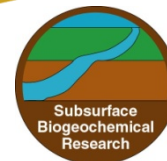


Simulation of October 2009 U(VI) Desorption Experiment

Glenn Hammond, Xingyuan Chen

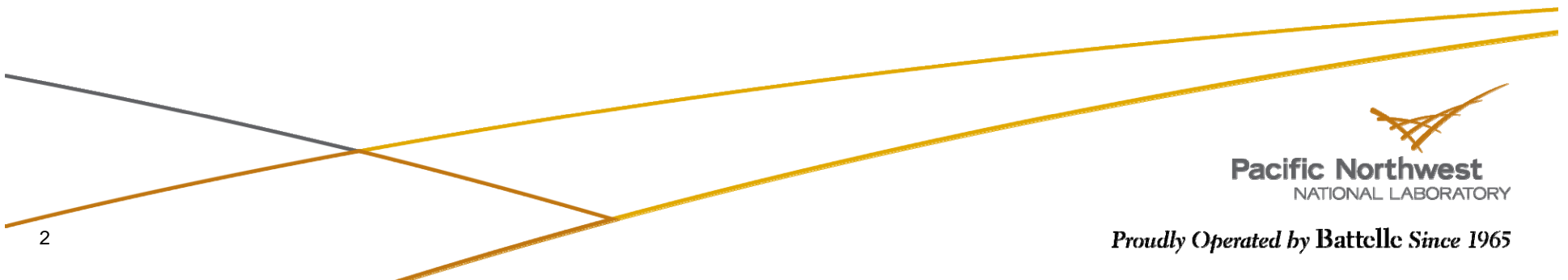
IFRC Project Meeting January 19-20, 2011



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Key Points

- ▶ Simulation results are most sensitive to boundary conditions (both flow and transport).
- ▶ Multirate kinetic surface complexation is more accurate than equilibrium at the IFRC site and time scale.
 - Equilibrium almost always undershoots observed U(VI) concentrations
- ▶ “Damage” to observed solute concentration data set due to wellbore flow may not be as terrible as originally thought.



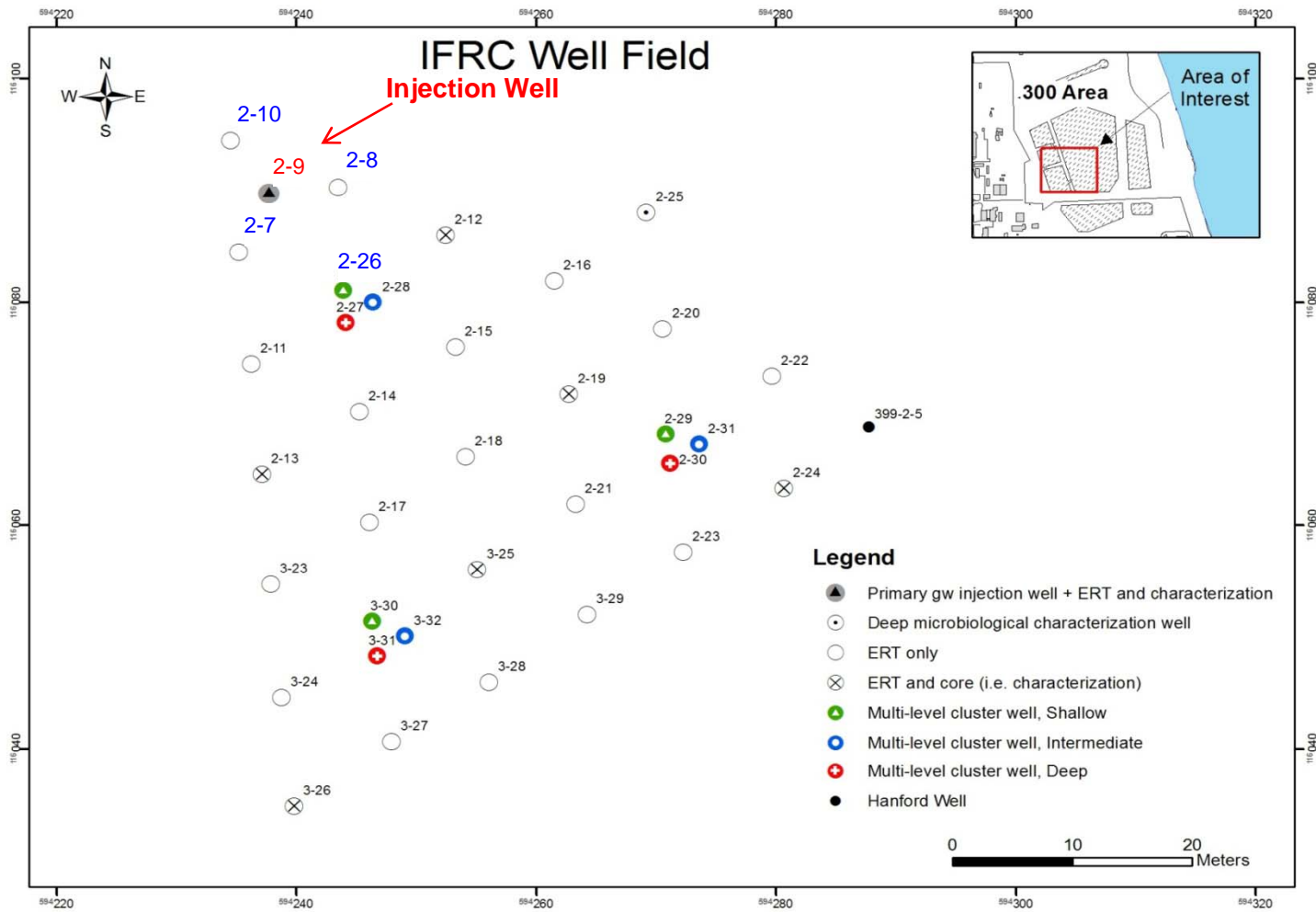
October 2009 Injection Scenario

▶ Simulation

- 120×120×15 meter domain (1×1×0.5 meter grid spacing)
- 15 primary, 88 secondary aqueous species
- 2 surface complexes (SOUO_2OH , $\text{SOHUO}_2\text{CO}_3$)
- Injection rate: 180 gpm (681.3 m³/min)
- IFRC U(VI) concentration: 35 ug/L
- Inject U(VI) concentration: 5 g/L
- Injection duration: 6.5 hrs
- Duration: 1000 hrs
 - Injection started at 255.5 hrs (3:30PM October 22, 2009)

