

PS Arsenic Mobilization in Shallow Aquifers Due to CO₂ and Brine Intrusion from Carbon Storage Reservoirs*

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Abstract

CO₂ enhanced oil recovery (CO₂-EOR) is a proven technology for improved oil production. In addition to economic benefits, ancillary associated CO₂ storage is causing recent renewed interest in the technology. Most CO₂-EOR targets exhibit not only excellent storage reservoirs bounded by effective seal layers, but also Underground Sources of Drinking Water (USDWs). Although risks to USDWs are definitively low, the potential leakage of CO₂, saline water and/or oil from the reservoir is a concern of commercial CO₂-EOR projects. Understanding of CO₂-water-sediment interaction mechanisms in USDWs and effective uncertainty assessments provide maximum protection for USDWs is critical for current policy as well as likely future USDW-specific regulatory protections. The primary focus of this research was the potential for release and migration of heavy metals in USDWs. Specifically, we developed an integrated framework of combined batch experiments and reactive transport simulations to quantify CO₂-water-sediment interactions and arsenic (As) mobilization responses to CO₂ and/or saline water leakage into USDWs. Experimental and simulation results suggest that when CO₂ is introduced, pH drops immediately, and initiates release of As from clay minerals. Calcite dissolution can increase pH slightly and cause As re-adsorption. Thus, the mineralogy of the USDW is ultimately a determining factor of the fate and transport of As and other such risks. Salient results of this research include: (1) Arsenic desorption/adsorption from/onto clay minerals is the major reaction controlling its mobilization, and clay minerals could mitigate As mobilization with surface complexation reactions; (2) dissolution of available calcite plays a critical role in buffering pH; (3) high salinity in general hinders As release from minerals; and (4) the magnitude and quantitative uncertainty of As mobilization are predicated on the values of reaction rates and surface area of calcite, adsorption surface areas and equilibrium constants of clay minerals, and cation exchange capacity. These results are intended to improve ability to quantify risks associated with potential leakage of reservoir fluids into shallow aquifers, in particular possible environmental impacts of As mobilization at CO₂-EOR and other types of carbon sequestration sites.

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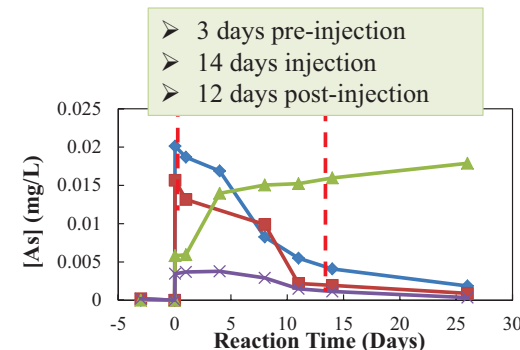
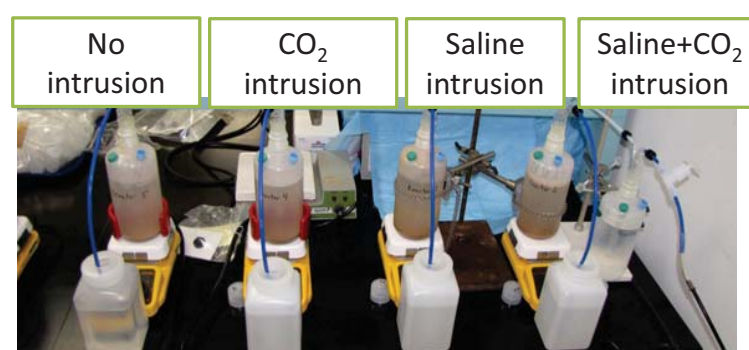
Introduction

The potential leakage of CO₂ and/or brine into Underground Sources of Drinking Water (USDWs) from the reservoir is considered as a major concern of geologic carbon storage projects. We developed an integrated framework of combined batch experiments and reactive transport simulations to quantify CO₂-water-sediment interactions and trace metal (arsenic) mobilization responses to CO₂ and/or brine leakage into USDWs. A field-scale model was also created with the kinetic parameters obtained from the integrated framework to forecast possible chemical impacts to USDWs with CO₂ and brine leakage. An active commercial-scale CO₂-enhanced oil recovery field, the Farnsworth Unit (FWU) overlain by the Ogallala aquifer was taken as a case study.

