Modeling Flow and Transport at DOE Sites:

Field-scale effects of heterogeneous coupled physical and biogeochemical processes.

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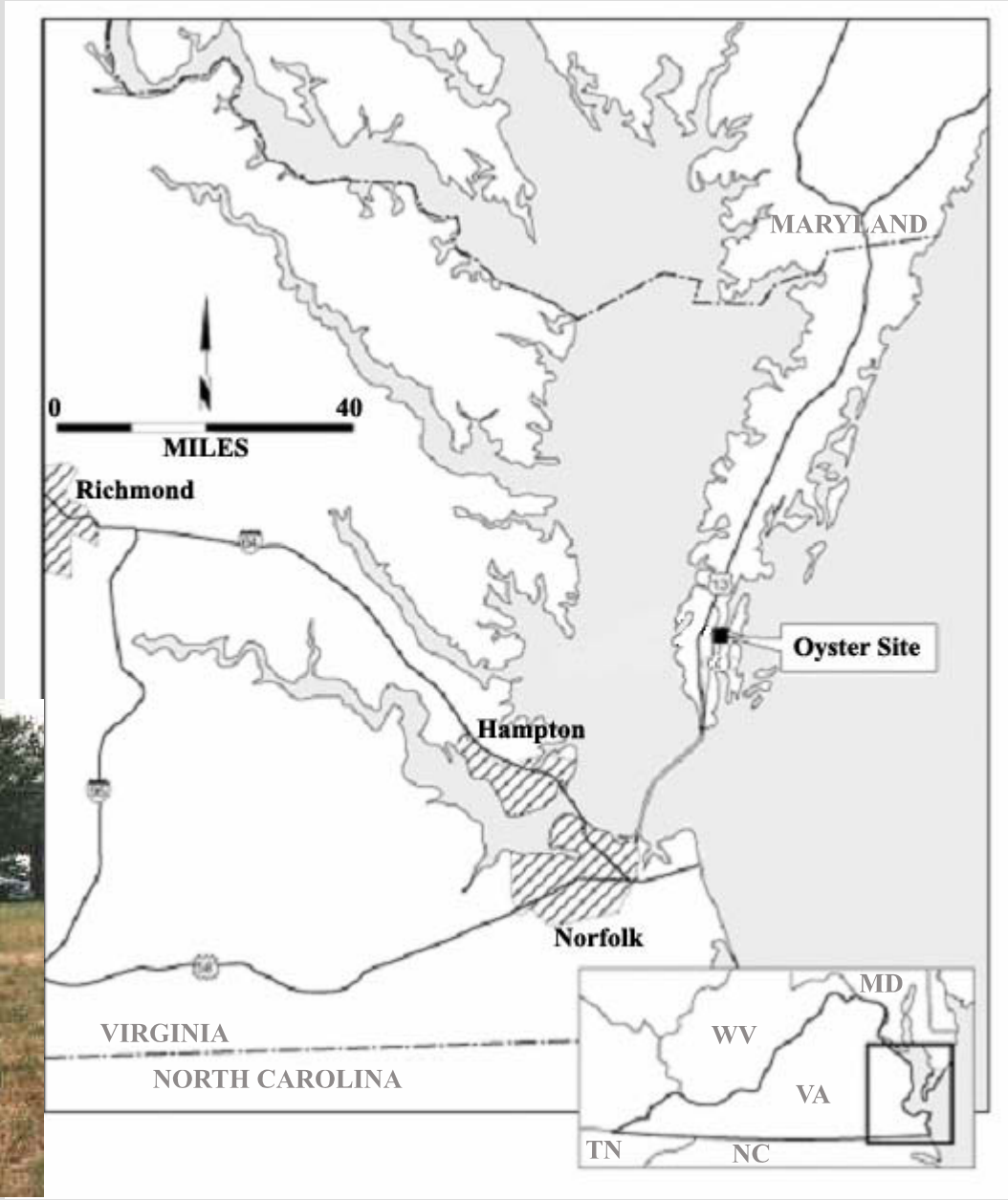
Reactive Transport Modeling

- Major strides have been taken in the last decade. Current models are relatively sophisticated and powerful, and have been successfully applied to field-scale problems.
- Some situations still confound modelers
  - Strong heterogeneity at multiple length scales (and in particular correlated physical and chemical heterogeneity)
  - Coupled flow, transport, and reaction processes
- Examples of DOE research sites where innovations in characterization and modeling have been applied

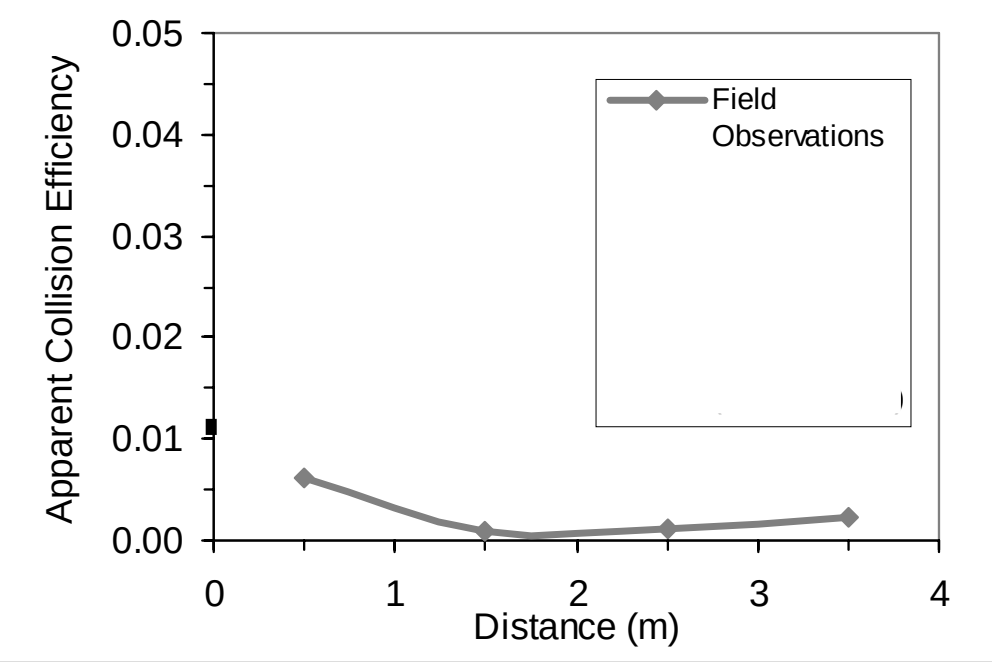
A Field Test

- South Oyster Focus Area (SOFA) – 2001
- Bacteria and tracer injected over 12-hour period; monitored over 7-day period



