PNNL-SA-60272

Hanford 300 Area IFC Flow and Transport Modeling Integration and Coordination

Mark Rockhold
Pacific Northwest National Lab

IFC Project Meeting, Richland, WA
April 29-30, 2008

Overview

- 3D numerical flow and transport models of the IFC plot and the greater 300 Area uranium plume-scale domains will be based on all available site characterization data and experimentally-based descriptions of geochemical reaction and mass transfer processes
- Calibrated 3D model results and associated data will provide the basis for determining the most parsimonius conceptual-mathematical model(s) of flow, geochemical reactions, and uranium mass transfer for the 300 Area
- Modeling will provide input to help inform and guide future remediation decisions

Basic requirements for modeling IFC flow and reactive transport experiments

- Three dimensional
- Variably saturated flow (vadose zone and aquifer experiments)
- Non-isothermal (heat as a tracer)
- Multi-component reactive transport (perturbations of aqueous chemistry, isotopic exchange, precipitation/dissolution reactions, etc.)

300 Area IFC codes

- **STOMP, STOMP-SC** (*PNNL*)
  - 3D variably saturated flow and transport
  - Coupled heat and mass transfer in multiple fluid phases (aqueous, gas, CO_2, NAPL, hydrates)
  - Multi-component reactive transport (with TVD)
- **FLOTRAN, PFLOTRAN** (*LANL*)
  - 3D variably saturated flow and transport
  - Coupled heat and mass transfer in two-phase systems (aqueous, gas, CO_2)
  - Multi-component reactive transport
- **MODFLOW / MT3DMS / PHT3D** (*USGS*, *U. Alabama, CSIRO*)
  - 3D variably saturated flow and transport
  - Single (aqueous) phase flow under isothermal conditions
  - Multi-component reactive transport (with TVD and particle tracking)

