Oak Ridge IFRC

**Modeling of Subsurface U(VI) Bioreduction and Uncertainties**

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Outline

• Background
• Site Characterization
• Batch Bioreduction Model
• Reactive Transport Model
• Discussion
U oxidation state, solubility and mobility

- Under aerobic conditions in natural waters
  - Quite mobile uranyle ion $\text{UO}_2^{2+}$ (pH < 5) and various uranyl-carbonate complexes (pH > 5)
- Under anaerobic conditions in aquifers
  - Practically insoluble uraninite $\text{UO}_2$
- Remediation Strategy
  - In-situ microbial reduction of U(VI) to U(IV) under anaerobic conditions
  - Precipitation of practically insoluble uraninite within contaminated aquifers
Enzymatic U(VI) Reduction

- Fe(III)-reducing bacteria (FeRB)
- Sulfate-Reducing Bacteria (SRB)
- Bioremediation Strategy:
  - Biostimulation of indigenous DMRB and SRB in the aquifer for immobilization of U in the aquifer
- Competing electron acceptors: nitrate, Fe(III) and sulfate
Site Characteristics

• Geochemistry
  – Low pH 3.4-3.9
  – High Nitrate ~10g/L
  – High Al, Ca, Mg, Na, and Ni
  – high U : 20 – 50 mg/L in GW & 700 mg/kg in sediments

• Stratigraphy
  – Matrix-fracture interactions
  – Heterogeneous, stratified aquifer

• Hydrogeology
  – Main pathway: unconsolidated intact saprolite
Batch Bioreduction Experiment

- Microcosm tests using three uranium contaminated sediments and groundwater amended with calcium oleate as an electron donor were performed.
- Oleate was degraded by indigenous microorganisms with acetate as a major product.
Batch Bioreduction Model Results

- The rapid removal U(VI) from the aqueous phase was observed associated with sulfate reduction.
- Bioreduction model
  - First order oleate degradation
  - Sulfate and U(VI) reduction using dual Monod rate law
Reactive Transport Model

- Physical transport processes
  - Advection + dispersion
  - Mass transfer between stagnant micro-pores and mobile flow zones
- Biogeochemical processes
  - Equilibrium aquatic geochemical reactions
  - Uranium sorption/desorption
  - Microbial reduction kinetics
Bioreaction Kinetics

- Ethanol injection
- Terminal electron-accepting process
  - Denitrification: $10^3$–$10^6$ cells/ml denitrifiers
  - Ferrihydrite Reduction: $10^2$–$10^3$ cells/ml FeRB
  - Sulfate Reduction: $10^4$–$10^5$ cells/ml SRB
  - U(VI) Reduction
- Biomass in mobile domain
Oak Ridge Area 3 Case

Modeling of Subsurface U(VI) Bioreduction and Uncertainties

Phase I        Phase II               Phase III

COD           pH

SO$_4^{2-}$  HCO$_3^{-}$

NO$_3^{-}$  U(VI)
Discussion

• Uncertainty Parameters
  – Aqueous speciation
  – SCM
  – Bioreaction kinetics
  – Microbial transformations
    Inhibition term \( K_{NO3} / (K_{NO3} + c_{NO3}) \)

• Model improvements
  – Sensitivity analysis to simplify the models
  – Extending to multiple types of biomass