A Field Test

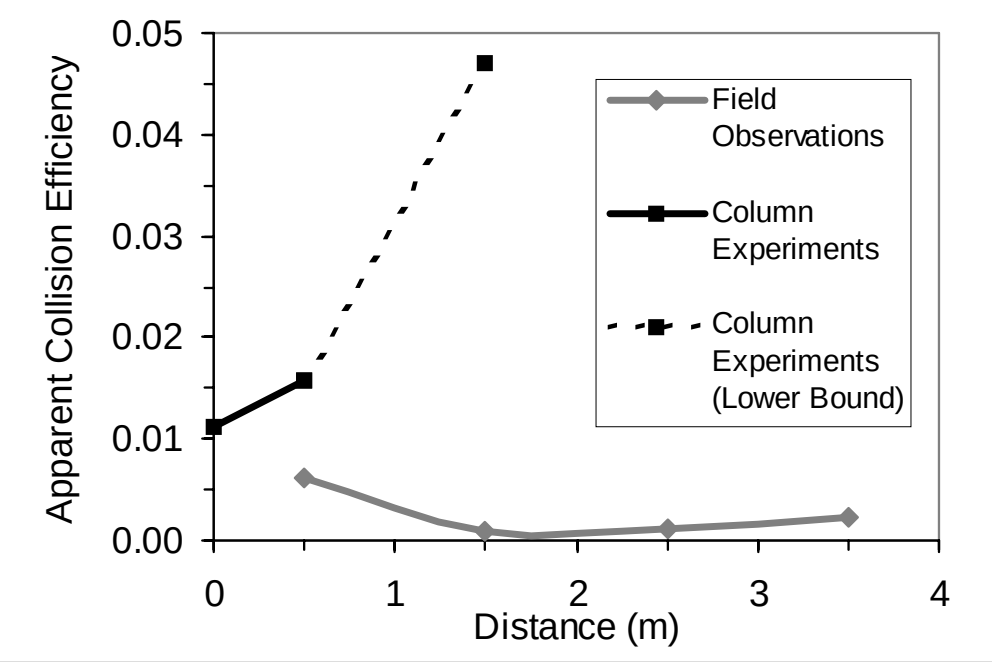
- Apparent field-scale collision efficiency decreases with transport distance…



Dong, H., T. D. Scheibe, W. P. Johnson, C. M. Monkman, and M. E. Fuller, "Change of Collision Efficiency with Distance in Bacterial Transport Experiments," *Ground Water*, 44(3): 415-429, 2006.

A Field Test

- Collision efficiency measured in columns **increases** with transport distance…



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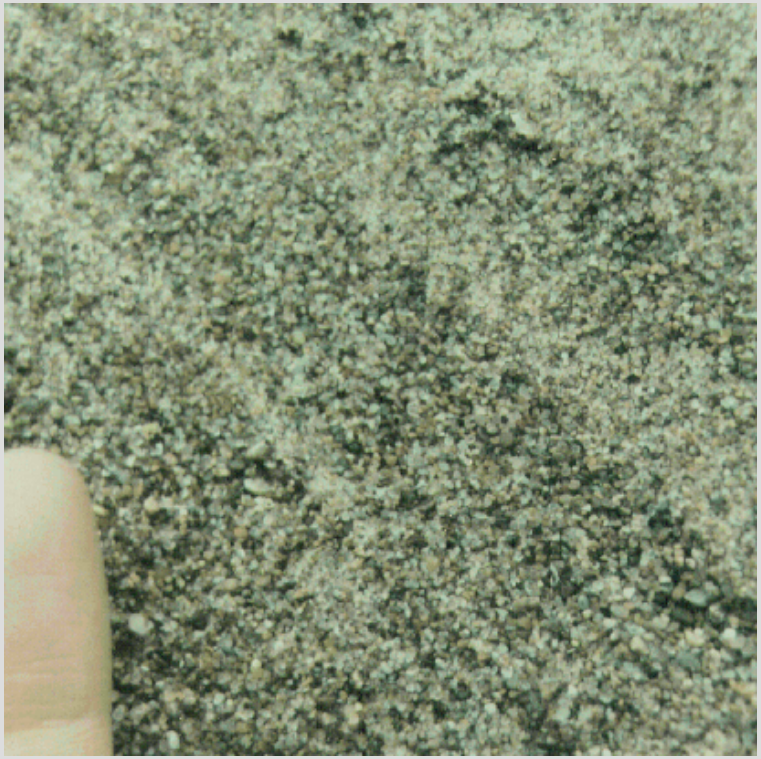
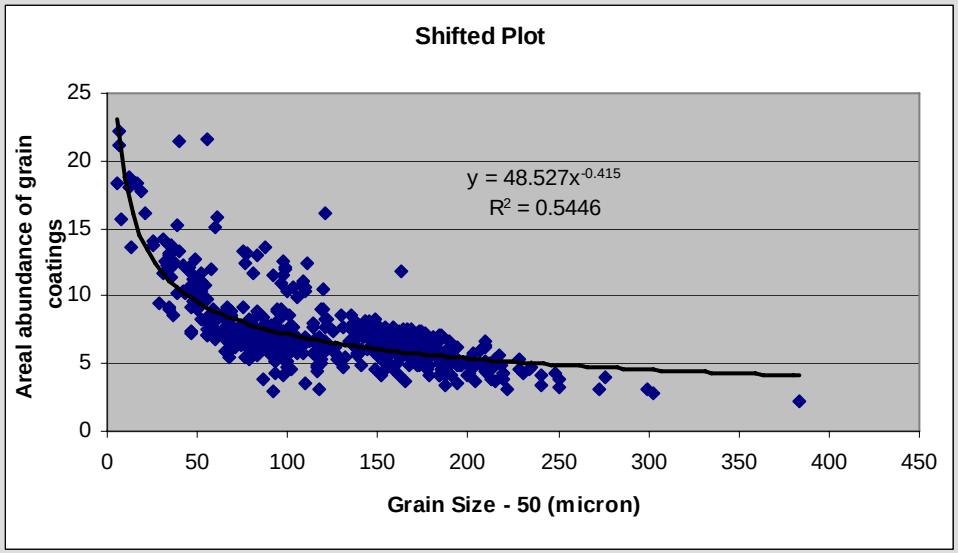
Hypothesis

- Local heterogeneity (correlated physical and chemical) could cause this effect…





A Numerical Experiment

- Use a previously-developed geostatistical model of hydraulic conductivity at the Oyster Site, conditioned to geophysical and borehole flowmeter data.

Scheibe, T. D. and Y.-J. Chien, An evaluation of conditioning data for solute transport prediction, *Ground Water*, 41(2): 128-141, 2003.

