Modelling Approaches and Issues

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Outline

► Modeling Challenges
► Site Characterization
  ● Physical and chemical properties
  ● U(VI) Source Term
► Scale Up
► Multiscale Models
► Need for High Performance Computing
Modeling Challenges

- 3D Domain: length and time scales
  - field scale domain (5-50m)
  - hourly river fluctuations, ~year predictions
- Complex chemistry: Na-K-Ca-Fe-Mg-Br-N-CO$_2$-P-S-Cl-Si-U-Cu-H$_2$O (~15 primary species)
- Multiscale processes (µm-m)
- Highly heterogeneous sediments
  - fine sand, silt; coarse gravels; cobbles
- Variably saturated environment
- Initial & boundary conditions

![Diagram showing saturated and unsaturated zones with dimensions $L_x \sim 50m$, $L_y \sim 50m$, and $L_z \sim 15m$.]
Site Characterization

- Porosity, permeability, relative permeability and capillary pressure relations
- U(VI) concentration in aqueous and solid phases
- Surface complexation site density
- Mineral surface areas, rate constants and abundances
- Multiscale model parameters
- Geostatistical model to generate multiple realizations
U(VI) Source Term

- Vadose zone source
- Release mechanisms
  - Fluctuating water table
  - Mineral dissolution
  - Desorption
  - Diffusion
- Infiltration
  - Chinook (~200 mm/d 1985)
  - Mean 200 mm/y
Sub-Grid Scale Model

- Mineral form (kinetic dissolution)
  - Co-precipitation of U(VI) with calcite
  - Metatorbernite \([\text{Cu(UO}_2\text{)}_2(\text{PO}_4\text{)}_2 \cdot 8\text{H}_2\text{O}]\)

- Sorbed form (surface complexation-local equilibrium)

- Intra-granular diffusion

- Sub-domain distribution
Scale Up

Spatial
- Small column ⇒ large column ⇒ field
- Core scale (column support data): 1-10 cm
- Field domain size: $L \sim 5$-50 m

Temporal
- Highly fluctuating river stage (~hourly)
- Time step $\Delta t$: 1 hour $= 1.14 \times 10^{-4}$ years
- $8.76 \times 10^6$ time steps to reach 1000 years

Methods
- Geostatistical methods to extrapolate between wells
- Fitting to column experiments
- Time averaging
Multiscale Models

- Multirate model

- Multiple interacting continuum model

1-Node Sub-Grid Model

3D Primary Continuum

1-D Sub-Grid Model

3D Primary Continuum
Two-Domain Model

▶ Primary continuum:

\[
\frac{\partial}{\partial t} \epsilon_{\alpha} \varphi_{\alpha} R_{j}^{\alpha} \Psi_{j}^{\alpha} + \nabla \cdot \epsilon_{\alpha} \Omega_{j}^{\alpha} = -\epsilon_{\alpha} \sum_{m} \nu_{jm} I_{m}^{\alpha} - \Gamma_{j}^{\alpha\beta} (\Psi_{j}^{\alpha} - \Psi_{j}^{\beta})
\]

▶ Secondary continua:

\[
\frac{\partial}{\partial t} \epsilon_{\beta} \varphi_{\beta} R_{j}^{\beta} \Psi_{j}^{\beta} + \nabla \cdot \epsilon_{\beta} \Omega_{j}^{\beta} = -\epsilon_{\beta} \sum_{m} \nu_{jm} I_{m}^{\beta} + \Gamma_{j}^{\alpha\beta} (\Psi_{j}^{\alpha} - \Psi_{j}^{\beta})
\]

▶ Mineral mass transfer:

\[
\frac{\partial \varphi_{s}^{\alpha}}{\partial t} = V_{s} I_{s}^{\alpha}, \quad \frac{\partial \varphi_{s}^{\beta}}{\partial t} = V_{s} I_{s}^{\beta}
\]
Multiple Interacting Continuum Model

Primary continuum ($\alpha = \text{primary fluid}$):

$$\frac{\partial}{\partial t} \epsilon_\alpha \varphi_\alpha R_j^\alpha \Psi_j^\alpha + \nabla \cdot \epsilon_\alpha \Omega_j^\alpha = -\epsilon_\alpha \sum_m \nu_{jm} I_m^\alpha - \sum_\beta a_{\alpha\beta} \Omega_j^{\alpha\beta}$$

Secondary continua ($\beta^{th}$ continuum):

$$\frac{\partial}{\partial t} \epsilon_\beta \varphi_\beta R_j^\beta \Psi_j^\beta + \nabla \cdot \epsilon_\beta \Omega_j^\beta = -\epsilon_\beta \sum_m \nu_{jm} I_m^\beta$$

Boundary conditions:

$$\Psi_j^\beta(0, t | r) = \Psi_j^\alpha(r, t), \quad \Omega_j^{\alpha\beta} = -\varphi_\beta D_\beta \left( \frac{\Psi_j^\alpha - \Psi_j^\beta}{d_{\alpha\beta}} \right)$$

Mineral mass transfer:

$$\frac{\partial \varphi_s^\alpha}{\partial t} = \overline{V}_s I_s^{\alpha}, \quad \frac{\partial \varphi_s^\beta}{\partial t} = \overline{V}_s I_s^{\beta}$$
Hanford Large Column Exp. NPP1-14
Multiscale Model of Hanford Large Column Exp.

Test model by comparing overall U(VI) mass balance
Number of Degrees of Freedom

\[ N_{\text{dof}} = N \times N_C + N \times N_C \times N_M \times N_K \]

**Storage**

- \( N \) = Number of primary domain nodes \( (3D: 10^7) \)
- \( N_K \) = Number of sub-grid classes \( (10) \)
- \( N_M \) = Number of nodes in each class \( (10) \)
- \( N_C \) = Number of chemical components \( (15) \)
- Total: \( 1.5 \times 10^{10} \)

- Employ sub-grid model only where needed
- Combine with adaptive mesh refinement
- Use efficient numerical schemes to rigorously “decouple” primary and secondary continua
  - Operator splitting
  - Fully implicit
Computational Resources

 Degrees of Freedom
Jaguar: 11,508 dual-core 2.6GHz AMD Opteron processors, 4 GB of memory (2 GB per core) for a total of 46 TB, 600 TB of scratch space, Cray Seastar router through Hypertransport interconnected in a 3D-torus topology providing very high bandwidth, low latency, and extreme scalability.
Multirate Model

Sorption model:

\[
\frac{\partial}{\partial t} \varphi C_j + \nabla \cdot F_j = - \sum_\beta \Gamma_j^\beta f_\beta K_j^d C_j - S_j^\beta
\]

\[
\frac{\partial S_j^\beta}{\partial t} = \Gamma_j^\beta f_\beta K_j^d C_j - S_j^\beta
\]

Not clear how to include mineral precipitation and dissolution
Time Step Control

- Groundwater velocity: $q \sim 500$ m/y (Darcy Vel.)
- Porosity $= 0.25$, $v_{\text{pore}} \sim 2$ km/y
- CFL $= v \Delta t/\Delta l \sim 1$, $\Delta t = 1$ hour, $\Delta l \sim 20$ cm