Surface complexation modeling of arsenic mobilization fromgoethite: Interpretation of in-situ experiments in a sedimentary basin of Inner Mongolia, China

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Sorption competition onto Fe-(oxyhydr-)oxides surfaces is a well-known mechanism controlling the release and mobility of arsenic (As) in subsurface (Dixit & Hering, 2006). Over the last decades, surface complexation models (SCMs) have been implemented to model interactions between sorbants and mineral-oxides surfaces by considering the thermodynamic properties underlying complexation and electrostatic interactions (Goldberg, 1992). However, SCMs development are typically based and/or applied on well-controlled laboratory experiments with simple aqueous systems rather than complex environmental groundwater conditions.

In this study, we present and compare conceptual and numerical modeling approaches developed to quantitatively interpret in-situ experiments that consisted in monitoring the temporal change of adsorbed-As concentration by incubating As-loaded goethite coated sand in the groundwater (Zhang, et al., 2017). Reactive transport models were developed using the Iphreeqc model coupling the geochemical code PHREEQC and MATLAB (Muniruzzaman & Rolle, 2016). The two surface complexation modeling approaches available in PHREEQC, the diffuse double layer (DDL) and the charge-distribution multisite complexation (CD-MUSIC) models (Hiemstra & Van Riemsdijk, 1996), were applied to simulate sorption competition assumed to be the only geochemical process leading to the release of As from goethite. Model parameters were calibrated through inverse modeling in order to simulate experimental results. Whereas a satisfying agreement with the measured As-adsorbed concentrations was obtained, the role of the aqueous species in the As desorption significantly differs between the predictions of the DDL and the CD-MUSIC models.

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