Iron oxides reactivity: A unified surface complexation modeling approach

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Iron oxides and oxyhydroxides are among the most reactive surfaces in the environment and various models have been developed to describe the reactivity of various phases such as goethite and ferrihydrite. Although surface complexation models (SCMs) provide a robust description of adsorption under various conditions, their application to mineral assemblages is still difficult, due to the high degree of complexity and parametrization.

In this study, we propose a *unified* SCM to describe chromate adsorption on three iron oxides: ferrihydrite, hematite and goethite. The unified approach focuses on employing a single set of electrolyte and specific adsorption equilibrium constants, while modeling surface charge using individual mineral structure and surface properties.

Specifically, a 3–site model was used to describe surface protonation using site densities derived from the structure and morphology, and protonation constants derived from the literature or fitted to mineral-specific charging curves. This approach has been able to capture the differences on points of zero net proton charge (PZNPCs) on various FH charging curves [1]. For chromate adsorption, insights from spectroscopy and batch adsorption experiments are incorporated to build a model that is able to simulate adsorption using a single set of electrolyte constants and a narrow range of surface complexation constants. Some results on simulating chromate adsorption on the three iron oxides are shown in Figure 1.

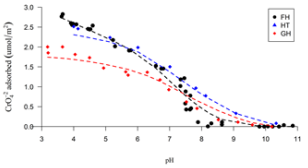

Figure 1. Chromate adsorption modeling on FH, HT and GH.

[1] Bompoti et al. (2016) *Chem. Geol.* doi:10.1016/j.chemgeo.2016.12.01.