Modeling the adsorption of selected metals onto nano-maghemite

M. KOMÁREK[1]*, C. M. KORETSKY[2], K. J. STEPHEN[2], D. S. ALESSI[3] AND V. CHRASTNÝ[1]

[1]Department of Environmental Geosciences, Faculty of Environmental Sciences, Czech University of Life Sciences Prague, Kamýcká 129, Prague 6 – Suchdol, 165 21, Czech Republic

[2]Department of Geosciences, Western Michigan University, 1187 Rood Hall, Kalamazoo, MI 49008, USA

[3]Department of Earth and Atmospheric Sciences, University of Alberta, 1-26 Earth Sciences Building, Edmonton, Alberta, T6G 2E3, Canada

Nano-maghemite is an interesting candidate for the removal of metals and metalloids from waters and contaminated soils. Additionally, nano-maghemite is one of the possible products of oxidation of nano-zerovalent Fe (nZVI), a commonly used remediation agent for waters and soils contaminated with metals (e.g., Cr(VI)) [1] [2]. The aim of this study is to measure and model the competitive adsorption of Cd(II), Cr(VI) and Pb(II) onto nano-sized maghemite. Spectroscopic data (XAS and XPS) and isotopic fractionation data (Cd, Cr and Pb) were used to gain insights into adsorption mechanisms. This, together with bulk adsorption and kinetic data, was used to constrain both semi-empirical and surface complexation models (SCM) describing competitive metal(loid) adsorption over a wide range of solution conditions [3].

Adsorption equilibrium was generally reached within 60 min for all metals. All three metals follow a pseudo-second order kinetics model. The fitted Langmuir parameters demonstrate that Pb(II) is the most efficiently adsorbed of the metals, with a maximum of 0.13 mmol g^{-1}. The log K values of protonation and deprotonation of the maghemite surface were modeled using a diffuse layer surface complexation model with a single amphoteric site in ProtoFit. Separate adsorption edges of the studied metals were modeled for a given reaction stoichiometry by optimizing stability constants for each separate metal based on single-metal experiments using FITEQL 4.0. These log K values were used for subsequent surface complexation modeling of the mixed systems using VisualMINTEQ. XPS spectra suggest that Cd(II) and Pb(II) are present as inner sphere complexes, and Cr K-edge XAS analysis of Cr-sorbed nano-maghemite further proved that Cr is present as Cr(VI).

[1] Mueller and Nowack (2010) *Elements* **6**, 395-400. [2] Jiang *et al*. (2013) *Chem. Eng. J*. **222**, 527-533. [3] Koretsky (2000) *J. Hydrol*. **230**, 127-171.