Methods

Batch Experiments

Two sets of experiments with “background” (BG, TDS ~ 200 mg/L) and “saline” (S, TDS ~ 4000 mg/L) synthetic groundwater were conducted.



Estimations of Key Parameters

TOUGHREACT models were simulated, considering aqueous species complexation, mineral dissolution/precipitation, adsorption/desorption, and cation exchanges.

Uncertainty parameters were estimated via inversion by minimizing the objective function J with PEST program:

$$J = \min \sum_{i=1}^N E_i(p); E_i(p) = \sum_{l=1}^{L_i} w_{li}^2 (u_i^l(p) - \tilde{u}_i^l)^2$$

where $E_i(p)$ is the sub-objective function from chemical species i , N is the number of chemical species, w_{li} is the weighting coefficient for the l th measurement of the i th species, which is computed with the inverse of the standard deviation of the experimental data, and u_i^l and \tilde{u}_i^l are the simulated and observed concentrations.

The Ogallala Aquifer Overlying the FWU

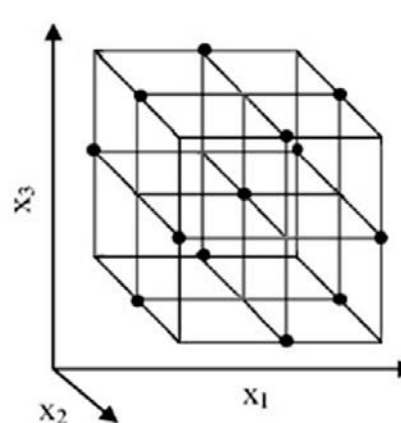


Hydrogeologic parameters for the FWU model

Model radius	10,000 m (1-D radial model)
Permeability	10 ⁻¹³ m ²
Porosity	0.3
Temperature	25 °C
Pressure	1 atm at the top
As concentration	3 µg/L (aquifer), 5 µg/L (brine)
Mineralogy	78% quartz, 11% calcite, 9% feldspar, 0.5% albite, 0.4% dolomite, 0.5% smectite
Simulation time	200 years

The Farnsworth Unit.

Response Surface Methodology (RSM)



Independent parameters for RSM of CO₂ and brine impacts to the groundwater (with Box-Behnken design)

Parameter name	Low (-1)	Mid (0)	High (+1)	Distribution
CO ₂ Leakage Rate: g/s	0	0.5	1.0	Uniform
Brine Leakage Rate: g/s	0	0.25	0.5	Uniform
Aquifer Thickness: m	40	120	200	Normal
Adsorbent SSA: m ² /g	1	50.5	100	Uniform

A second-order RSM equation is used to account for and quantify curvature:

$$y = \beta_0 + \sum_{i=1}^n \beta_i X_i + \sum_{i<j} \beta_{ij} X_i X_j + \sum_{i=1}^n \beta_{ii} X_i^2 + \varepsilon$$

Conclusions & Environmental Implications

- ✓ Arsenic desorption/adsorption from/onto clay minerals is the major reaction controlling its mobilization, and clay minerals could mitigate As mobilization with surface complexation reactions.
- ✓ Dissolution of available calcite plays a critical role in buffering pH.
- ✓ The magnitude and quantitative uncertainty of As mobilization are predicated on the values of reaction rates and surface area of calcite, adsorption surface areas and equilibrium constants of clay minerals, and cation exchange capacity.
- ✓ Arsenic may be considered an insignificant long-term concern in a CO₂ rich USDW environment because of clay adsorption.
- ✓ Increased salinity of USDW via the leaked saline water may likely be a larger concern than associated released trace metals.
- ✓ Results of this study are intended to improve ability to quantify risks associated with potential leakage of reservoir fluids into shallow aquifers, in particular the possible environmental impacts of As mobilization at carbon sequestration sites.

