Developing A Predictive Model for the Kinetics of Heavy Metal Adsorption/Desorption in Soil

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The adsorption/desorption reaction is a key process controlling the reactivity and bioavailability of heavy metals in soil. Predicting the kinetics of heavy metal adsorption/desorption in soil requires consideration of multiple heterogeneous soil binding sites and variations of reaction chemistry conditions. However, so far there is no work on developing a mechanistic-based model to describe heavy metal adsorption and desorption kinetics by simultaneously considering metal binding to various sites of both soil organic matter (SOM) and soil minerals.

In this study, based on the equilibrium models WHAM 7 and CD-MUSIC, we developed a unifying model for the kinetics of heavy metal adsorption/desorption in soil, which specifically considers metal kinetic reactions with multiple binding sites of SOM and Al/Fe (hydr)oxides simultaneously. The key idea of our model is to constrain the adsorption and desorption rate coefficients for each specific binding site through the equilibrium partition coefficient and constrain the variations of desorption rate coefficients among different binding sites through the metal binding constants of various sites. Thus, the model had only one fitting parameter for each soil binding phase, and all other parameters were derived based on WHAM 7 and CD-MUSIC. A stirred-flow method was used to study the kinetics of Cd, Cu, Ni, Pb and Zn adsorption and desorption on several soils under various pH and metal concentrations, and the kinetics model was able to reproduce most of the kinetic data. The model can be further used to predict the dynamic behavior of heavy metals in soil under various natural conditions.