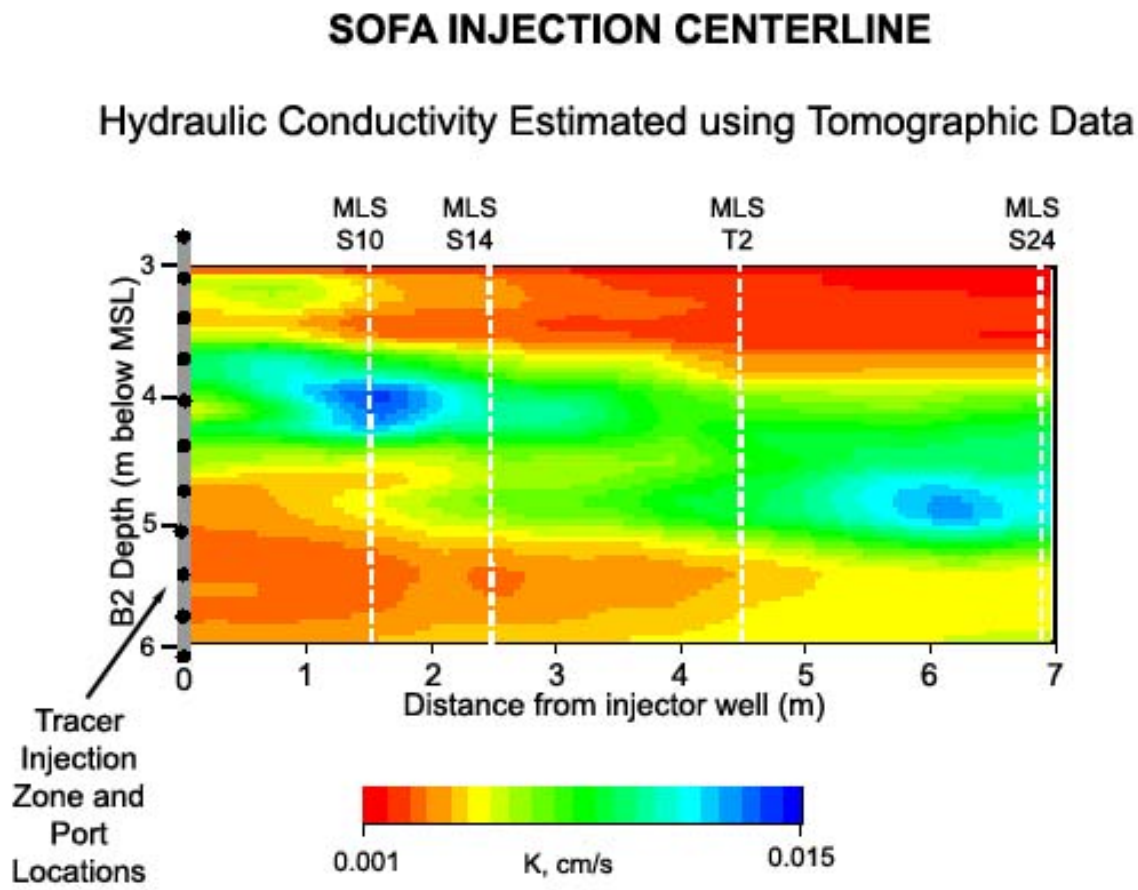
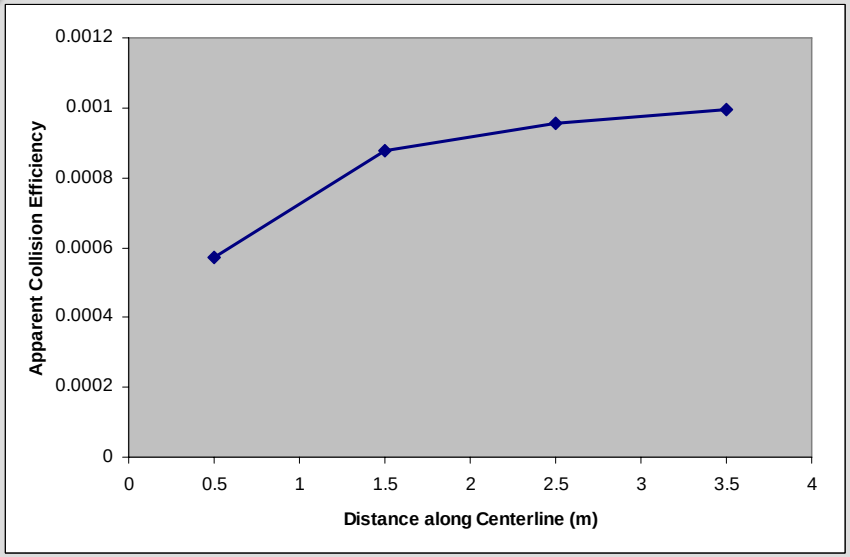
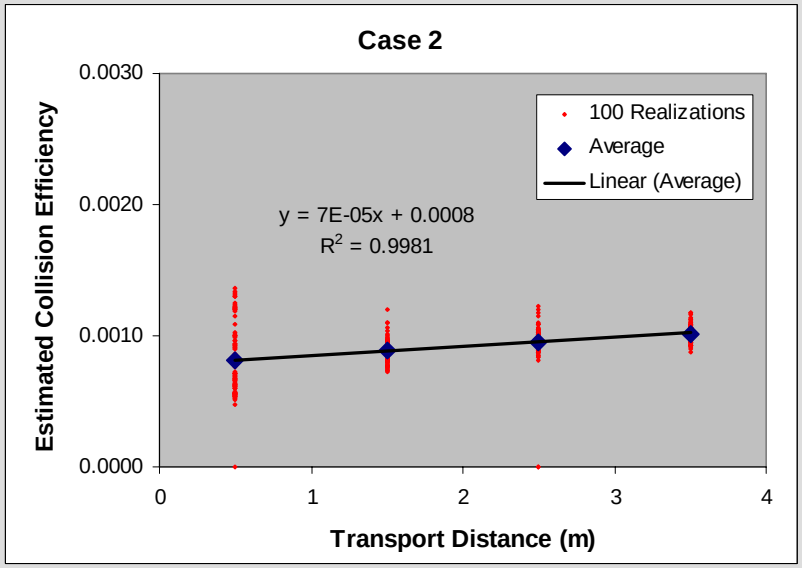


