Surface complexation modeling for chromate adsorption on Al - ferrihydrite

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Ferrihydrite (FH) is a poorly crystalline oxyhydroxide with high surface reactivity and, therefore, has an important role in the transport of contaminants in the subsurface. Although naturally occuring FH often contains impurities such as Al substitutions, however the impact of these on surface properties are not yet fully understood. True substitution of Al occurs only up to ~20% molar basis [1], however sorption studies typically focused on higher levels that lead to distinct Fe-Al assemblages [2]. A recent study of low-substitute Al-Fh indicated that the speciation of chromate, selenate and sulfate on the surface changed substantially with increased Al content [3].

In this study, synthetic Al – substituted FH (0, 6 and 18 % mol Al/(Al+Fe)) was characterized with transmission electron microscopy (TEM) to examine differences in morphology and particle size. Batch adsorption studies for chromate were performed and indicated that while the maximum adsorption capacity was similar, the slope around neutral pH increased with increased Al substitution.

The SCM modeling efforts employed a CD - MUSIC approach tied with a Basic Stern electrostatic model, utilizing distinct sites for Fe and Al binding of chromate and taking into account the different species present. To our knowledge, this is the first surface complexation modeling study for Al-FH. Sensitivity analysis for surface complexation and specific adsorption equilibrium constants was performed.

[1] Cismasu et al. (2012) *Geochim. Cosmochim. Acta* 92, 275-291.[2] Liu & Hesterberg (2011) *Environ. Sci. Technol.* **45,** 283–6289. [3] Johnston & Chrysochoou (2016) *Environ. Sci. Technol*. 50, 3589–3596