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Article

Arsenic in Petroleum-Contaminated Groundwater Near Bemidji, Minnesota Is Predicted to Persist for Centuries

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Supplementary Materials

Table S1. Physical and chemical properties of bulk oil. Modified from Table 3 in [28].

Parameter	Value
Bulk oil	
Density (g/cm^3)	0.854
Initial total mass (g/m of aquifer thickness)	7.77 x10^6
BEX (mass fraction of initial oil)	0.010
Toluene (mass fraction of initial oil)	0.0035
NVDOC (mass fraction of initial oil)	0.40
Short-chain n-alkanes (mass fraction of initial oil)	0.074
Long-chain n-alkanes (mass fraction of initial oil)	0.1

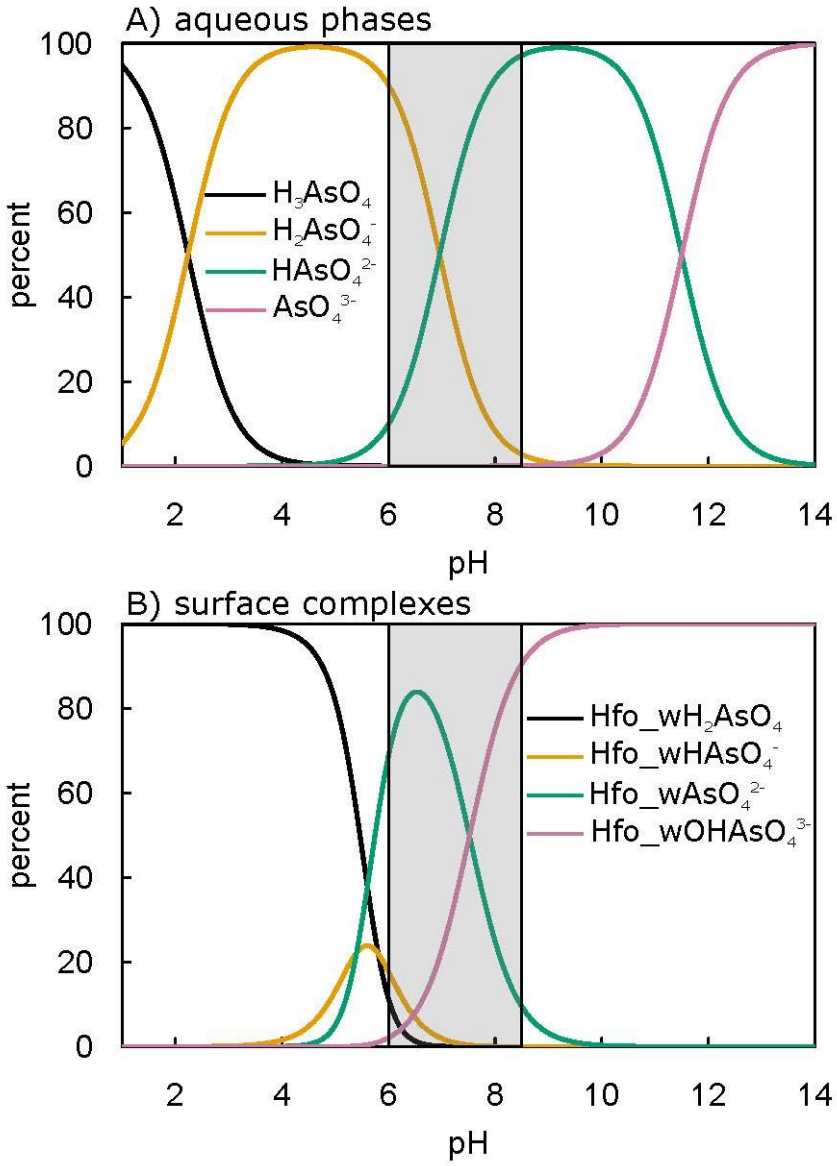

Figure S1. Generalized relative abundances of aqueous As(V) species (top) and As(V) surface complexes on $Fe(OH)_3$ (bottom). Aqueous species are determined from acid dissociation constants in Table 1. Surface species are determined from intrinsic complexation constants in Table 1. Modeled As(V) species are triprotic (black; H_3AsO_4/Hfo_wH_2AsO_4), diprotic (gold; $H_2AsO_4^-$/Hfo_w$HAsO_4^-$), monoprotic (green; $HAsO_4^{2-}$/Hfo_wAsO_4^{2-}), and unprotonated (pink; AsO_4^{3-}/Hfo_w$OHAsO_4^{3-}$). The monoprotic surface species (green) is omitted from [59]. The gray box indicates the pH range of most groundwaters (6-8.5).