PNNL-SA-77568


Hanford 300 A IFRC Site

Hydrologic and Tracer Experiment Simulations

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Modeling Approaches

- A multi-tiered approach to cope with field experiments of increasing complexity and an increasing number of coupled processes
  - Conservative solute and heat tracer modeling analyses to identify physical heterogeneity and transport processes
  - 2-D cross sectional modeling of multi-rate mass transfer processes under idealized scenarios to gain new insights and conceptual understanding
  - 3-D field-scale modeling of uranyl tracer experiments to quantify processes and parameters that control the fate and mobility of uranium

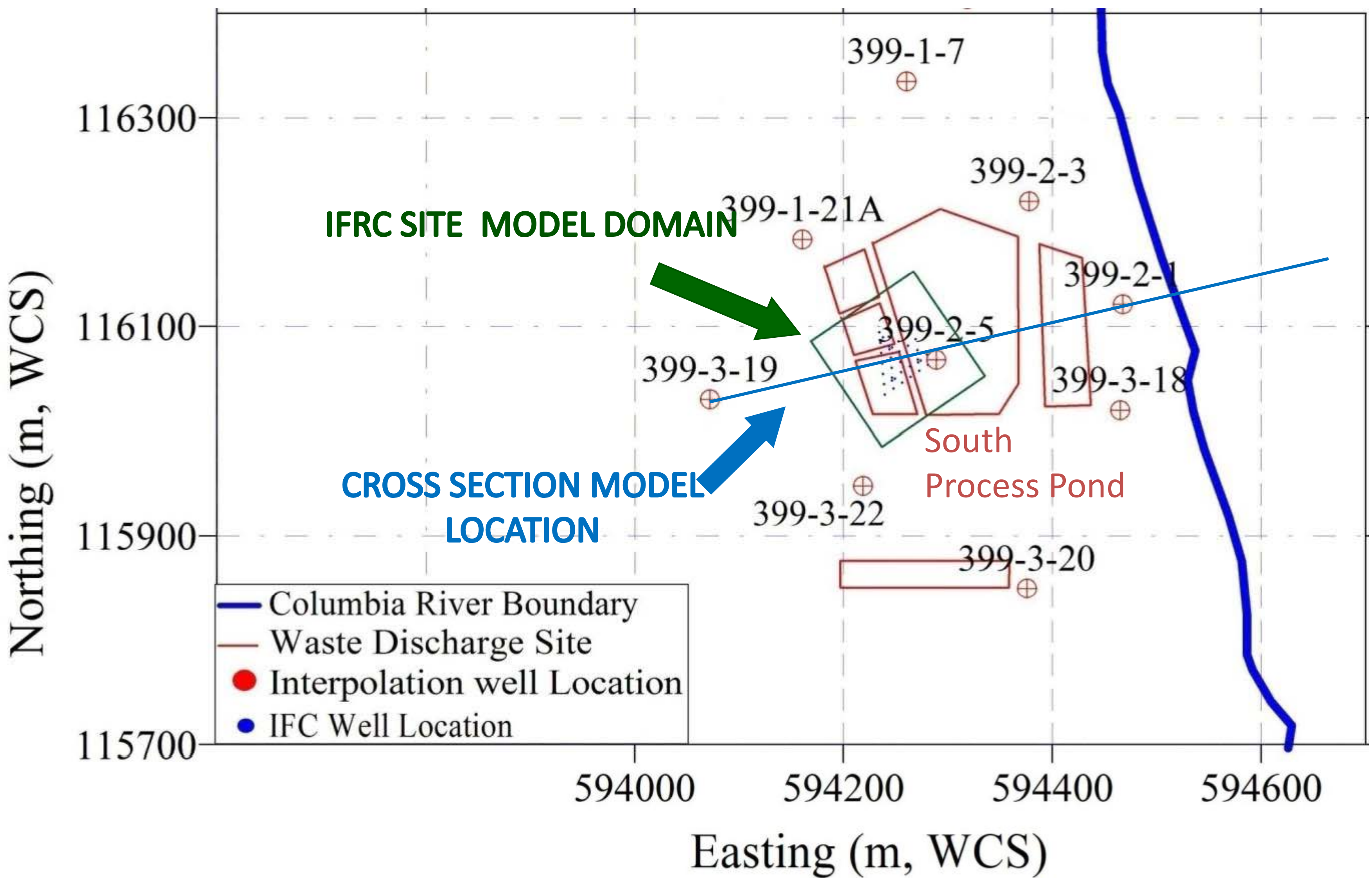
Previous Work (Conservative Tracers)

