Kinetics of heavy metal reactions with soil organic matter (SOM): the roles of SOM binding sites

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Soil organic matter (SOM) is the most important ligand in soil that controls the reactivity of heavy metals. SOM contains multiple heterogeneous binding sites that account for metal binding. So far, how those individual SOM binding sites control the metal adsorption and desorption rates is still largely unknown, which limits our ability to accurately predict dynamic behaviour of heavy metals in soil. Furthermore, the chemical compositions of SOM may vary significantly, which complicates how to model the kinetics of heavy metal reactions with SOM.

We have developed a mechanistic-based kinetics model for heavy metal adsorption/desorption reactions with SOM by integrating chemical speciation model WHAM into the kinetics model, which is able to account for the nonlinear binding of heavy metal ions to heterogeneous SOM binding sites and the variations of solution chemistry conditions [1,2]. Based on metal reactions with various carboxylic and phenolic binding sites of humic substances, we have attempted to constrain the adsorption/desorption rate coefficients through the equilibrium partition coefficients for each of the humic substance binding sites. We have developed the relationship between the metal adsorption/desorption rate coefficients and the metal binding constants among different humic substance binding sites. Based on the model we developed, we analyzed the kinetic data collected from the laboratory kinetic experiments and published in literatures during past three decades and obtained global model parameters for each heavy metal. The desorption rate coefficients varied signifiantly among different heavy metals and spread to a wide range among different binding sites of humic substances. Our results indicate that the molecular structure of SOM and the specific binding forms significantly affect the rates of metal reactions with SOM, which should be considered in modeling the dynamic behavior of heavy metals in the environment.

[1] Zhenqing Shi, et al. (2013) *Env. Sci. Technol*. **47**, 3761−3767.

[2] Zhenqing Shi, et al. (2016) *Env. Sci. Technol*. **50,** 10476-10484.