A Process-based model for iron mineral transformation

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Iron (Fe) (oxy)hydroxide minerals play a key role for determining the mobility of a wide range of contaminants in groundwater systems. [1].

Successive transformation of the meta-stable reactive mineral ferrihydrite to more thermodynamically stable Fe minerals has been observed in many natural environments and reproduced under controlled laboratory conditions [2]. Catalysis by aqueous and sorbed Fe^{2+} has consistently demonstrated a key role in the rate of Fe mineral transformation, where the terminal Fe mineral products have included: lepidocrocite, goethite, hematite and magnetite. To date the rates and pathways of the transformation processes have not been closely examined within any quantitative framework that describes the complex relationships between the transforming minerals and surface-associated as well as aqueous Fe^{2+}. Therefore, this study was aimed at developing a geochemical kinetic modeling framework reliant on surface complexation reactions to describe Fe mineral transformation rates and pathways.

The resulting model was able to reproduce experimental data collected from two studies investigating the transformation of ferrihydrite to lepidocrocite, goethite and magnetite across a range of circumneutral pH conditions and aqueous Fe^{2+} concentrations [3,4]. The model highlighted the crucial role of sorbed Fe(II) and ligand type on controlling the transformation rates and secondary mineralization pathways, as sorbed Fe(II) concentration varied by close to an order of magnitude across the investigated pH range of 6.2 to 7.2. Finally, the impact of competing metal(loid)s for sorption sites on Fe minerals was investigated using the model to quantify how it affects Fe mineral transformation rates, pathways and overall contaminant mobility.

[1] Pedersen et al., GCA 70, 4116-4129 (2006) [2] Hansel et al., GCA 67, 2977-2992 (2003) [3] Boland et al., ES&T 48, 5477-5485 (2014) [4] Hansel et al., ES&T 39, 7147-7153 (2005)