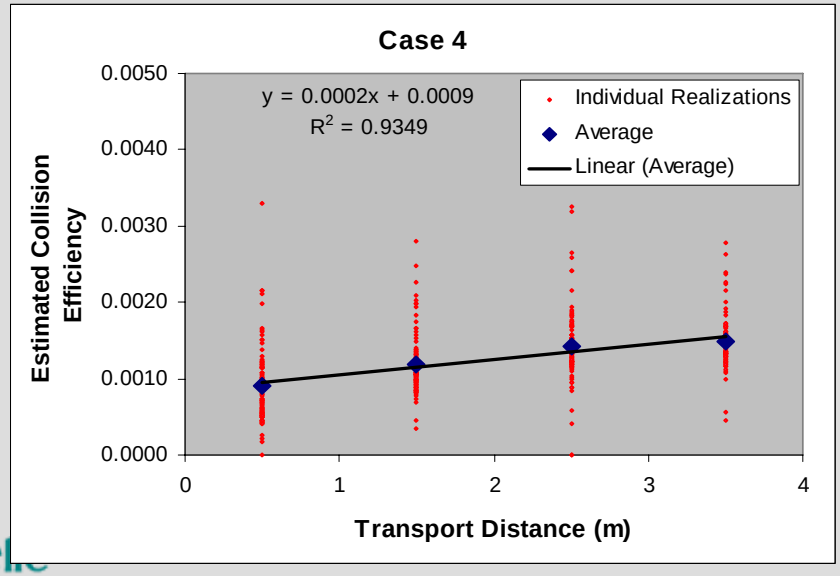
Image courtesy of Susan Hubbard, LBNL

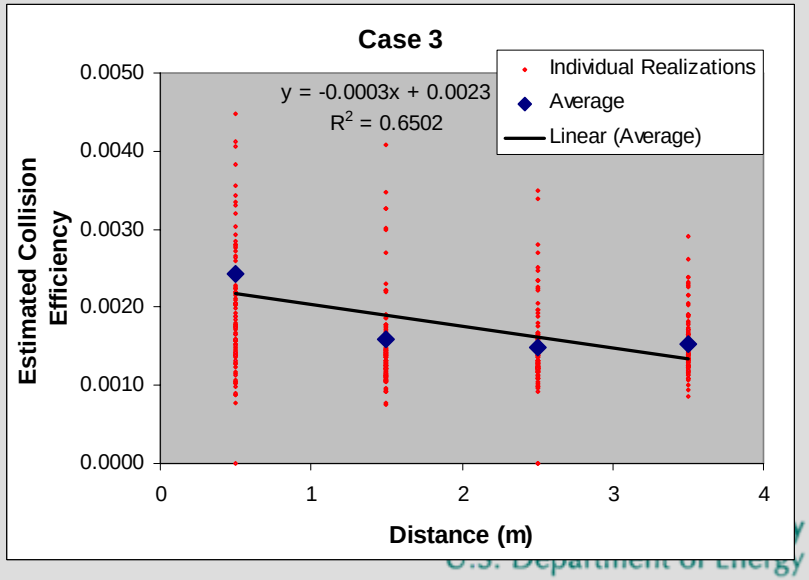
Scheibe, T. D., H. Dong, and Y. Xie, "Correlation Between Bacterial Attachment Rate Coefficients and Hydraulic Conductivity and its Effect on Field-Scale Bacterial Transport," *Advances in Water Resources*, in press.

