

Thermodynamics defines the driving force and the maximum extent of Tr uptake, but real challenge in modelling the “sorption continuum” is how to impose time-dependent *additional metastability constraints* reflecting physically plausible mechanisms. Can the competitive Langmuir isotherm in site-balance-based SCMs be replaced with BET-type sorption isotherms for more realistic modelling of Tr surface binding and precipitation? How this can help implementing SCMs on labile surfaces (C-S-H, Fe-LDH, carbonates)? How to combine very slowly equilibrating 2:1 clay structures (illite, smectite) with faster, yet different sorption kinetics on planar and edge surfaces? Still a lot to investigate!