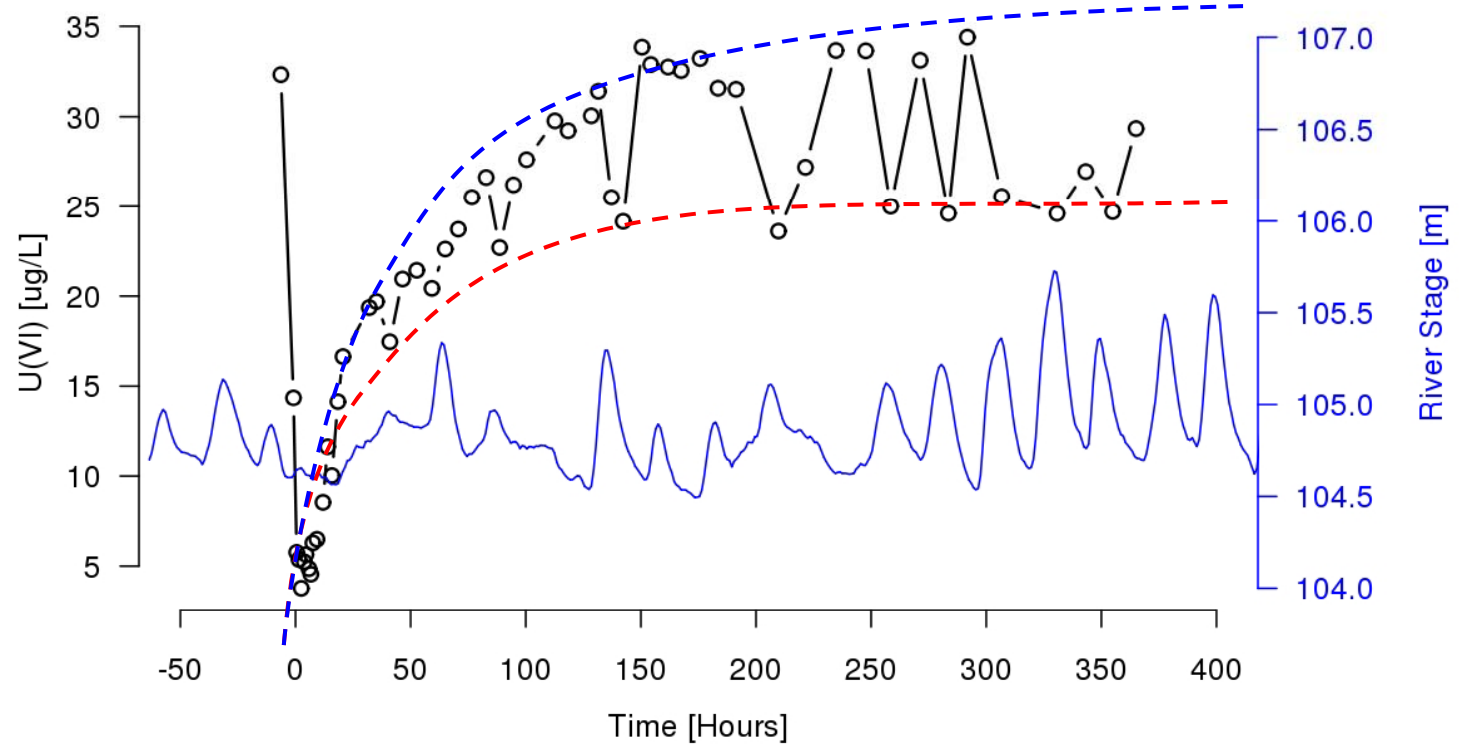
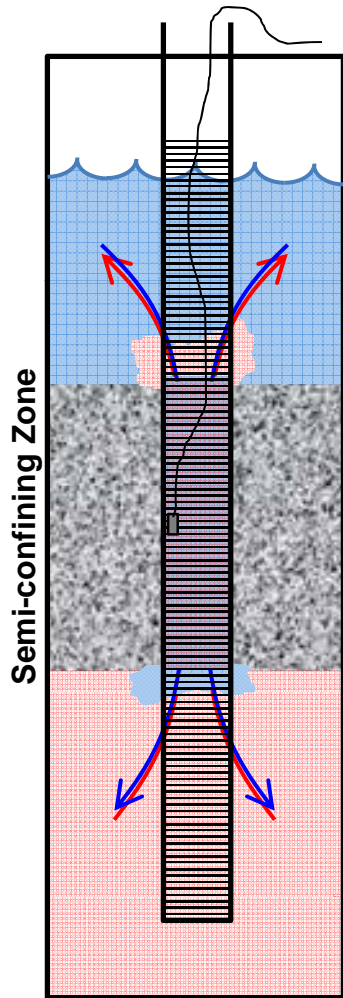
▶ Stochastic Simulations

- 500 realizations of permeability per scenario
- 2 hours to run on 64,000 processor cores