- Developed a method to obtain relatively reliable boundary conditions to simulate the March 2009 Br and heat tracer experiments
- Obtained a relatively reliable 3D K field as a result of model calibration using data from the Br and heat tracer experiments as constraints
- Demonstrated the importance of considering and accounting for intraborehole flows and solute mixing for the interpretation of tracer tests

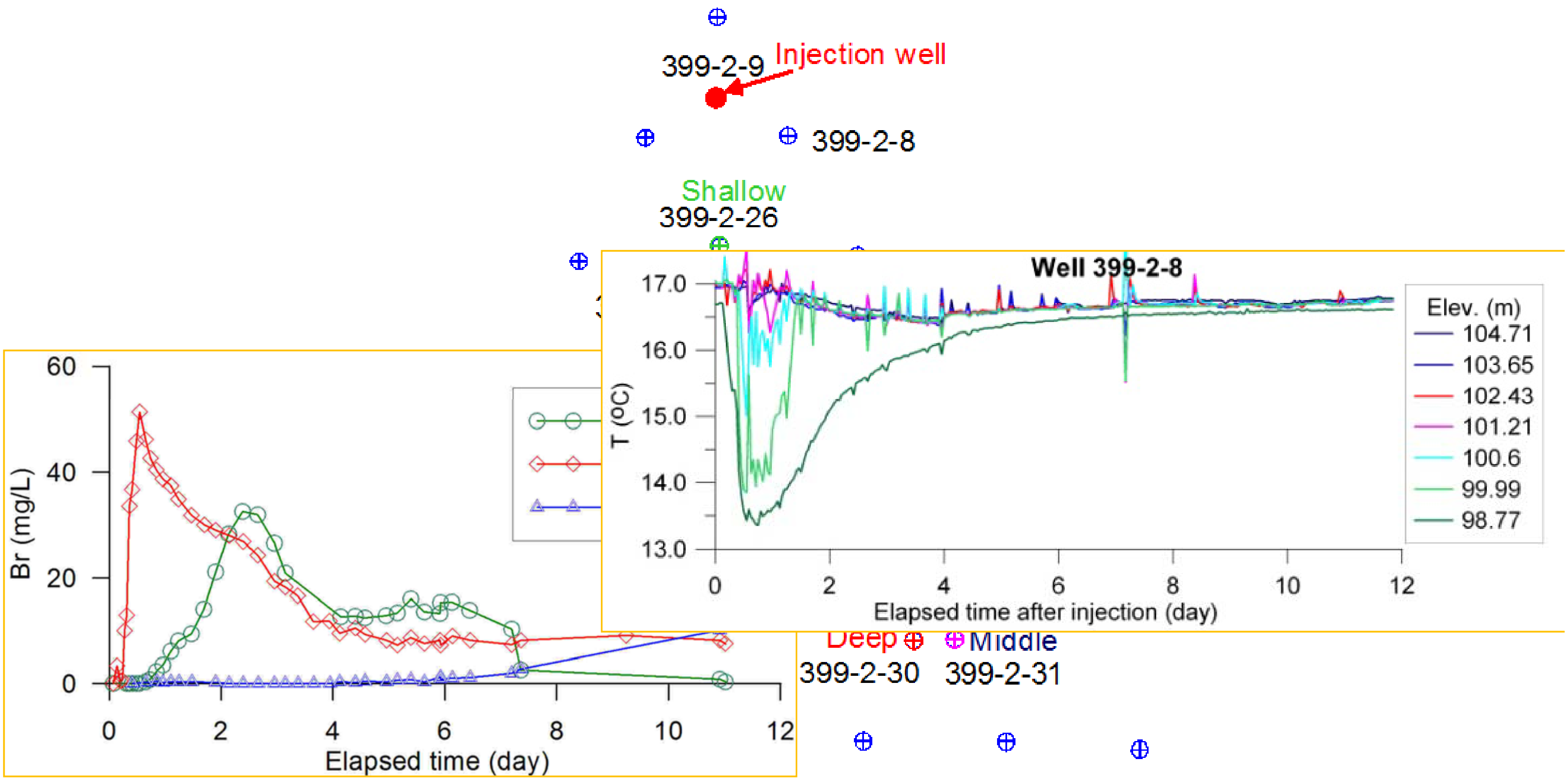
Previous Work (Reactive Transport)

