Modeling kinetic reactions of heavy metals with DOM and ferrihydrite: effect of DOM and ferrihydrite interactions

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Both dissolved organic matter (DOM) and ferrihydrite (Fh) are important adsorbents in the environment and affect the fate and bioavailability of heavy metals. Quantitatively understanding the kinetics of heavy metal reactions with DOM and Fh are crucial for accurately predicting the fate and transport of heavy metals in the environment. In the previous work, we have developed mechanistic kinetics models for metal complexation/dissociation reactions with DOM based on WHAM 7 model [1, 2], and for ion adsorption/desorption reactions on Fh based on the CD-MUSIC model [3]. The interactions between DOM and Fh have been reported to affect the chemical properties of DOM and Fh, but how such interactions affect the reactivity of DOM and Fh as well as the kinetic behavior of heavy metals are still unclear.

In this study, we first systematically investigated the kinetics of metal dissociation from DOM and metal adsorption/desorption kinetics on DOM-Fh composites, and developed quantitative models for predicting the kinetic reactions. The kinetics models integrated both WHAM 7 and CD-MUSIC into a multi-site kinetics model to account for the heterogeneity of binding sites of DOM and Fh. Both EXAFS and Cs-STEM were empolyed to explore the reaction mechanisms at molecular levels and sub-nano scales, and the impact of DOM-Fh interactions on metal reactions was specifically considered in our kinetics model. Moreover, FT-ICR-MS analysis and molecular modeling were employed to investigate the variations of DOM compositions and chemical properties and to further illustrate the effects of DOM-Fh interactions on the reactivity of DOM at the molecular levels. Our results contribute to developing a comprehensive model for predicting metal behavior in the environment.

[1] Shi, et al. *Environ. Sci. Technol.* **50** (2016), 10476-10484.
[2] Wang, et al. *Chemosphere*. **221** (2019), 254-262.
[3] Tian, et al. *Environ. Sci. Technol.* **51** (2017), 10605-10614.