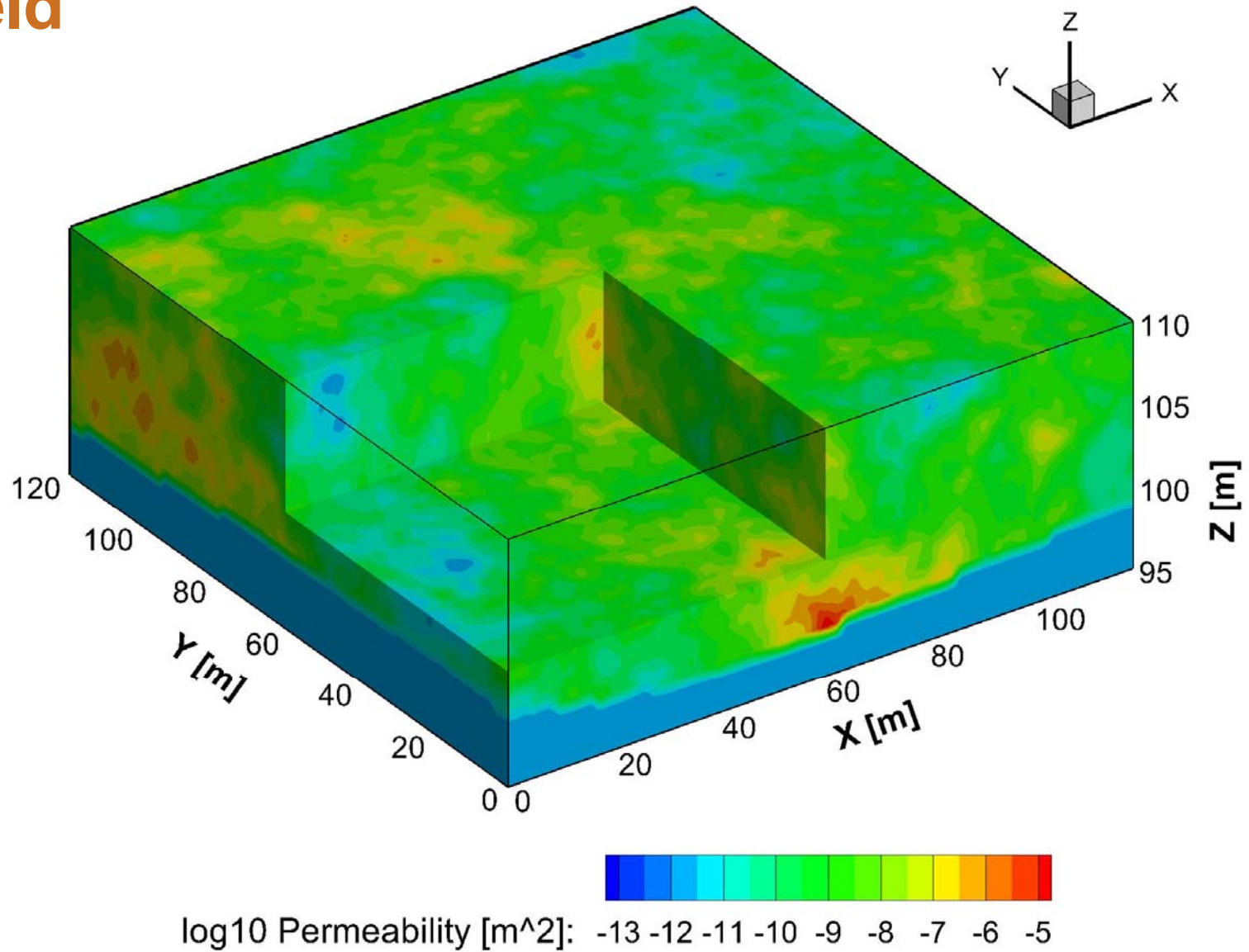


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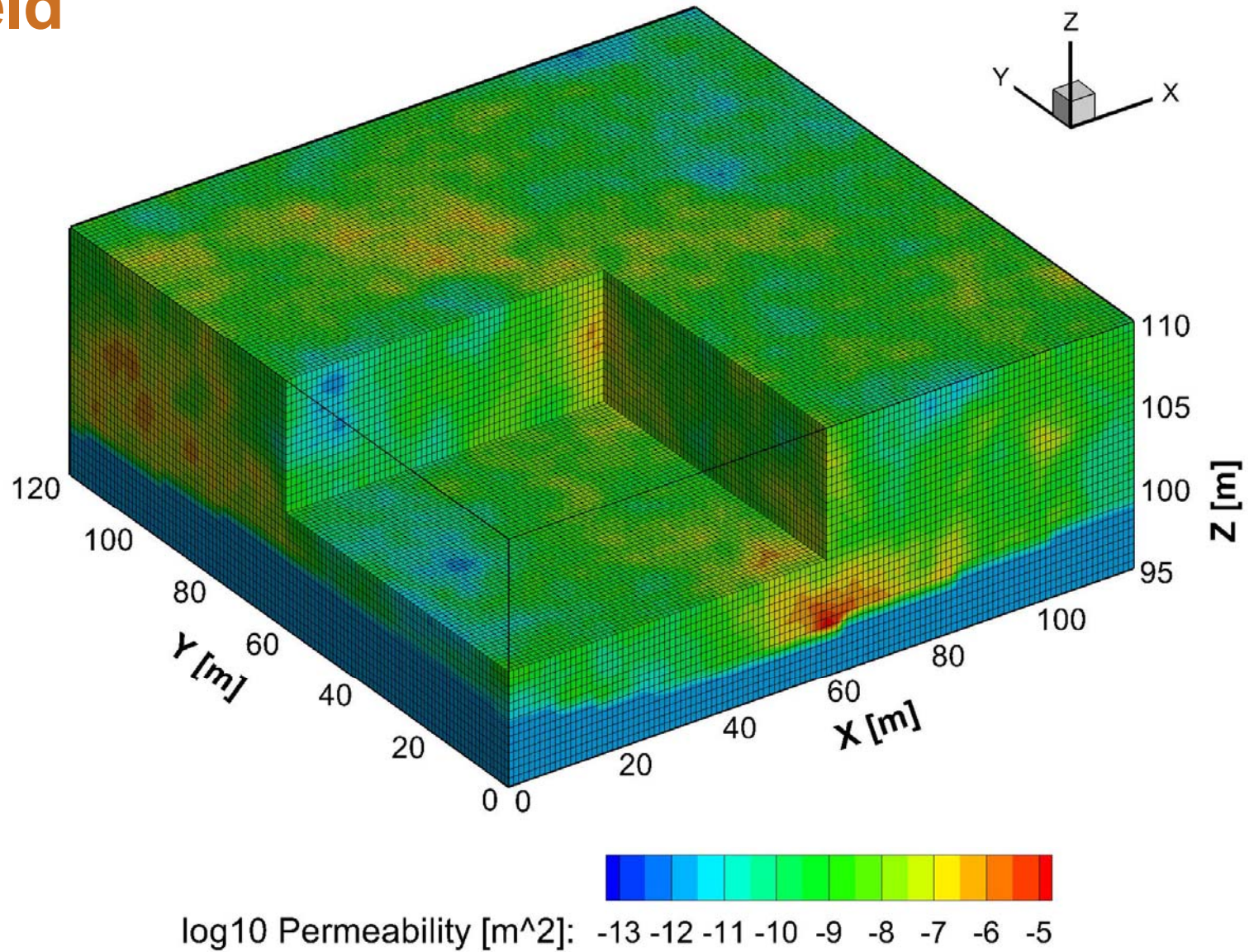
U(VI) Concentration Sampled at Well 2-9 vs. River Stage



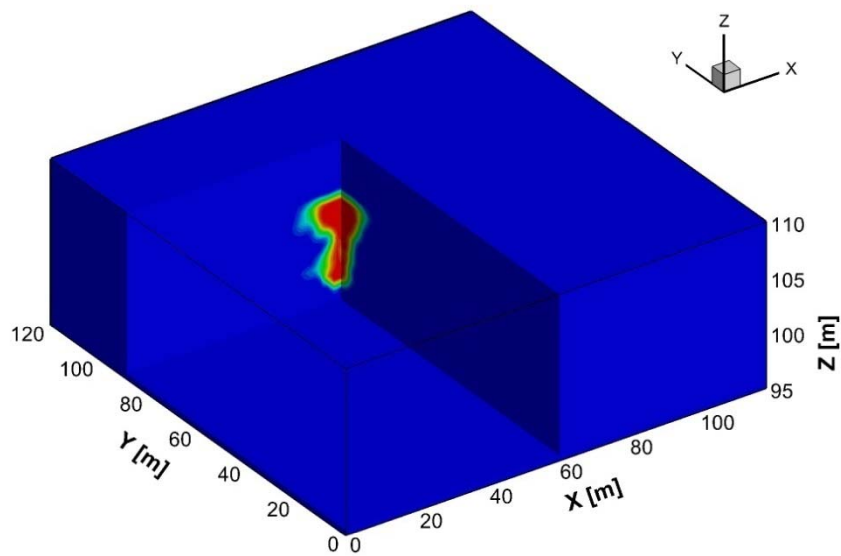
Representative Heterogeneous Permeability Field



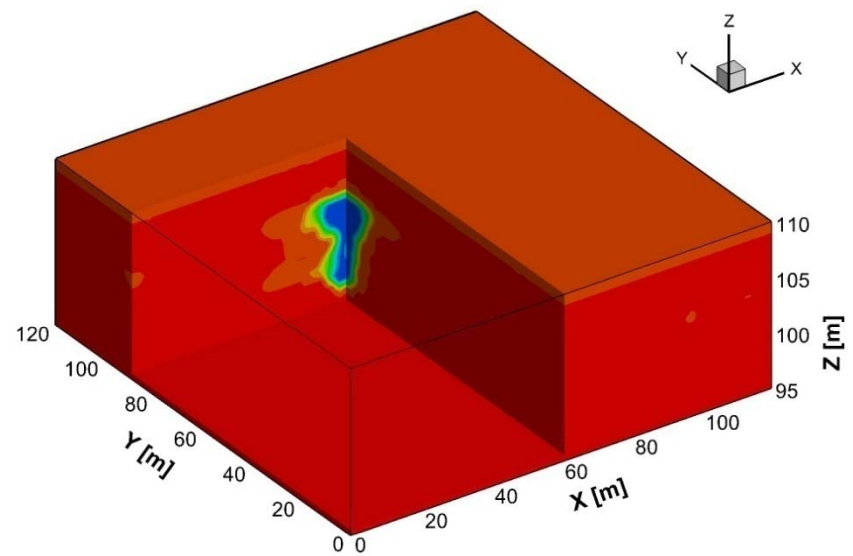
Representative Heterogeneous Permeability Field



