Modeling of iron mineral transformations and arsenic fate under sulfate reducing conditions

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A critical step in the development of modelling tools for the prediction of arsenic (As) behaviour under field-relevent conditions is validation against well-constrained experiments. In this study a mechanistic reactive transport modeling framework for Fe reductive dissolution and remineralisation, surface complexation and associated As fate under SO_4 reducing conditions has been developed. Data from previously published column experiments [1] were used to guide and constrain the model development. Different conceptual models that incorporate the pH dependence of hydrous Fe(III) oxide tranformation and As fate were tested with the reactive transport simulator PHT3D. All processes were simulated using a thermokinetic approach.

The selected reaction network accurately simulates the reductive dissolution of ferrihydrite by the sulfide produced during sulfate reduction, whereby the associated production of native sulfur and Fe(II) acts as the driving process for Fe mineral transformations and release of As.

The model also captures correctly the transformation of ferrihydrite to goethite and the formation of makinawite as influenced by the abundance of aqueous Fe(II). The simulations illustrate that the surface loading of Fe(II) on Fe(III) mineral surfaces rather than the aqueous concentrations determine the remineralisation pathway and corresponding reaction rates. The model framework developed will be applicable to the investigation of a wide range of other problems where the reductive dissolution and remineralisation of Fe (hydr)oxides influences the fate and transport of contaminants such as As.

[1] Burton, E.D., S.G. Johnston, and R.T. Bush, Microbial sulfidogenesis in ferrihydrite-rich environments: Effects on iron mineralogy and arsenic mobility. *Geochimica Et Cosmochimica Acta*, 2011. **75** (11): p. 3072-3087