

# Coupled chemical-hydrodynamic modelling of iron oxyhydroxide precipitation in dynamic aqueous environments

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Iron is ubiquitous in natural environments and used widely in engineered treatment systems as a coagulant or adsorbent. When iron is introduced to such systems, it forms a variety of species dependent upon the pH of the solution with this pH very dependent upon the particular concentration of iron added. In an attempt to better understand the relative importance of factors controlling iron oxide precipitation, we modelled the dynamic formation of iron oxides on addition of ferric (or ferrous) iron to a solution of well-defined hydrodynamic characteristics. The hydrodynamics of this system and the transport of iron species from the Fe injection point were modelled using COMSOL while the speciation and kinetic calculations were performed using the speciation program PHREEQC with the coupling of hydrodynamic and speciation aspects undertaken using a modified version of the method described by Wissmeier and Barry [1].

Fe was introduced in to the system at a controlled rate at a particular location and the concentrations of the various Fe(III) hydrolysis products determined by a charge balance at each element in the simulation domain for each time step. This model enables description of the formation of amorphous ferric oxides (AFOs) as a result of Fe(III) polymerization and subsequent changes in Fe concentration in the system as a function of pH. The rate of Fe(III) polymerization was calculated as a function of Fe(III) speciation and associated water-loss rates.

The distribution of pH and all Fe species in the simulation domain were determined at every time step and the AFO distribution in the simulation domain also modelled providing insight into the spatial-species dependant mechanisms and their contribution to the observed kinetics of AFO formation. The time scale of mixing was also obtained from the hydrodynamics of the system and will be used in subsequent studies of adsorptive uptake of contaminants on the freshly forming AFO.

[1] Wissmeier & Barry (2011) *Env. Mod. & Soft.* **26**, 210-218