Tracer and U(VI) Concentration at End of Injection

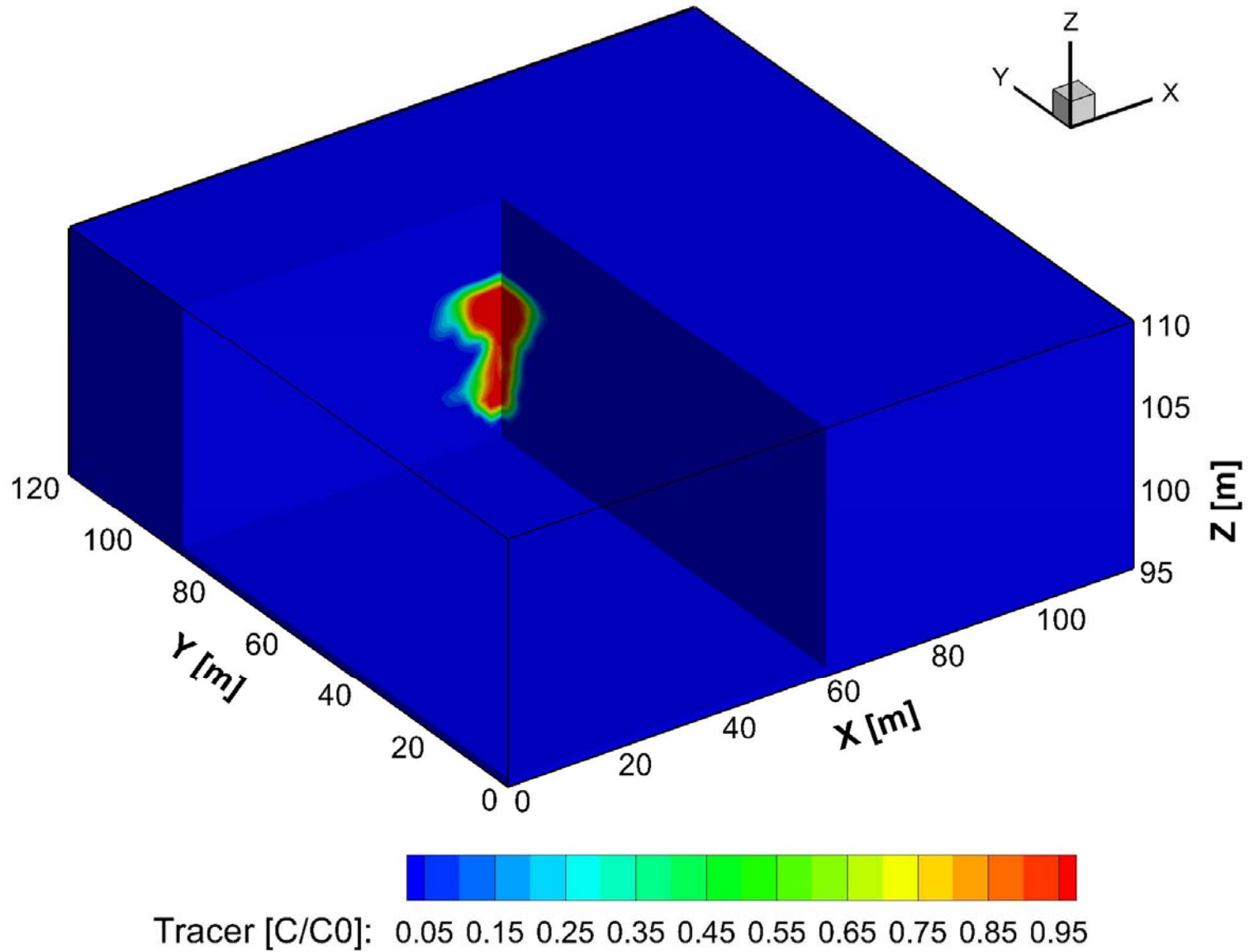


Tracer [C/C0]: 0.05 0.15 0.25 0.35 0.45 0.55 0.65 0.75 0.85 0.95

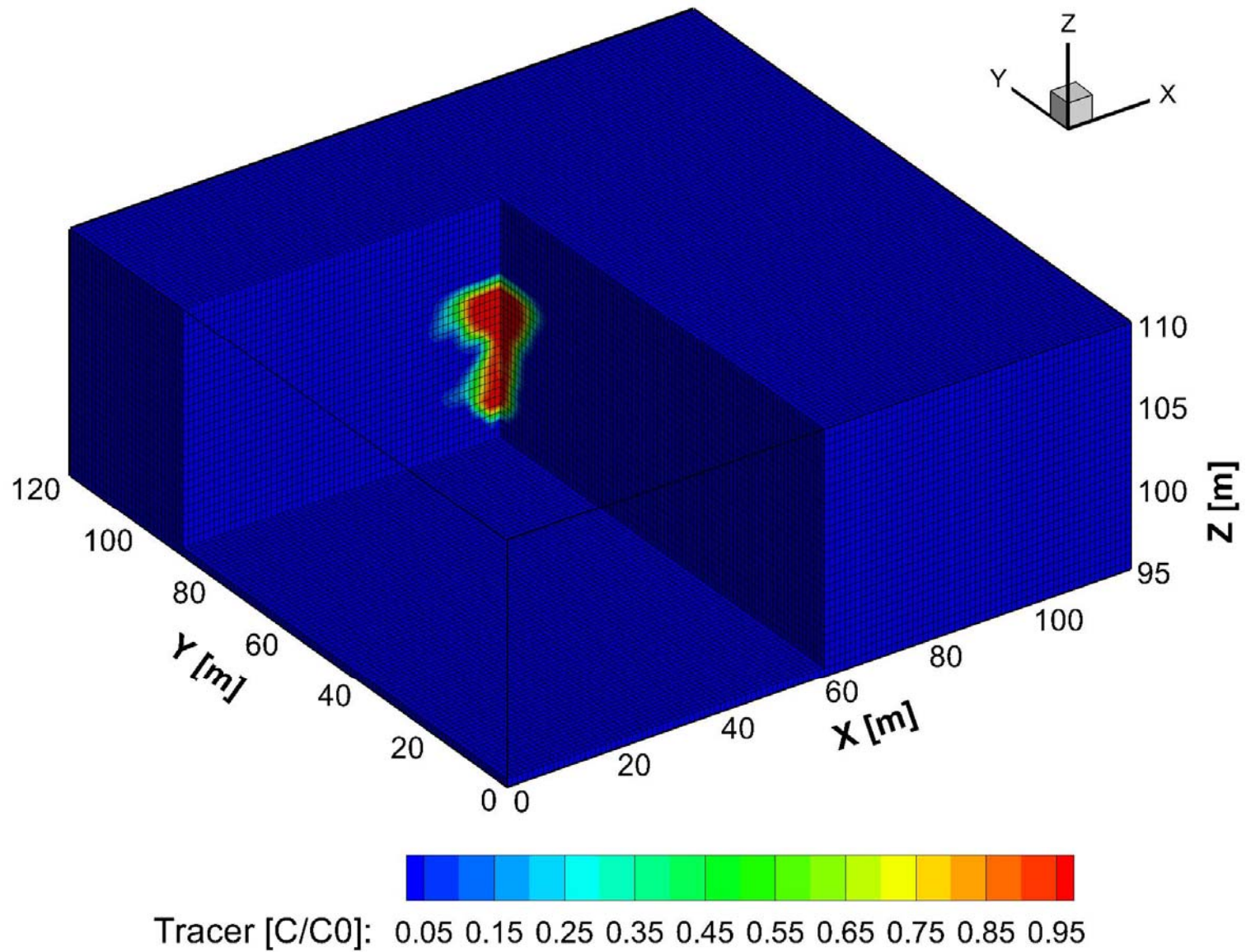


U(VI) [$\mu\text{g/L}$]: 5 7.5 10 12.5 15 17.5 20 22.5 25 27.5 30 32.5 35

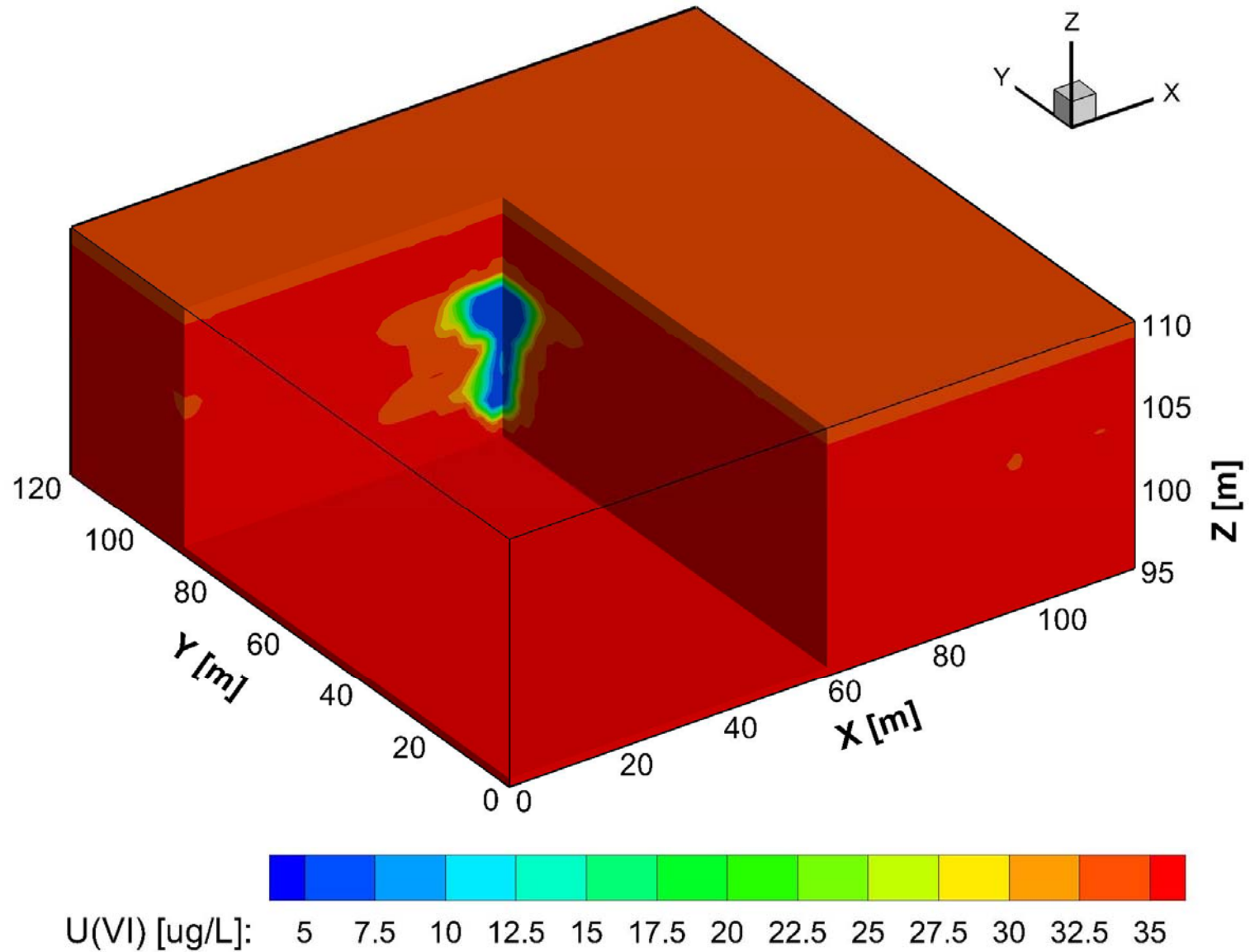
Tracer Concentration at End of Injection