A Numerical Experiment



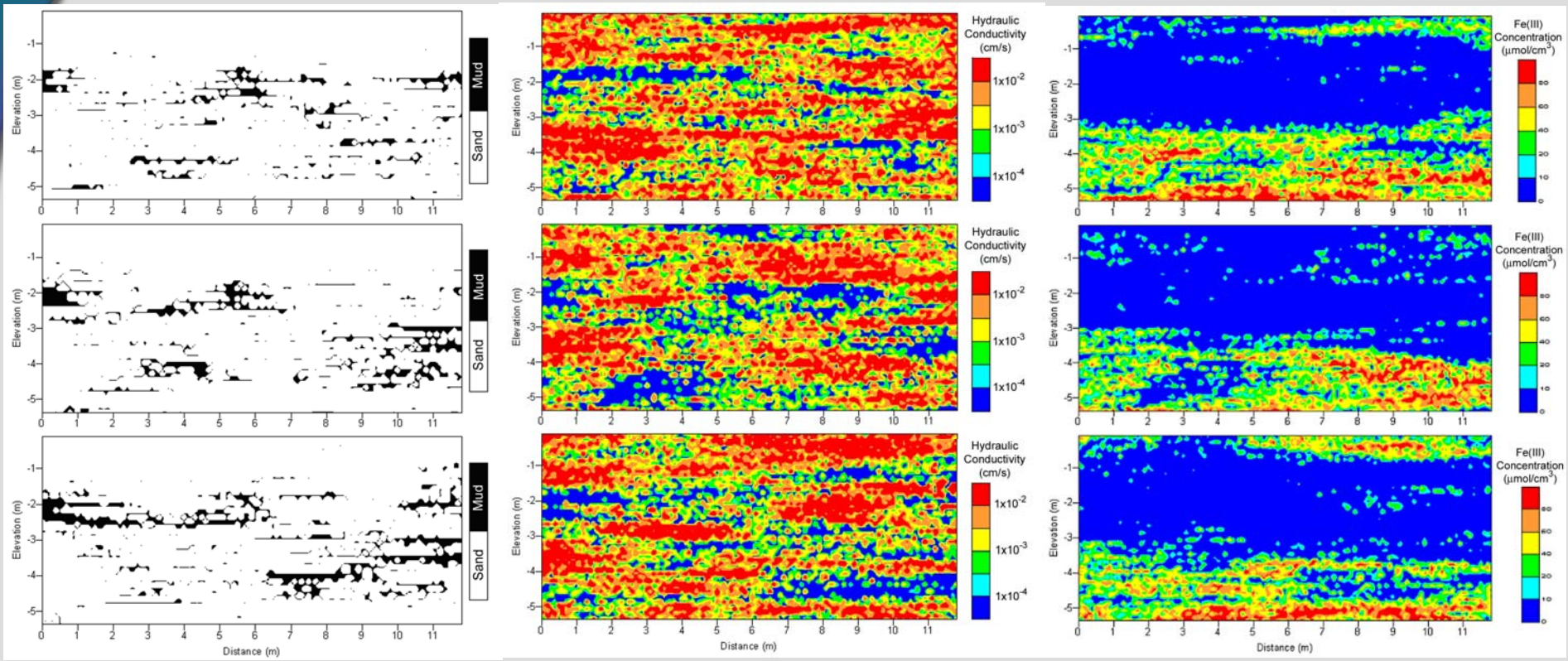






Simulation of (Hypothetical) Uranium Bioremediation

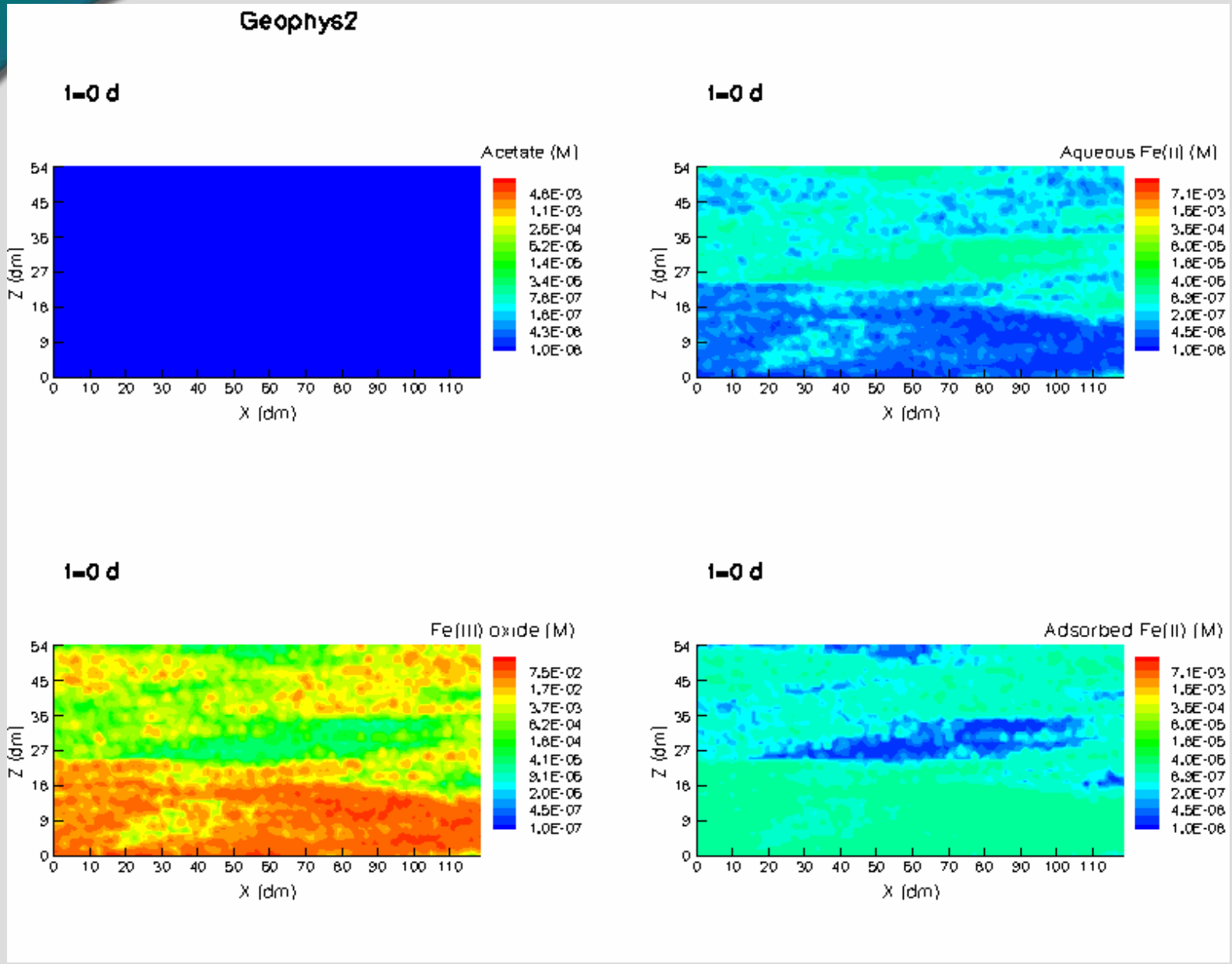
Geophysical Characterization of Physical and Chemical Heterogeneity



Scheibe, T. D., Y. Fang, C. J. Murray, E. E. Roden, J. Chen, Y.-J. Chien, S. C. Brooks, and S. S. Hubbard. “Transport and biogeochemical reaction of metals in a physically and chemically heterogeneous aquifer”, *Geosphere* 2(4): 220-235, 2006.

Acetate

Fe(III) Oxide (solid)



Fe(II) (aqueous)

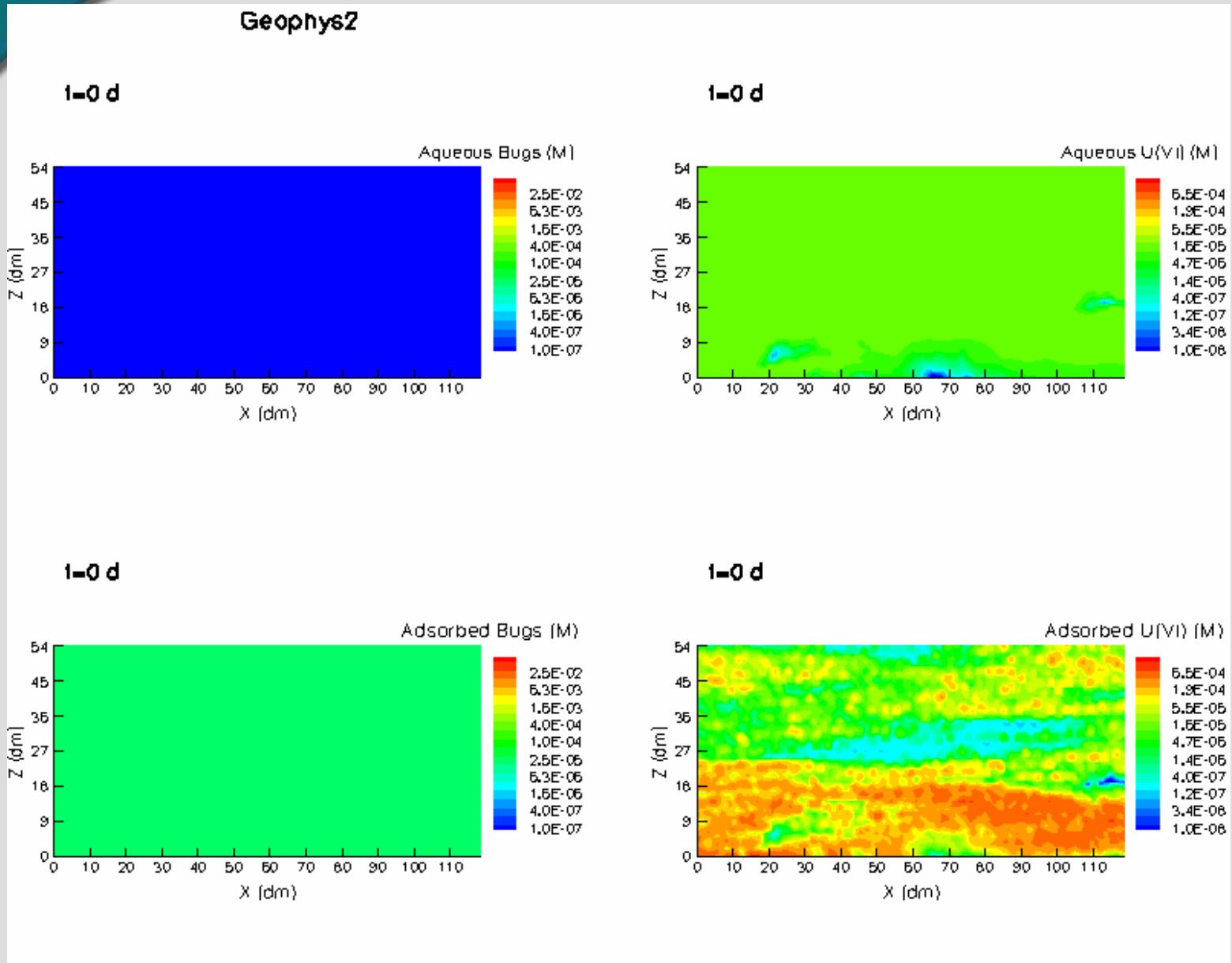
Fe(II) (adsorbed)

