

Model-based interpretation of arsenic release during in-situ exposure of iron oxides

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Sorption at mineral/solution interfaces and the coupling with the iron cycling are key controls for the release and mobility of arsenic in groundwater. Despite the significant advances in understanding these mechanisms, an apparent research gap still exists between controlled laboratory and natural field conditions.

In this study we consider recent in-situ experiments that have been conducted to directly assess the transient release of arsenic and the change of known mineral phases by exposing synthesized As-loaded ferrihydrite and goethite to natural groundwater conditions. We propose and develop a modelling framework to provide a quantitative understanding of the experimental datasets and to corroborate the description of As behaviour, observed in different monitoring wells, with detailed process knowledge essentially developed in laboratory studies. Arsenic desorption from goethite, resulting from the continuous supply of dissolved groundwater solutes, is simulated using surface complexation reactions and comparing the DDL and CD-MUSIC models [1]. In the case of ferrihydrite, the model accounts for the interplay of the abiotic and biogeochemical processes (i.e., surface complexation, reductive dissolution, formation of secondary iron minerals and arsenic sequestration into the newly formed minerals) important for the transformation of Fe-oxides and controlling arsenic mobility [2].

The formulation of modelling scenarios and the evaluation of the sensitivity of the surface composition to changes in hydrochemical conditions were used to disentangle the contributions of different mechanisms and to identify the aqueous species affecting the mobility of arsenic at the field site. The results show that the complex interplay between charged species in sorption processes and their individual effects on mineral transformation need to be considered to quantitatively capture As release and sequestration from/into iron minerals under natural groundwater conditions.

[1] Stolze et al. (2019) *Geochim. Cosmochim. Acta* **248**, 274-288. [2] Stolze et al. (2019) (*in review*).