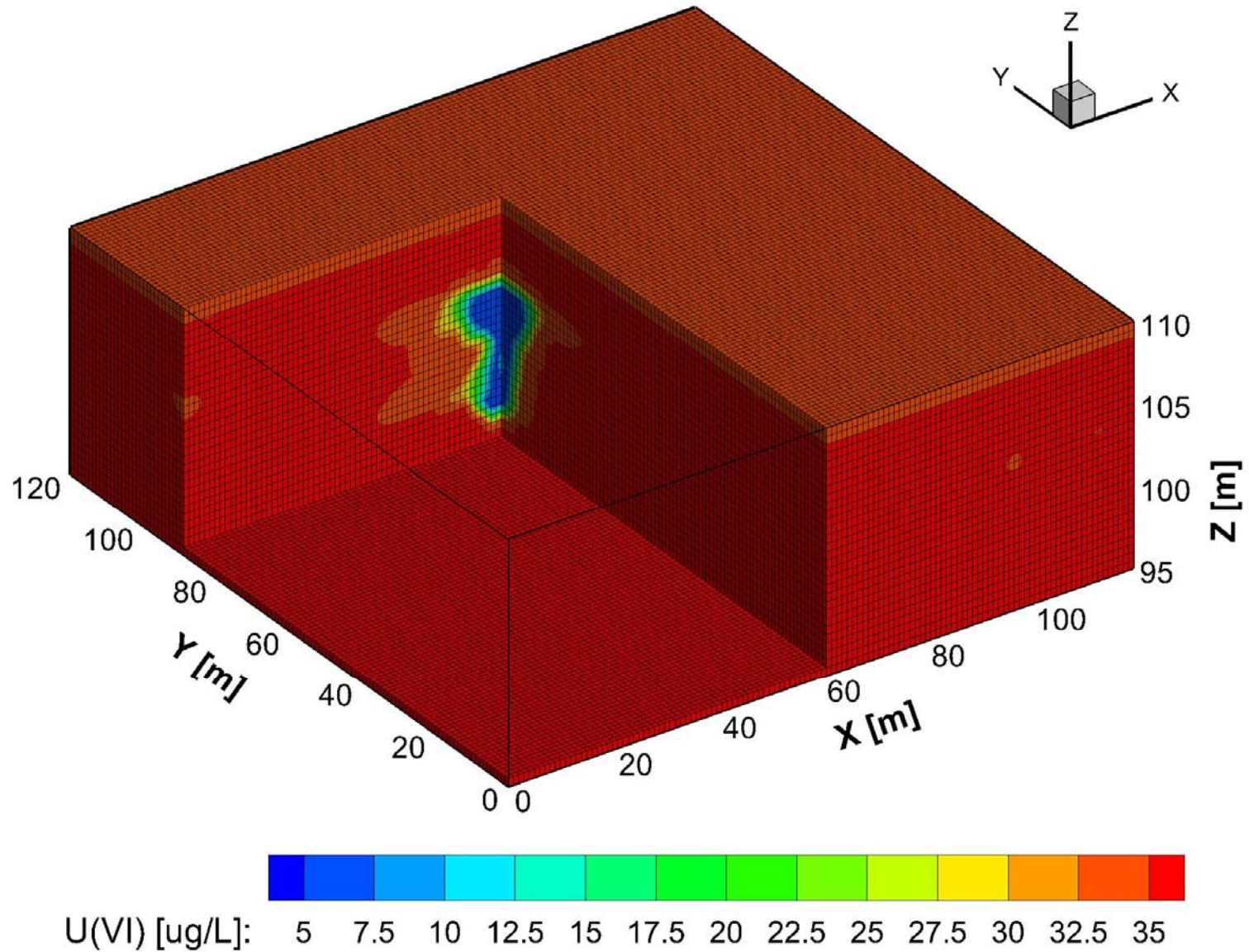
Tracer Concentration at End of Injection