Biomass (aqueous)

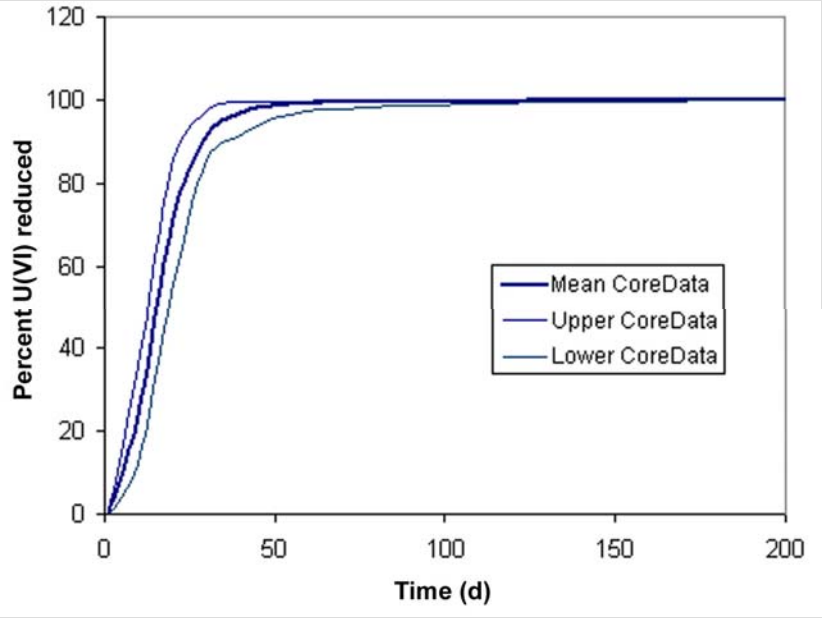
U(VI) (aqueous)

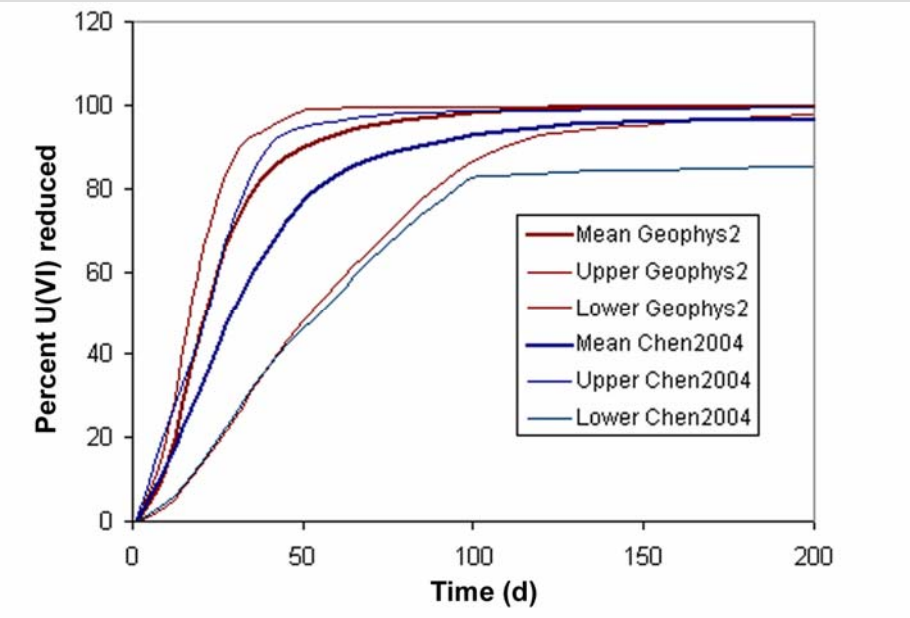
Biomass (adsorbed)

U(VI) (adsorbed)



