Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Arsenic Transport in Natural Porous Media

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Clusters
Lichtenberg II Cluster Darmstadt

Additional Software
PHREEQC-3

Institute
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Introduction

Arsenic (As) contamination of groundwater is a severe global health problem, affecting millions of people worldwide. The transport and concentration of arsenic in groundwater are largely controlled by sorption onto mineral surfaces. However, we still lack a comprehensive, mechanistic understanding of As partitioning under complex natural conditions. This knowledge gap critically limits our ability to predict where and when arsenic in groundwater will occur and to design effective, long-term mitigation strategies for safe drinking water. To address this challenge, our project aims to develop a comprehensive, physics-based numerical model. The model is designed to simulate arsenic transport through natural mineral assemblages, using a rich experimental dataset for validation across a broad range of hydrochemical conditions. The complexity of these natural systems, involving numerous interacting physical and chemical processes, makes it a formidable computational task. Exploring multiple scientific hypotheses and calibrating the model to find the parameters that best match reality requires running thousands of simulations. This large-scale exploration is computationally intractable on standard computers, making access to the parallel processing power of the Lichtenberg HPC an essential requirement for the success of this research.

Methods

The model mathematically describes the physical transport of aqueous species and a series of geochemical reactions. These reactions include the binding of arsenic to reactive mineral surfaces and the formation and transport of new mineral

particles. To numerically implement this model, we developed a transport simulation framework in Python that is coupled with the powerful geochemical code PHREEQC-3. This coupling allows for a robust, iterative calculation where the physical transport and the thermodynamically-constrained chemical reactions continuously inform one another. Although a single simulation is demanding, the primary computational challenge lies in the model calibration. To find the set of parameters that allows our model to accurately reproduce the experimental data, we employ a global optimization algorithm. This automated procedure, also implemented in Python, systematically runs the simulation thousands of times to identify the optimal solution. This large-scale, iterative search for the correct parameters is computationally intensive and is precisely the task for which HPC resources are indispensable.

Results

The project has been divided into two main phases. In the initial phase, our efforts focused on developing the reactive transport code and using it as a tool for scientific discovery. By running large ensembles of simulations on the Lichtenberg HPC, we explored multiple competing hypotheses that could potentially explain our experimental observations. This systematic, computation-driven comparison allowed us to identify the key physical and geochemical processes that exert the most significant control on arsenic transport. Our findings highlight three critical mechanisms: (i) the facilitated transport of arsenic that binds on secondary mineral particles that form and flow through the porous medium; (ii) the transfer of arsenic from the mobile pore water to the static mineral surfaces that occurs over multiple time scales; and (iii) the strong feedback loop between water chemistry and the electrical charge on mineral surfaces, which ultimately governs how strongly arsenic binds to them. In the second phase, we successfully calibrated the model to reproduce the experimental results from two distinct types of natural porous media. The results of this calibration show that while the geochemical mechanisms controlling the mobility of arsenic are consistent between the two systems, the speed and timing of the arsenic mass-transfer differ significantly. This leads to important variations in the rate at which arsenic is released in pore water.

Discussion

The model we have developed is now capable of reproducing the data obtained in the complex flow-through experiments. These results are highly encouraging, providing new quantitative insights into the fundamental mechanisms controlling arsenic mobility in natural aquifers. The next step is to refine the model-data fit and translate these findings into impactful scientific publications.

Publications

Lucien Stolze: Earth and Environmental Sciences Area, Lawrence Berkeley National Laboratory (USA)

Reference

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