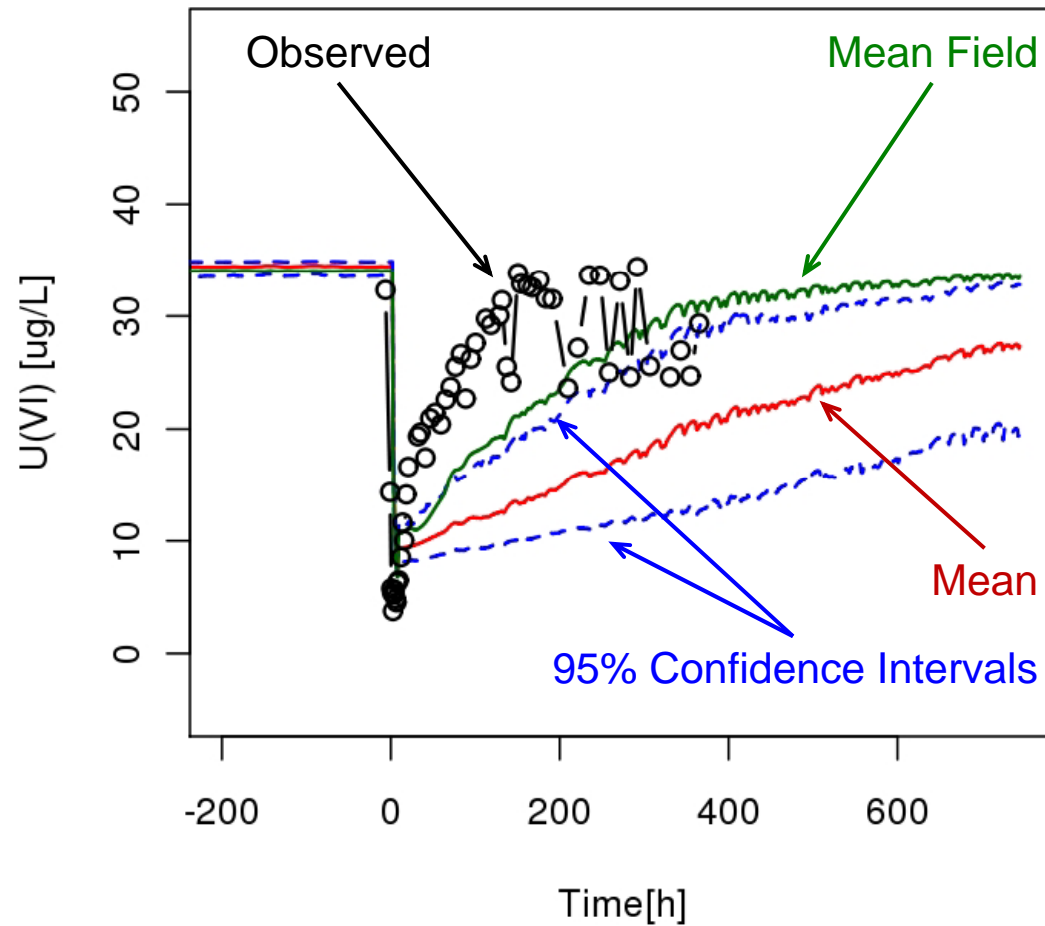
U(VI) Concentration at End of Injection



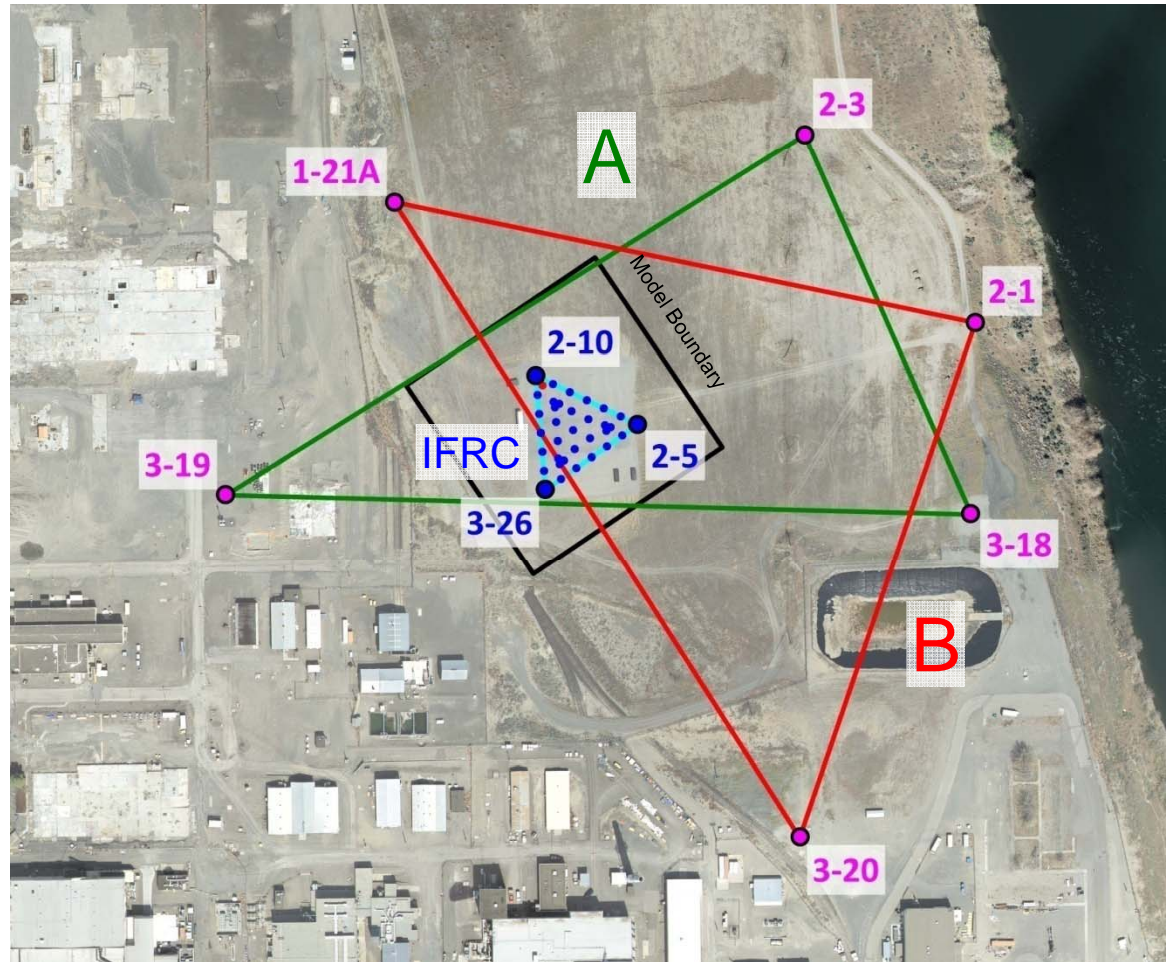
U(VI) Concentration at End of Injection



Explanation of U(VI) Desorption Simulation Results



Wells Employed in Boundary Conditions



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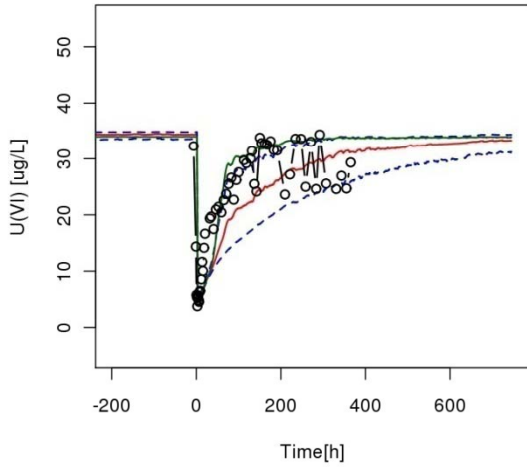
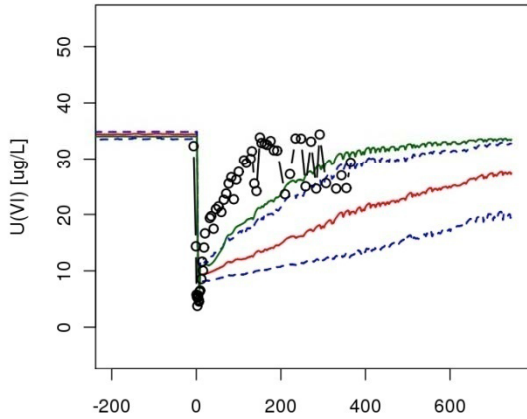
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Flux Averaged U(VI) Conc. at Well 2-9 vs. Boundary Condition vs. Surface Complexation

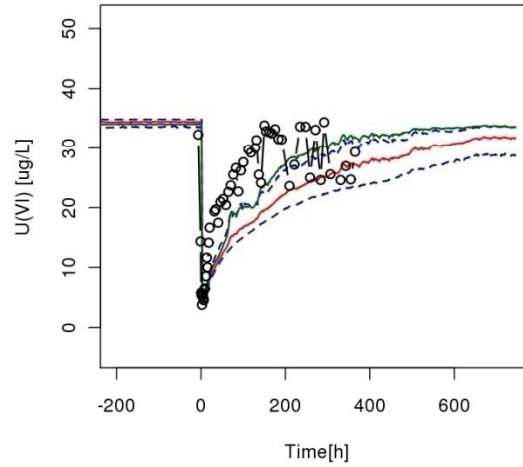
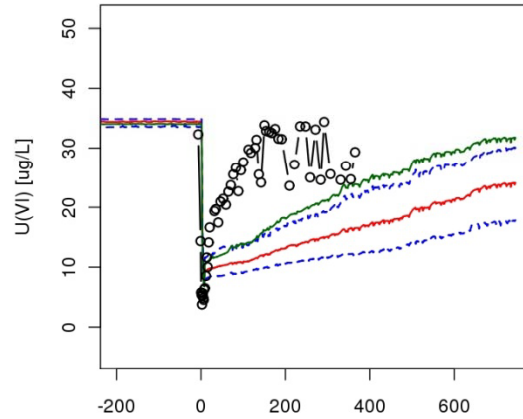
Equilibrium

Multirate Kinetic

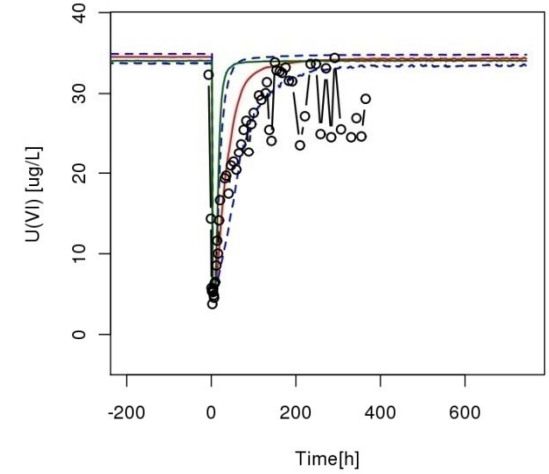
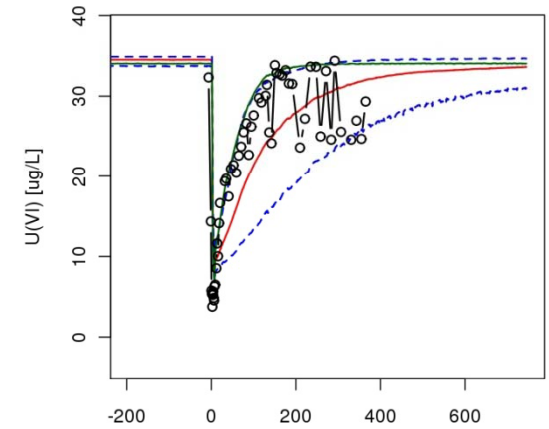
A



