Towards consistent models of Cd(II), Cu(II), Pb(II) and Zn(II) adsorption onto Fe oxides

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We provide complementary robust adsorption data for Cd, Cu, Pb, Zn and ubiquitous Fe (oxyhydr)oxides, which are commonly found in soil environments: goethite, hematite, lepidocrocite, maghemite, magnetite. Equilibrium and kinetic adsorption experiments were performed in open atmosphere. Data obtained from the kinetic experiments were fitted to pseudo-second-order equations and isotherm parameters were obtained from the measured data using non-linear least squares regression. Acid-base titrations were performed for the selected oxides at different ionic strengths (0.001-0.1 M $NaNO_3$) using a CO_2-free chamber with N_2 as the inert gas. The obtained surface charge curves were used to optimize surface protonation models; thus, (de)protonation constants and surface site densities were calculated. Adsorption edges were constructed under atmospheric conditions at different initial metal concentrations (10^{-6}-10^{-4} M) and ionic strengths (0.001-0.1 M $NaNO_3$). Adsorption edges for all the studied metals were modeled using the DLM and CD-MUSIC. Stability constants were optimized for each individual edge, i.e., each ionic strength and metal concentration, with a given reaction stoichiometry. The obtained data are easily implementable into various geochemical codes and will be beneficial for researchers using SCM for developing multisurface predictive models of metal behavior in various aqueous environments and soil systems. Usually, only a general Fe oxide (i.e., HFO) is used for this purpose.