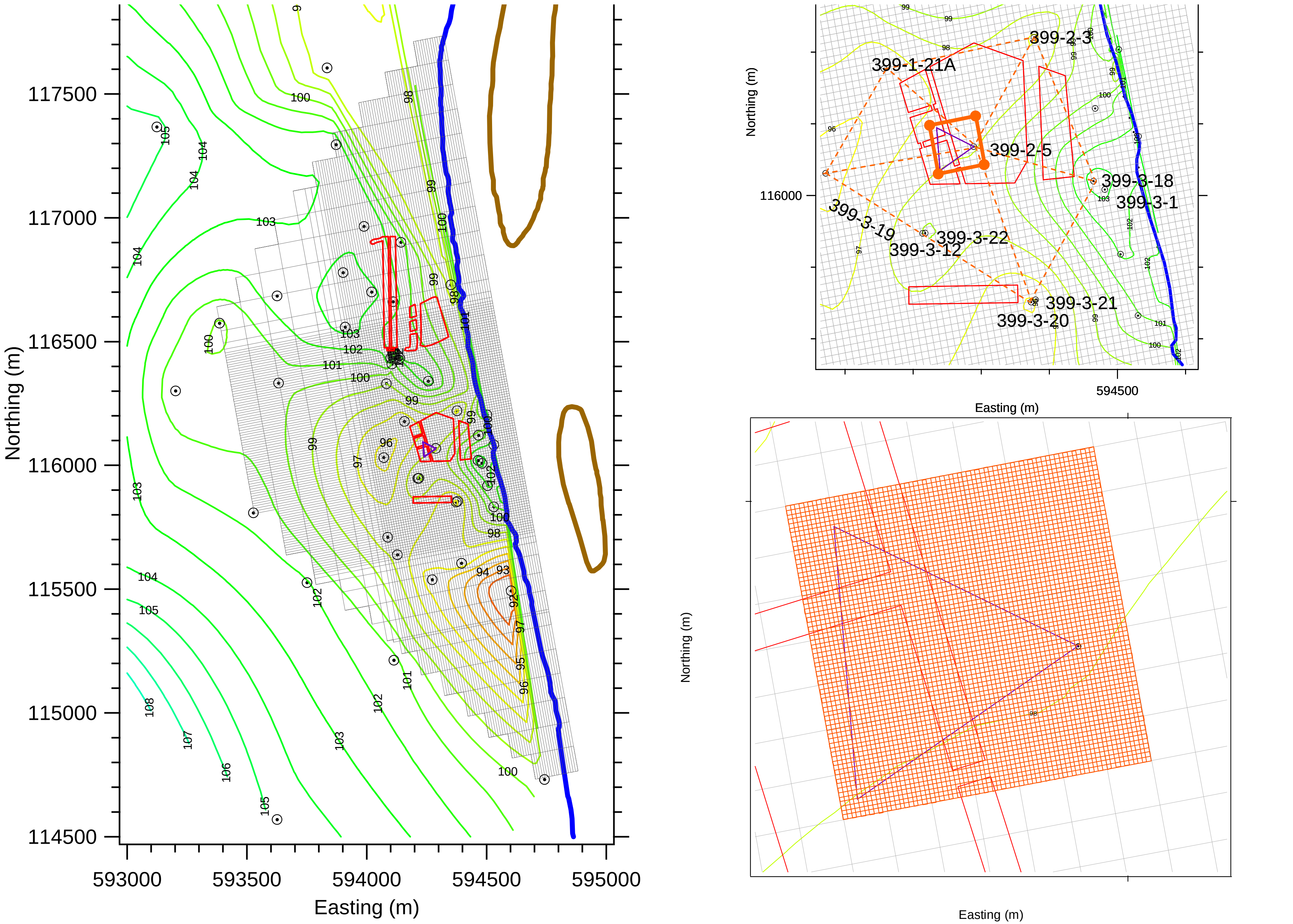
Code commonalities and differences

- For simple systems - single (aqueous) phase flow and non-reactive transport – *these codes all solve essentially the same governing equations*
- Codes differ in
  - Capabilities for solving single- vs. coupled, multi-fluid flow problems
  - Single- vs. multi-continuum model formulations for flow and transport
  - Numerical schemes for transport and reactions
    - e.g. Implicit vs. explicit advection operators (e.g. TVD)
  - Parallelization methods, scalability, problem sizes they can handle
  - Inverse modeling
    - Linkages to UCODE vs. PEST vs. SCEM-UA vs. TAO
  - Capabilities for modeling coupled hydrogeophysical data
    - Resistivity (e.g. response to saline tracer, etc.)
  - Ease of use
    - GUI (e.g. Visual MODFLOW)
  - User base, on-site applications experience, and developer support
  - Speed of execution
    - Dependent on development goals

Defining roles for modeling groups

- STOMP(-SC), (P)FLOTRAN and MODFLOW / MT3DMS / PHT3D will all be used for developing and testing alternative conceptual-mathematical models of uranium mass transfer and reactions at 300 Area IFC Experimental Site
- STOMP models of 300 Area
  - 3-D uranium plume-scale flow and transport model (Peterson et al. 2008; Williams et al., in review)
  - 2-D multi-component U transport models w / wo mass transfer (Kd, GCSCM, Multi-rate) (Yabusaki et al. 2008)
  - STOMP models are currently being used in support of remedial decisions for the 300 Area uranium plume – STOMP is qualified for use in Hanford regulatory analyses
- MODFLOW – MT3DMS models of 300 Area
  - 3-D uranium plume-scale flow and transport model (Meyer et al. 2007)
- PFLOTRAN model of 300 Area
  - Preliminary 3-D plume scale flow model (Hammond & Lichtner, 2008)

STOMP 300 Area uranium plume- and IFC plot-scale model grids



Goals for model coordination

1. Maximize scientific contributions, peer-reviewed publication of results, and benefit to DOE and stakeholders
2. Take advantage of strengths of each code, experience of developers, users, and available tools (e.g. utilities)
3. Minimize intra- and inter-group repetition, and maximize synergy through different approaches and perspectives
4. Focus on the science and the conceptual-mathematical models (not on the "codes")

The quality and usefulness of modeling results will depend on the types and quality of the characterization data and field experimental results, the <u>level of effort and creativity in data assimilation and model parameterization</u>, and on the ability of the computer models to represent the physical and (bio)geochemical processes.

Multiple conceptual-mathematical models

- Predictive uncertainty attributed to:
  - ***Conceptual model uncertainty***
    - Multi-scale heterogeneities
      - Topography of Hanford / Ringold fm contact and channel features
      - Facies distributions
    - Models of reaction and mass transfer
      - Multi-rate kinetic, surface complexation, dissolution, etc.
      - Single- vs. dual- vs. multi-continuum model formulations
    - Boundary conditions
      - Sparse well coverage for defining heads along inland boundaries
  - ***Parameter uncertainty*** (model-dependent physical, hydraulic, geochemical, and electrical parameters)
    - e.g. K_x, K_y, K_z, ϕ, λ, h_b, D_x, D_y, D_z, A_s, β_i, γ_i, κ_i
  - ***Scenario uncertainty***
    - Remedial actions (e.g. polyphosphate, apatite, bioreduction, etc.)
    - Future land use
    - Climate change and Columbia R. hydropower operations

Conceptual model uncertainty can not be addressed without developing multiple conceptual / mathematical models of the site

"Strawman" for modeling

1. Define small set of test problems related to the 300 Area IFC that each code must solve, for which analytical solutions exist, e.g.
    a. 3D tracer transport under steady flow in homogeneous aquifer
    b. 3D tracer transport under steady flow through variably-saturated porous media
    c. 3D reactive transport under steady flow in homogeneous aquifer
2. Compare analytical and numerical results for code verification and benchmark testing

Strawman (cont.)

