Reactive Transport Simulation of In-Situ Uranium(VI) Bioremediation Experiment

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Introduction

A reactive-transport model is developed based on travel-time discretization to simulate an in-situ bioremediation experiment for demonstrating enhanced bioreduction of uranium(VI) at Oak Ridge, TN. Breakthrough curves of a conservative tracer are used to derive the space to travel-time transformation from the injection well to the observation points. Reactive transport is solved numerically in time and travel-time coordinates. Breakthrough curves of reactive components are obtained by weighting the solutions of the reactive transport model with the travel-time distributions. By assuming linear transport systems, we estimate the first-order consumption rates of injected electron donor at both observation and extraction wells. By considering nonlinear reaction kinetics, the breakthrough curves of major components are estimated at the observation point.

Governing Equations

$$\frac{\partial \mathbf{c}^m_{aq}(t,\mathbf{x})}{\partial t} + \frac{\partial \mathbf{c}^m_{sorb}(\mathbf{c}^m_{aq})}{\partial t} + \mathbf{v}(t,\mathbf{x})\cdot\nabla \mathbf{c}^m_{aq}(t,\mathbf{x})$$

$$\leftrightarrow im\,(\mathbf{c}^m_{aq},\mathbf{c}^{im}_{aq}) + \mathbf{r}_{equi}(\mathbf{c}^m_{aq}) + \mathbf{r}_{microbial}(\mathbf{c}^m_{aq},t)$$

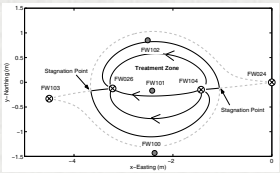
$$\tau(\mathbf{x}) = \int_{\mathbf{x}_{in}}^{\mathbf{x}} \frac{d\xi}{\|v_\xi\|}$$

$$\frac{\partial \mathbf{c}^m_{aq}(t,\tau)}{\partial t} + \frac{\partial \mathbf{c}^m_{sorb}(\mathbf{c}^m_{aq})}{\partial t} + \frac{\partial \mathbf{c}^m_{aq}(t,\tau)}{\partial \tau}$$

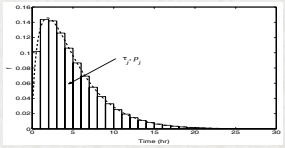
$$\leftrightarrow im\,(\mathbf{c}^m_{aq},\mathbf{c}^{im}_{aq}) + \mathbf{r}_{equi}(\mathbf{c}^m_{aq}) + \mathbf{r}_{microbial}(\mathbf{c}^m_{aq},t)$$

$$\mathbf{c}^m_{aq}(t) = \sum_j p_j(\tau_j)\,\mathbf{c}^m_{aq}(t|\tau_j)$$

Nonuniform Flow Field

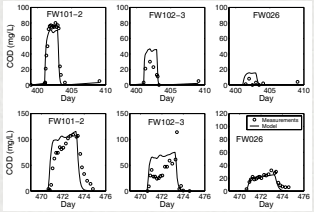


Travel-Time *pdf* at FW101-2



Model I: First-order model

To approximate first-order electron donor consumption rates; Linear system assumption; Method of transfer function



***K*=0.1/hr**

Model II: Nonlinear reaction model

Reaction kinetics include:

- Aquatic equilibrium geochemistry
- Uranium sorption/desoprtion (Surface-Complexation Model)
- Kinetic mass transfer
- Denitrification, sulfate reduction, and U(VI) reduction

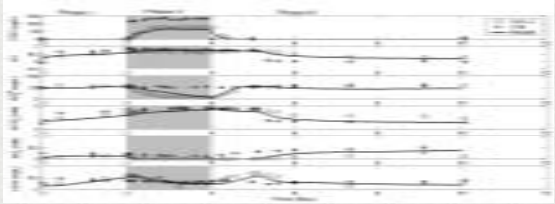
Model implementation:

- Travel-time domain by PhreeqC and MATLAB
- Aqueous speciation: Grenthe et al. (1992), calcium-uranyl-carbonate complexes and Wateq4f
- Surface chemistry: Dzombak and Morel (1990) and Waite et al. (1994)

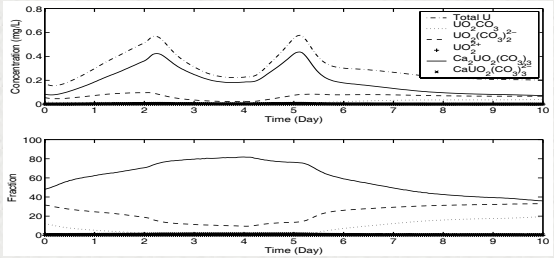
Parameters to be determined:

- Effective reduction rate of U(VI)
- Sorption site distribution

Concentration Breakthrough Curves at FW101-2



Aqueous U(VI) Species and Fraction



Conclusions

- Effective electron-donor consumption rate: 0.1/hr;
- Effective U(VI) reduction rate: 1mmol/mgSRB-day;
- U(VI) sorption/desorption is kinetically controlled, and highly influenced by pH and bicarbonate levels which va during the bioreduction experiment.
- Inhibition by nitrate was absent due to complete remova and impact of calcium on reduction rate may be present, which may strongly influence the level of bioavailable U(species.

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