Effect of Integrating Geophysics

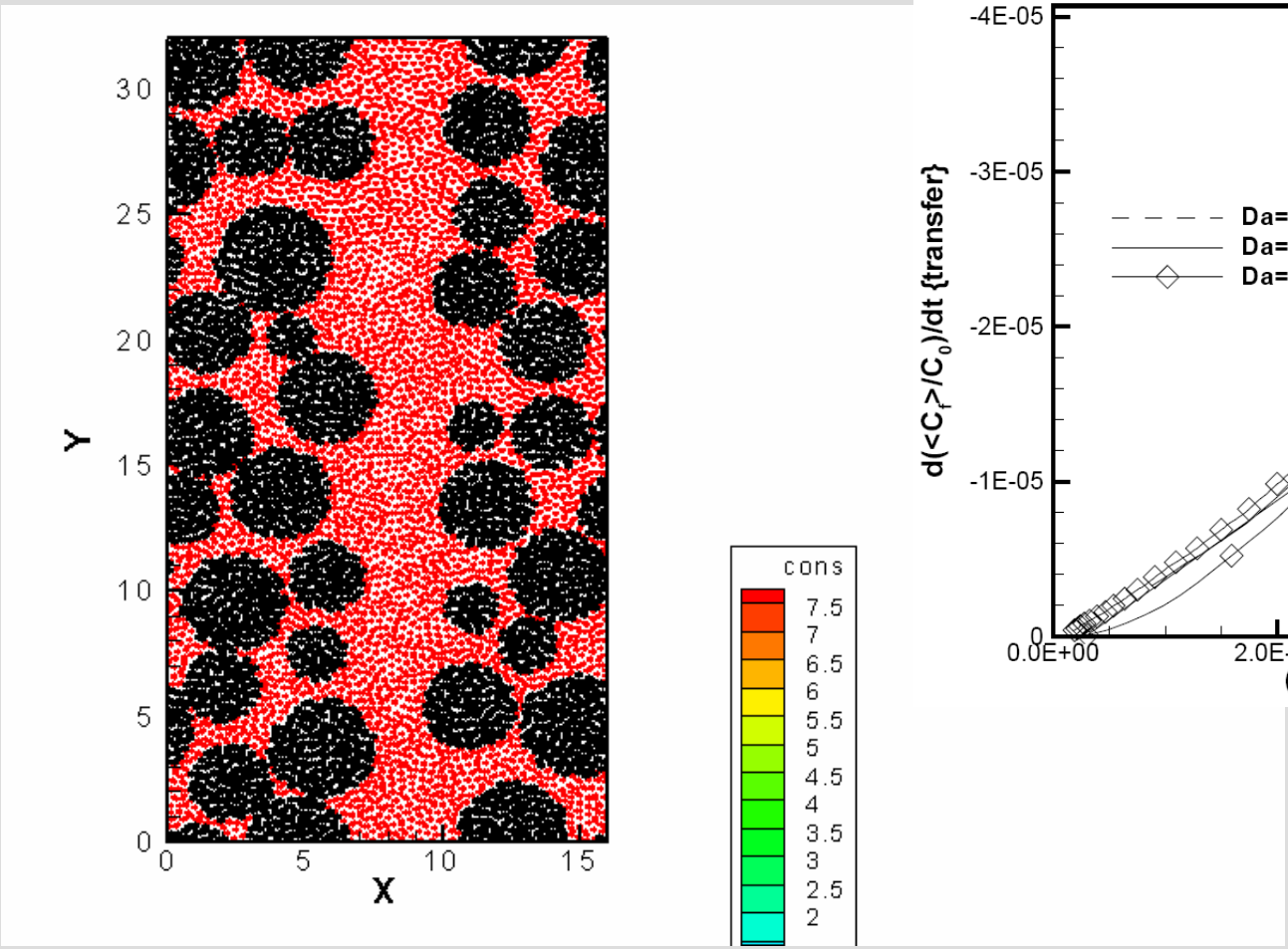


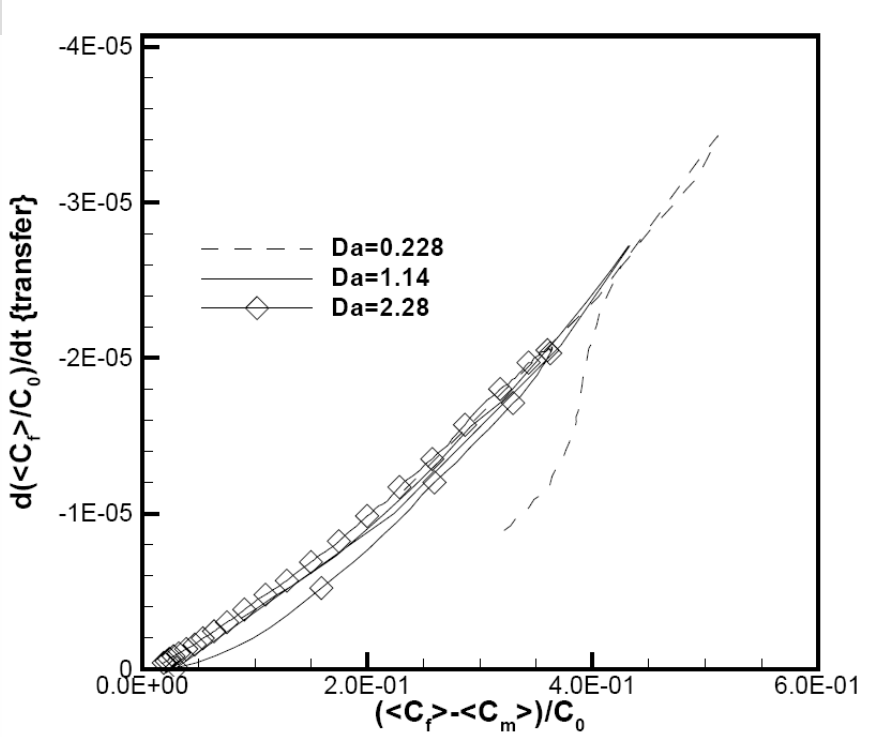


Coupled Processes

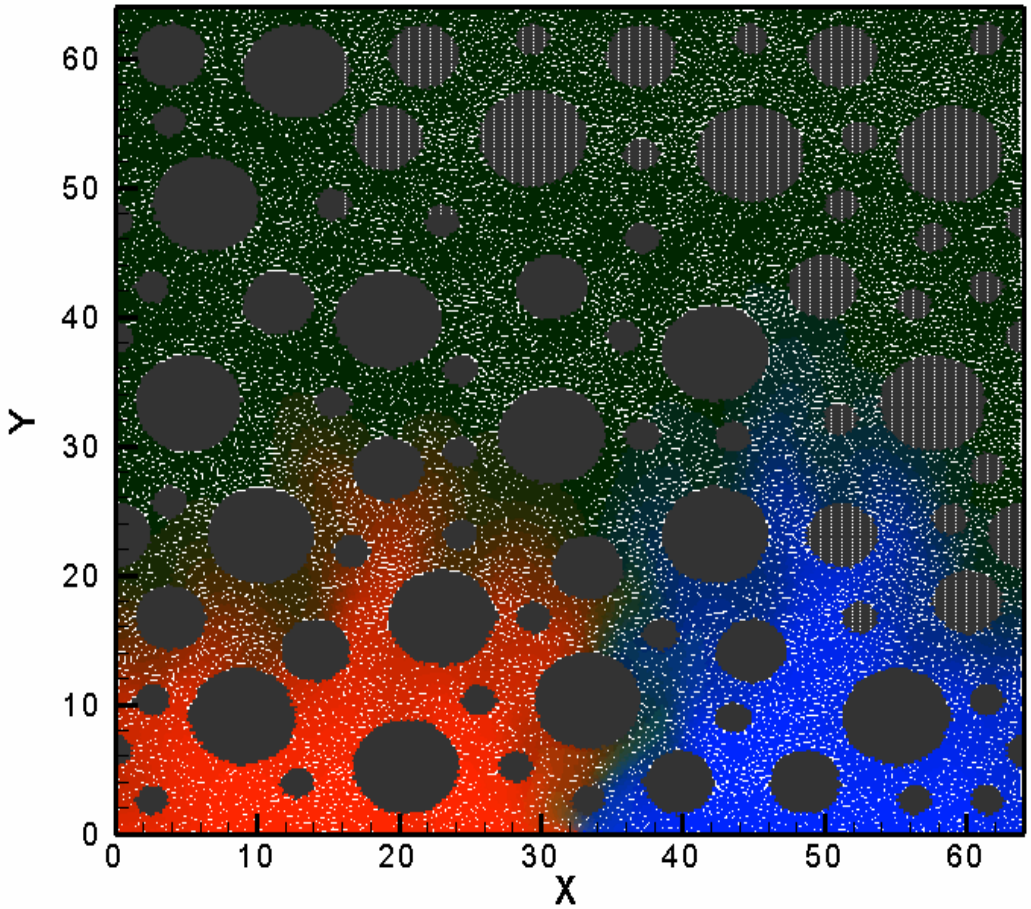
- Can “create” their own heterogeneity
- Feedback among flow, transport, and reaction
- Innovative characterization and modeling methods:
  - Pore-scale characterization and modeling
  - Biological characterization (genetic methods) and *in silico* modeling