3. IFC Team will postulate discrete set of alternative conceptual models based on IFC characterization and field experiments
   a. Physical system structure and heterogeneities
   b. Reaction and mass transfer processes within the system
4. Assign probabilities to the alternative conceptual models (e.g. equal weights, subjective weighting, or based on synthetic test cases)
5. Assign conceptual models to modeling teams for implementation

Strawman (cont.)

6. All modeling teams will perform “blind” pre-experiment modeling of first IFC tracer test (aquifer injection of NaBr, PFBA, etc.)
7. Perform first IFC tracer test
8. Compare observed and simulated results

Strawman (cont.)

9. Provide site characterization data, boundary condition information (water level data), and tracer test results to all modeling teams
10. Have modeling teams *calibrate* their models to the field tracer test data
11. Perform quantitative comparisons of observed and simulated results
12. Rank the conceptual-mathematical models using objective criterion (e.g. Kashyap or Akaike information criterion - overly complex or over-parameterized models are penalized.)

Strawman (cont.)

13. Design subsequent IFC tracer or reactive transport experiment (aquifer injection)
14. All modeling teams will do pre-experiment modeling (predictive mode – no model calibration)
15. Perform reactive transport experiment
16. Compare observed and simulated results

Office of Science
U.S. DEPARTMENT OF ENERGY

Strawman (cont.)

17. Provide data from reactive transport experiment to modelers
18. Calibrate the models
19. Compare observed and calibrated simulation results and rank the models
20. Evaluate joint conceptual model and parameter uncertainty using MLBMA(???) (Meyer et al. 2007)
21. Repeat steps 12-19 for each field experiment

Strawman (cont.)

- Verification and benchmark comparisons will establish basic equivalencies of code numerics (to shift focus from “codes” to the conceptual-mathematical models of geochemical reaction and mass transfer that we are trying to test)
- Predictive modeling, subsequent calibration, and ranking of simulation results using objective criterion will determine most parsimonious conceptual-mathematical models of flow, geochemical reaction, and uranium mass transfer for the IFC experimental domain
- Results can be transferred to 300 Area uranium plume-scale flow and reactive transport models
  - Note: Plume-scale modeling will require additional effort related to larger-scale structural features and heterogeneities

Strawman summary

- For each field experiment

1. Perform “blind” pre-experiment modeling using different conceptual-mathematical models
2. Perform field experiment
3. Compare observed and simulated results
4. Calibrate the models
5. Perform quantitative comparisons of goodness of fit
   a. Point comparisons, spatial moments, mass fluxes, particular emphasis on late-time BTC behavior
6. Rank the models
   a. Kashyap and Akaike information criteria (overly complex or over-parameterized models are penalized)

- Postulate refined conceptual-mathematical models and repeat steps 3 – 6, as needed.

References

- Hammond, G. and P. C. Lichtner. 2008. High Resolution Simulation of the Hanford 300 Area, DOE ERSP Annual PI Meeting, Lansdowne, Virginia.
- Meyer, P. D., M. Ye, M. L. Rockhold, S. P. Neuman, and K.J. Cantrell. 2007. Combined Estimation of Hydrogeologic Conceptual Model, Parameter, and Scenario Uncertainty with Application to Uranium Transport at the Hanford Site 300 Area, NUREG/CR-6940, PNNL-16396, U.S. Nuclear Regulatory Commission, Washington, D.C.
- Peterson, R. E., M. L. Rockhold, R. J. Serne, P. D. Thorne, and M. D. Williams. 2008. Uranium Contamination in the Subsurface Beneath the 300 Area, Hanford Site, Washington. PNNL-17034, Pacific Northwest National Laboratory, Richland, Washington.
- Williams, M. D., M. L. Rockhold, P. D. Thorne, Y. Chen. 2008. Three-Dimensional Groundwater Models of the 300 Area at the Hanford Site, Washington. In review, Pacific Northwest National Laboratory, Richland, Washington.
- Yabusaki S. B., Y. Fang, and S. R. Waichler. 2008. Building Conceptual Models of Field-Scale Uranium Reactive Transport in a Dynamic Vadose Zone-Aquifer-River System. *Water Resources Research* (in press February 2008).
- Zachara, J. et al. 2006. Multi-Scale Mass Transfer Processes Controlling Natural Attenuation and Engineered Remediation: An IFC Focused on Hanford's 300 Area Uranium Plume. Proposal to U.S. DOE, Office of Biological and Environmental Research, LAB 06-16 – Environmental remediation Science Program, Integrated Field-Scale Subsurface Research Challenge.