Modeling Working Group

Coordination Plans and Opportunities

NABIR FRC Workshop
September 22-24, 2003

Survey of Current Modeling Efforts

- General project information
- Objectives of modeling efforts
- Code documentation, availability, capabilities and limitations
- Sources/values for FRC input parameters

In Situ Immobilization of Uranium in Structured Media via Biomineralization

Schiebe, Roden and Zachara

- Modeling objectives

  - Basis for iterative design and interpretation of field experiments

  - Identify mechanisms and reaction parameters
- HBGC123D – 3-D transport with biogeochemical rxs and FRAC3DVS – 3-D explicit fracture transport
- Simulations in progress for experimental design
- Summary of model parameters from site investigations and the literature being compiled

Evaluation of Biostimulation for Remediation of Uranium Contaminated Groundwater

Criddle, Kitanidis, et al.

- Objectives:
  - Determine optimal design of multiwell extraction systems
  - Predict field-scale flow and reactive transport
  - Identify mechanisms and reaction parameters
- ComCZAR and SRG3D – flow field/capture zone models
- UPHREEQC – PHREEQC variant for uranium geochem
- Model parameters from in situ flowmeter, seismic & tracer tests, column studies and literature

Factors Controlling In Situ Uranium and Technitium Bioreduction and Reoxidation

Istok, Krumholtz, Gu and McKinley

- Objective:

  Identify and quantify biogeochemical reactions controlling uranium and technitium during push-pull testing
- PHREEQC2 –batch or 1-D steady flow with equilibrium/kinetic geochemical rxs
- No biogeochemical modeling of field experiments planned
- Schiebe plans to utilize data from field experiments for parameter estimation/model validation

Influence of Reactive Transport on Reduction of U(VI) in Presence of Fe(III) and Nitrate

Wood, Szecsody, Liu and Zachara

- Modeling objective

  - Simulate lab column experiments to invert for physical and biogeochemical parameters

- CXTFIT – analytical transport model inversion (1-D)
- RAFT – numerical model for transport with user-prescribed equilibrium and/or kinetic reactions (3-D)

Ion Reduction and Radionuclide Immobilization: Kinetic, Thermodynamic, Hydraulic Constants and Reaction-based Modeling

Burgos and Yeh

- Modeling objectives

  - Determine optimum forms of kinetic rate equations that are consistent across a wide spectrum of conditions

  - Determine thermodynamic and kinetic coefficients for chemical and microbially-mediated reactions
- HBGC123D and variants – flow/transport with biogeochemical reactions
- Simulate lab batch and column experiments for parameter estimation and validation of reaction formulations

Overview of Model Parameters

- Hydraulic and transport variables – K, recharge/pumping, unsat properties, dispersivities, fracture/matrix parameters (most straightforward to determine but high spatial variability)
- Equilibrium chemical rxs – equilibrium constants, exchange capacity
- Chemical kinetics – forward/backward rate coefficients
- Microbial kinetics – rate constants for substrates, nutrients and e-receptors, lag/inhibition coefficients, microbial growth/death coefficients
- How much detail is needed vis a vis chemical components, microbial populations, soil heterogeneity, etc.?

Model Uses and Benefits

- Extend research results to different conditions/sites with minimal additional effort <u>if model is mechanistically accurate</u>
- Facilitate interpretation of lab and field data by mathematically separating complex interacting processes
- Design lab/field scale experiments to obtain the greatest amount of useful information per research dollar
- Scale-up process descriptions from lab/pilot to full-scale, predict remediation effectiveness, optimize design and extrapolate to sites with different conditions
- Determine what factors are most important to remediation success to better focus research efforts

Coordination Objectives

- Achieve maximum leverage on investments in expensive field and lab data collection
- Encourage consistent parameterization where possible to maximize data portability among projects (e.g., kinetic models)
- Minimize redundant model development and calibration efforts across current and future projects (archiving of codes and data files, parameter tabulations, site hydrologic data, etc.)
- Provide model sensitivity results for use in evaluating critical research needs and as guidance for lab/field studies

Issues for Consideration …

- What are the "most critical" model parameters?

"*Research leverage*" = $\sigma_p S_p E_p$

where σ_p = std deviation of parameter p

S_p = sensitivity of (cost)/benefit to parameter p

E_p = research efficiency: reduction in σ_p per research $

- Is current research addressing these issues?

Coordination Tasks

- Tabulate reaction models utilized by various PIs to facilitate coordination of modeling approaches
- Develop a database of model parameters as well as “raw” data to facilitate extrapolation to different conditions and sites and avoid redundant efforts across projects
- Improve pre-/post-processing capabilities of existing numerical models applicable to FRC to facilitate use by PIs
- Site-wide FRC model would serve as base for integrating results from diverse studies, as starting point for project-specific modeling efforts and for eventual consideration of field-scale remediation alternatives