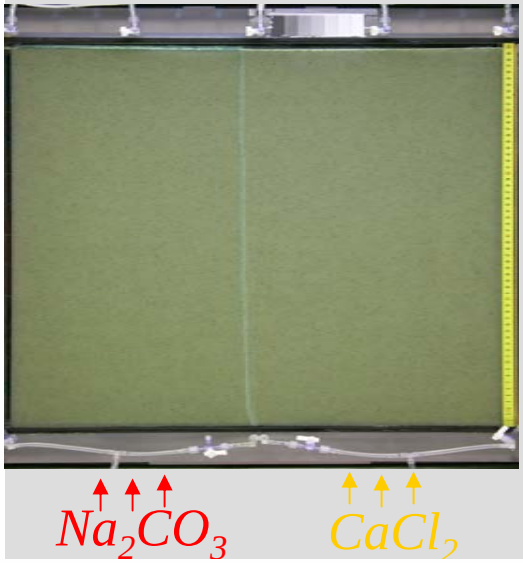
Importance of Mixing Assumptions

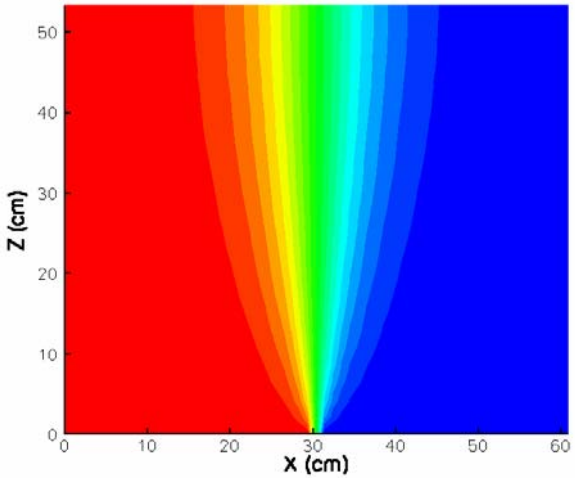




Side-by-side injection of reacting solutions into two halves of a two-dimensional granular porous medium.



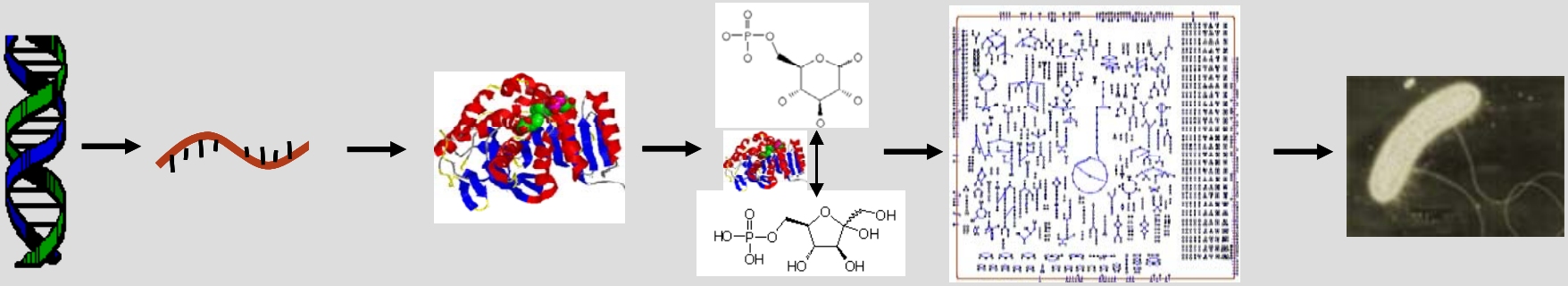




Biological Characterization/Modeling

Slide material from R. Mahadevan (Univ. of Toronto)

Increasing Complexity



DNA RNA Protein/Enzyme Reaction Reaction Network Cell

$$R_{Fe(III)} = V\max_{Surf} \frac{[Cells]}{Km_{Cells} + [Cells]} [Fe(III)Surf_{Free}] f(\Delta G_{rxn})$$

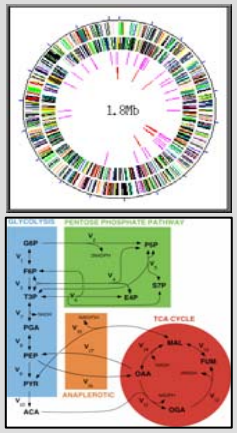
Monod-Type Kinetics

In reality, many different reaction pathways exist within the cellular mechanisms; which are optimal under specific environmental conditions?

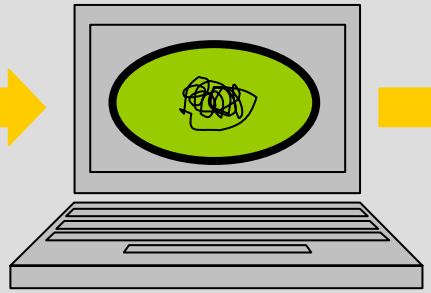
Constraint-Based *In Silico* Modeling

- Genetic characterization of reaction pathways
- Laboratory characterization of flux constraints
- Optimization under specific conditions

Slide material from R. Mahadevan (Univ. of Toronto)



Biological Information



In silico Cellular Models

- Understand Metabolism
- Predict Growth Physiology
- Analyze high-throughput data

Summary

- For problems with strong multiscale heterogeneity and/or coupled reaction/flow/transport processes, innovative characterization methods linked to advanced numerical models are needed.
  - **Field-scale:** Geophysical characterization; stochastic simulation (account for cross-correlation between physical and chemical processes)
  - **Pore-scale:** 3D geometric methods combined with discrete or continuum models to simulate coupled processes
  - **Cell-scale:** Innovative biological characterization and modeling are exciting areas for future advancement
  - **Hybrid Multiscale Simulation:** Develop models with multiscale representations of physics/chemistry/biology (adaptive)

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  - Office of Science, Biological and Environmental Research, Environmental Remediation Sciences Program (ERSP)