B

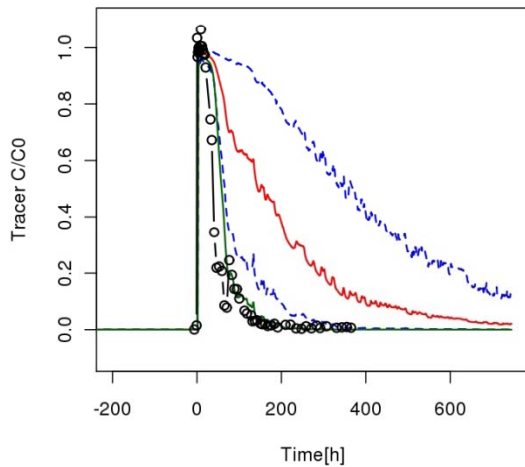


IFRC

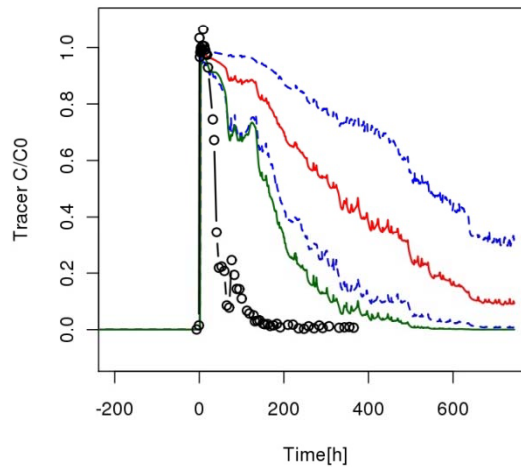


Flux Averaged Tracer Conc. at Well 2-9 vs. Boundary Condition

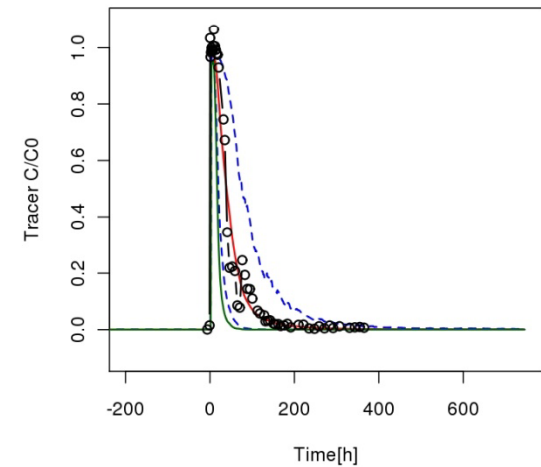
A



B

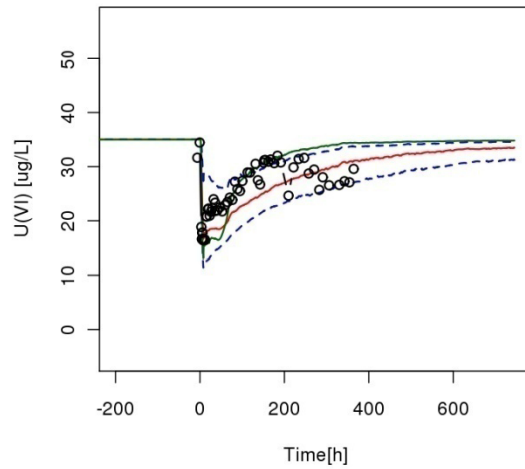


IFRC

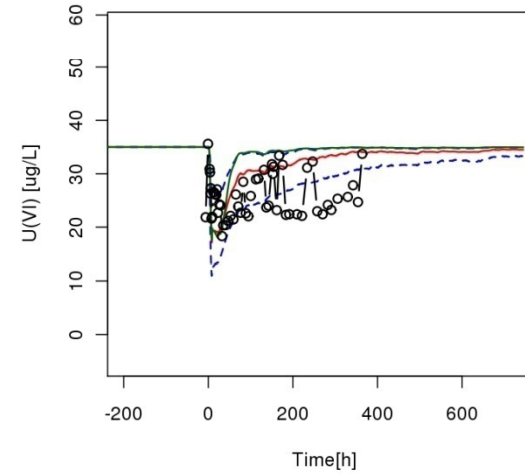


Flux Averaged U(VI) Concentration at Wells (Boundary Condition A, Multirate Kinetic)

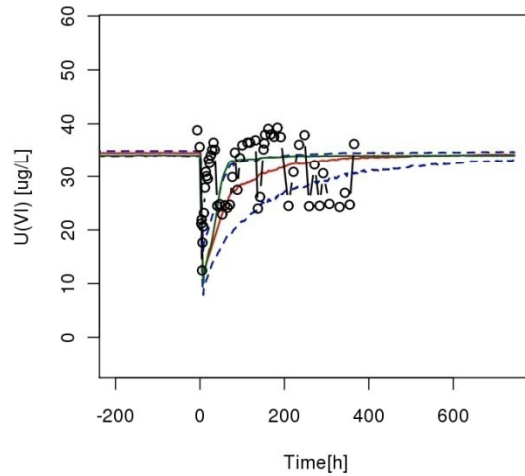
2-7



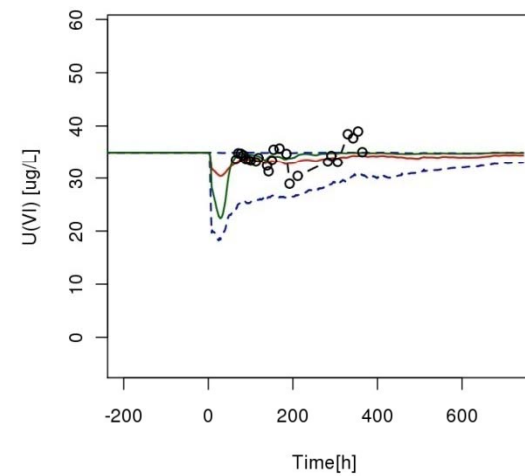
2-8



2-10

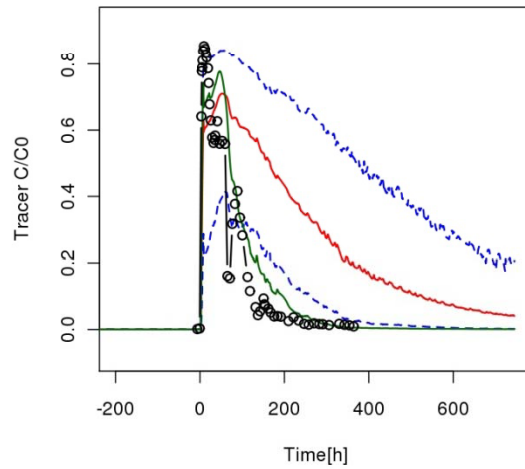


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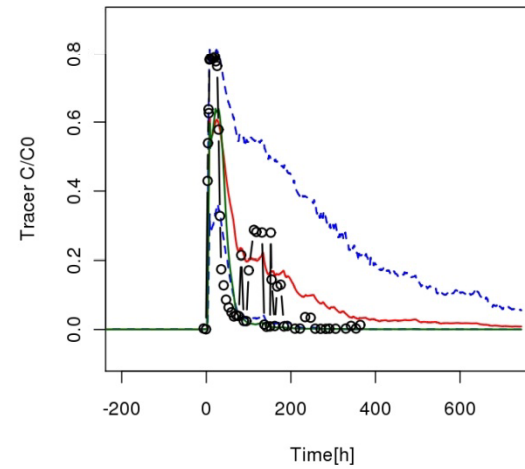


Flux Averaged Tracer Concentration at Wells (Boundary Condition A)

