Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Arsenic Transport in Natural Porous Media



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Project Term
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Clusters
Lichtenberg II Cluster Darmstadt

Additional Software
PHREEQC-3

Institute
Institute of Applied Geosciences

University
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Partners
Earth and Environmental Sciences Area, Lawrence Berkeley National Laboratory, USA

Introduction

Arsenic (As) contamination of groundwater is a problem of enormous scale and affects the health of millions of people. Arsenic mobility in groundwater is mainly controlled by sorption onto mineral surfaces. However, we still lack robust mechanistic description of As partitioning under natural conditions. This knowledge gap hinders our capability to predict the occurrence of arsenic in groundwater and to implement effective mitigation strategies. In order to advance scientific knowledge on As mobility, we use a rich experimental dataset to implement a numerical physics-based model that describes the transport of arsenic in a natural mineral assemblage and under a broad range of hydrochemical conditions. We use the large computational capabilities of the Lichtenberg HPC to conduct model parameter estimation and explore multiple modeling scenarios with an automated procedure.

Methods

The model mathematically describes the physical transport of aqueous species and a series of geochemical reactions that include the complexation of arsenic onto reactive mineral surfaces and the precipitation and transport of secondary mineral phases. The model is numerically implemented using a Python-based simulator describing the transport of aqueous species. This simulator is coupled to the geochemical code PHREEQC-3 using the reaction module PhreeqcRM. Such coupling enables to carry out the thermodynamically-constrained geochemical reaction and transport calculations iteratively. Model parameter estimation is performed adopting a

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global optimization algorithm and using an automated procedure implemented in Python.

Results

In the initial phase of the project, we have developed and implemented the reactive transport code described above. This versatile numerical approach has allowed us to explore multiple model hypotheses that could potentially explain the experimental dataset. By performing numerical simulations and systematically comparing the results with the experimental dataset, we restrained the number of candidate solutions. We have now identified physical mass-transfer and geochemical processes that significantly affect the transport of arsenic under the experimental conditions. These processes include (i) the colloid-facilitated transport of arsenic by sorption onto secondary mineral phase precipitate and their elution through the porous media, (ii) the kinetic mass transfer of arsenic between the mobile pore water and the reactive surface of the porous matrix encompassing multiple time scales, and (iii) the strong mutual influence between the hydrochemical conditions and the mineral surface charge which determine sorption of arsenic.

Discussion

The model is now capable to reproduce a large part of the experimental dataset. Although these results are encouraging and already shed light on the mechanisms controlling arsenic transport under natural conditions, additional work is required in order to improve the model-data fitting, finalize the model implementation, and turn these results into scientific publications.

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