Acknowledgement

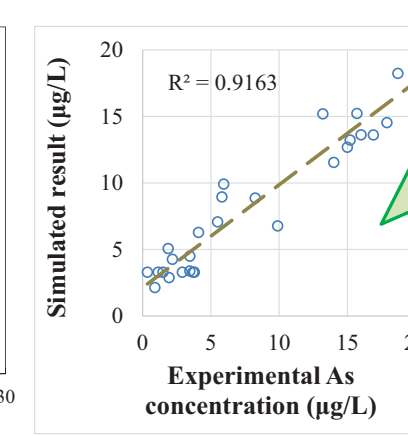
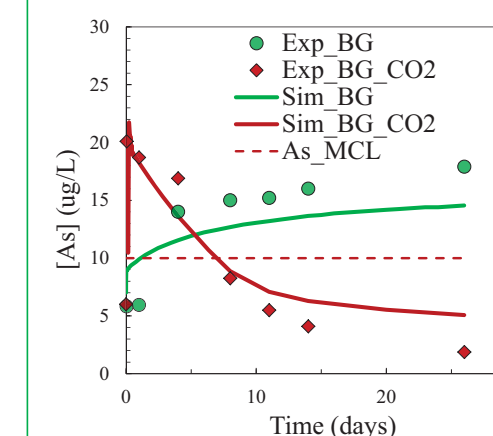
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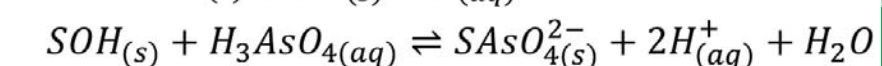
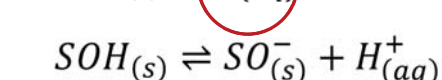
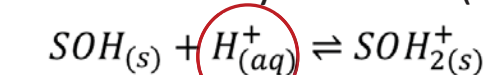
Results and Discussion

Arsenic mobilization mechanisms



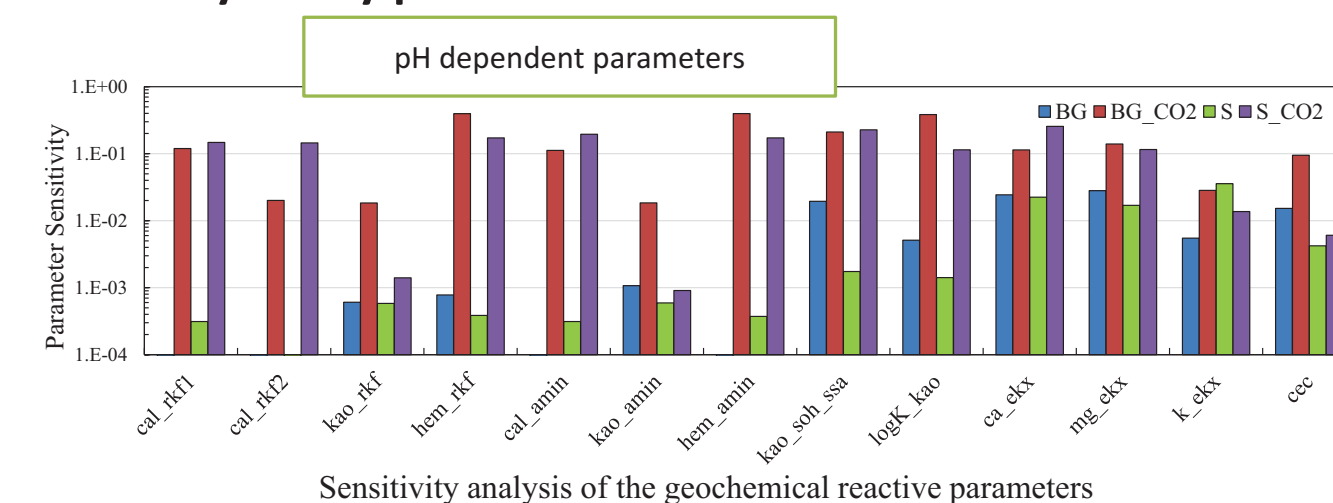
- Simulation results match with the experimental measurements.
- Without CO₂ intrusion, aqueous [As] approaches equilibrium with sediment (increase in this case).
- With CO₂ intrusion, [As] increase at the initial time and decrease slowly afterwards.