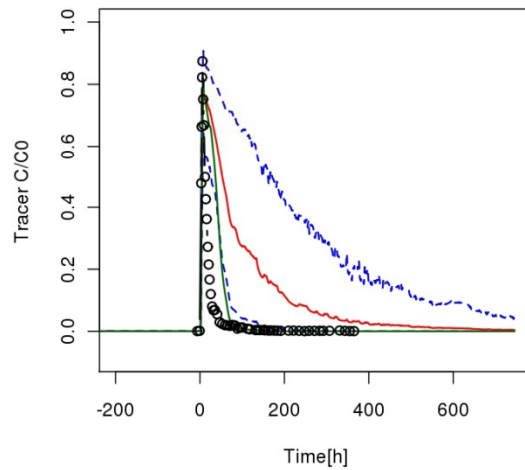
2-7



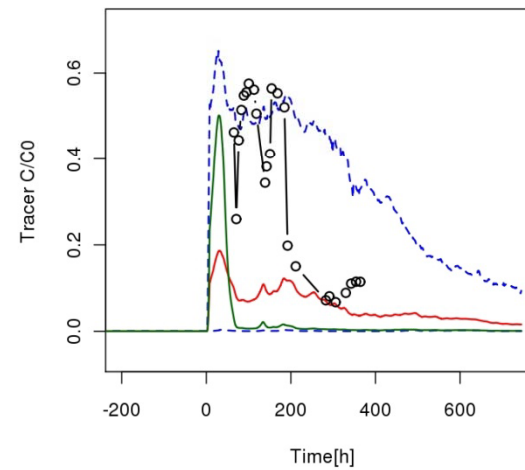
2-8



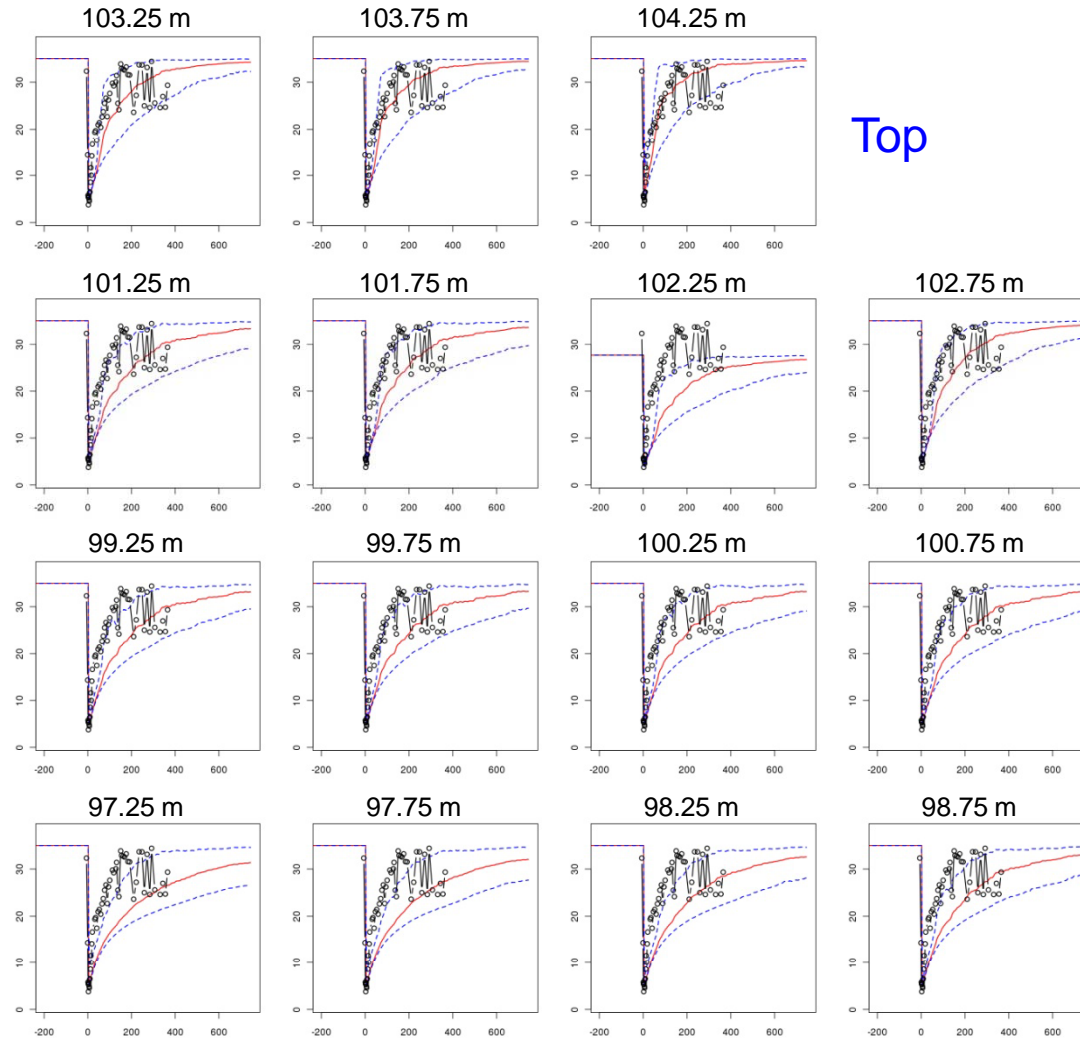
2-10



2-26



Depth Discrete U(VI) Concentration at Well 2-9 (Boundary Condition A, Multirate Kinetic)



Top

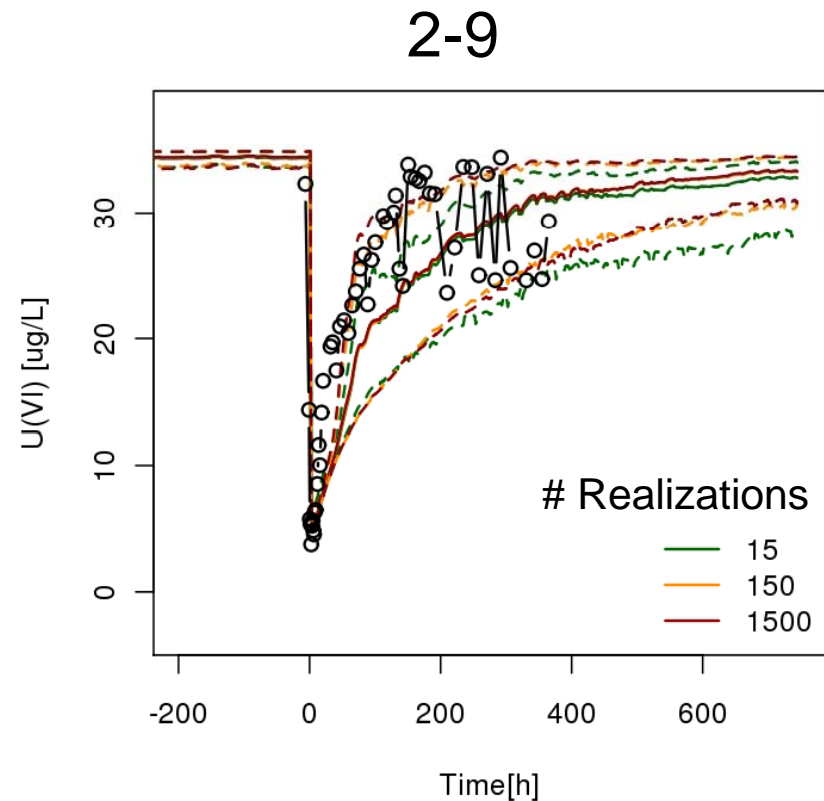
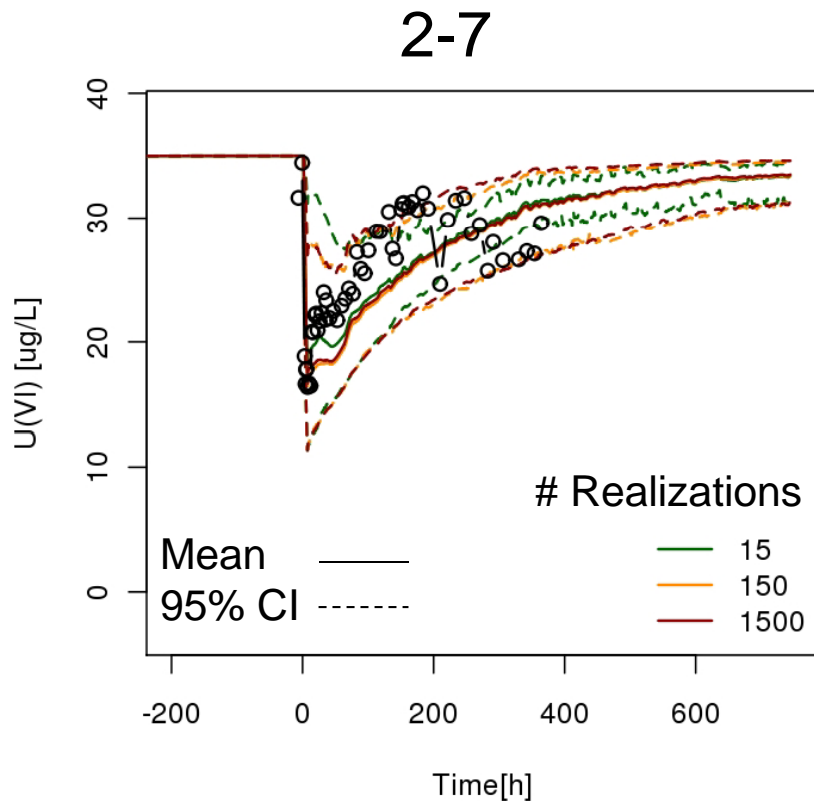
Bottom



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Convergence of Mean and 95% Confidence Interval as a Function of # of Realizations (Boundary Condition A, Multirate Kinetic)



Future Directions

- ▶ Integrate updated field characterization results to generate random fields
- ▶ Calibrate multirate model parameters
- ▶ Quantify non-labile U(VI) source term(s)