Adsorption/desorption onto/from the surfaces of clays controls As mobilization with water-rock-CO₂ interactions. The surface complexation reactions of the clay minerals (S represents mineral sites) could be written as:

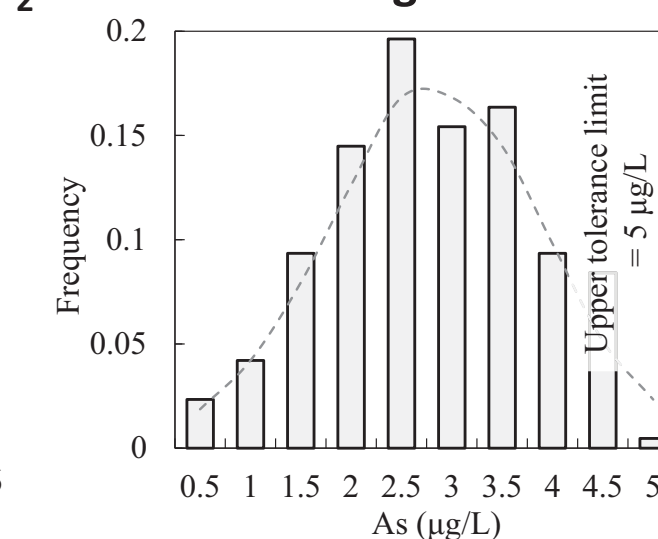
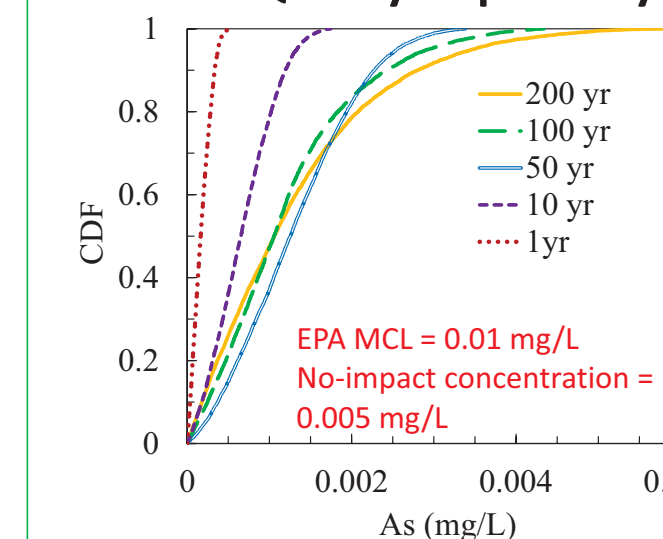


- Arsenic and H ions compete for mineral sites.
- With calcite dissolution, it consumes H⁺ for gradual As adsorption onto clay minerals.

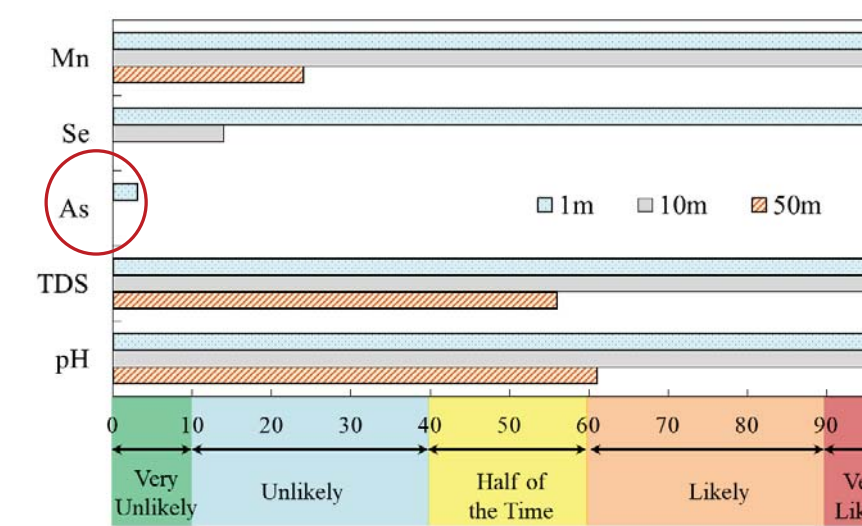
Sensitivity of key parameters



USDW Quality Impacts by CO₂ and Brine Leakage at the FWU



Cumulative distribution function of As concentration 1 m away from the leaky well (left). It shows only 3% probability of the concentration exceed the No-impact concentration based on site monitoring data (right).



Probability of occurrence of pH, TDS, As, Se and Mn exceeding the No-impact threshold at 1 m, 10 m and 50 m away from the leaky well after 200 years. Arsenic may be considered an insignificant long-term concern at the FWU. Salinity and pH changes might be a larger concern.