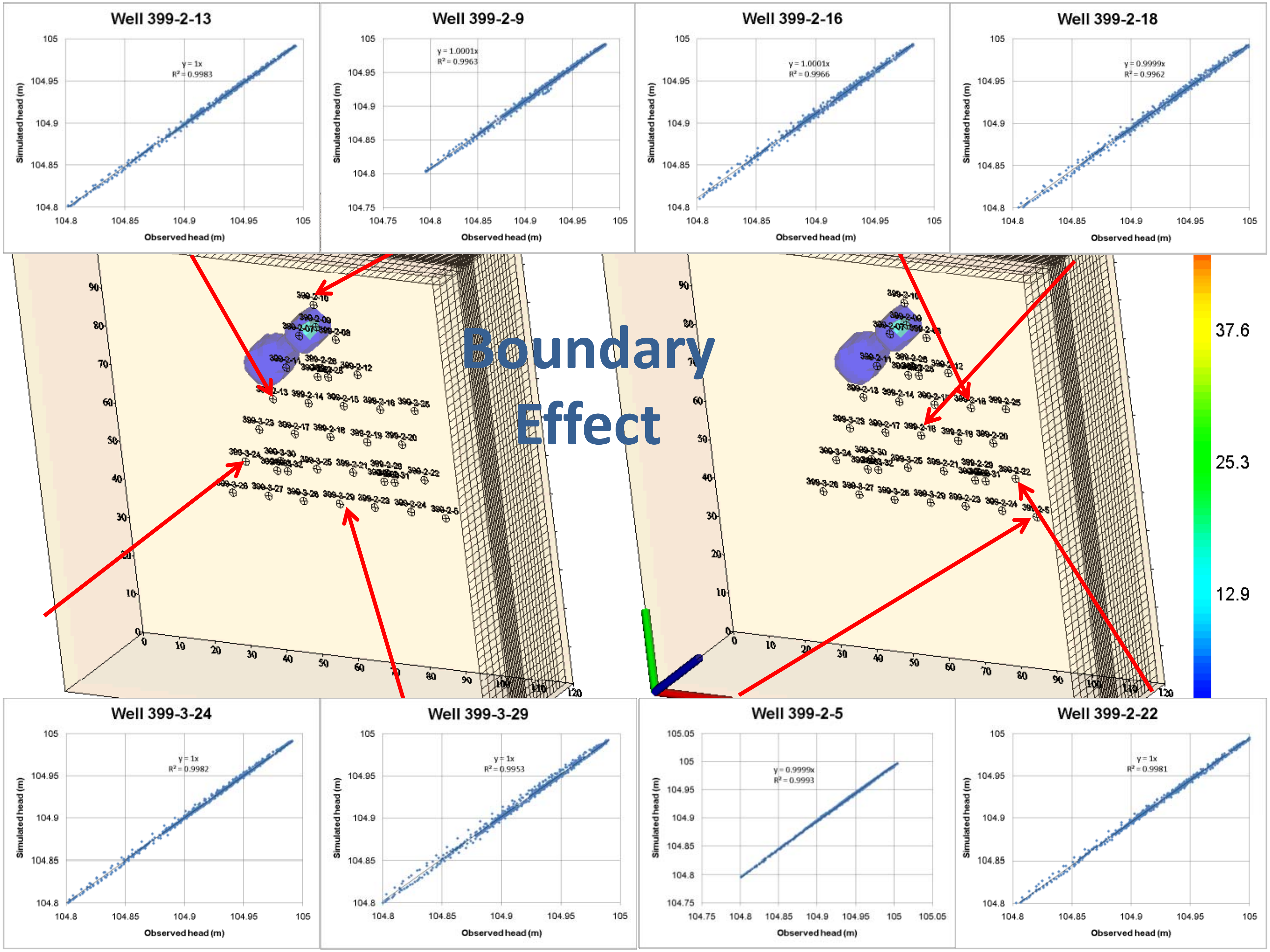
- First application of multi-rate mass transfer processes to the field scale using PHT3D
- Analysis of parameter sensitivities to identify *to what extent* the importance of processes and parameters controlling reactive transport of uranium agree between laboratory and field scales
- Investigation of the influence of calcite and its distribution on uranium mobility and U discharge patterns
- Comparison of physical non-equilibrium model and chemical non-equilibrium model to describe intra-grain diffusion and surface reactions

Model Domains

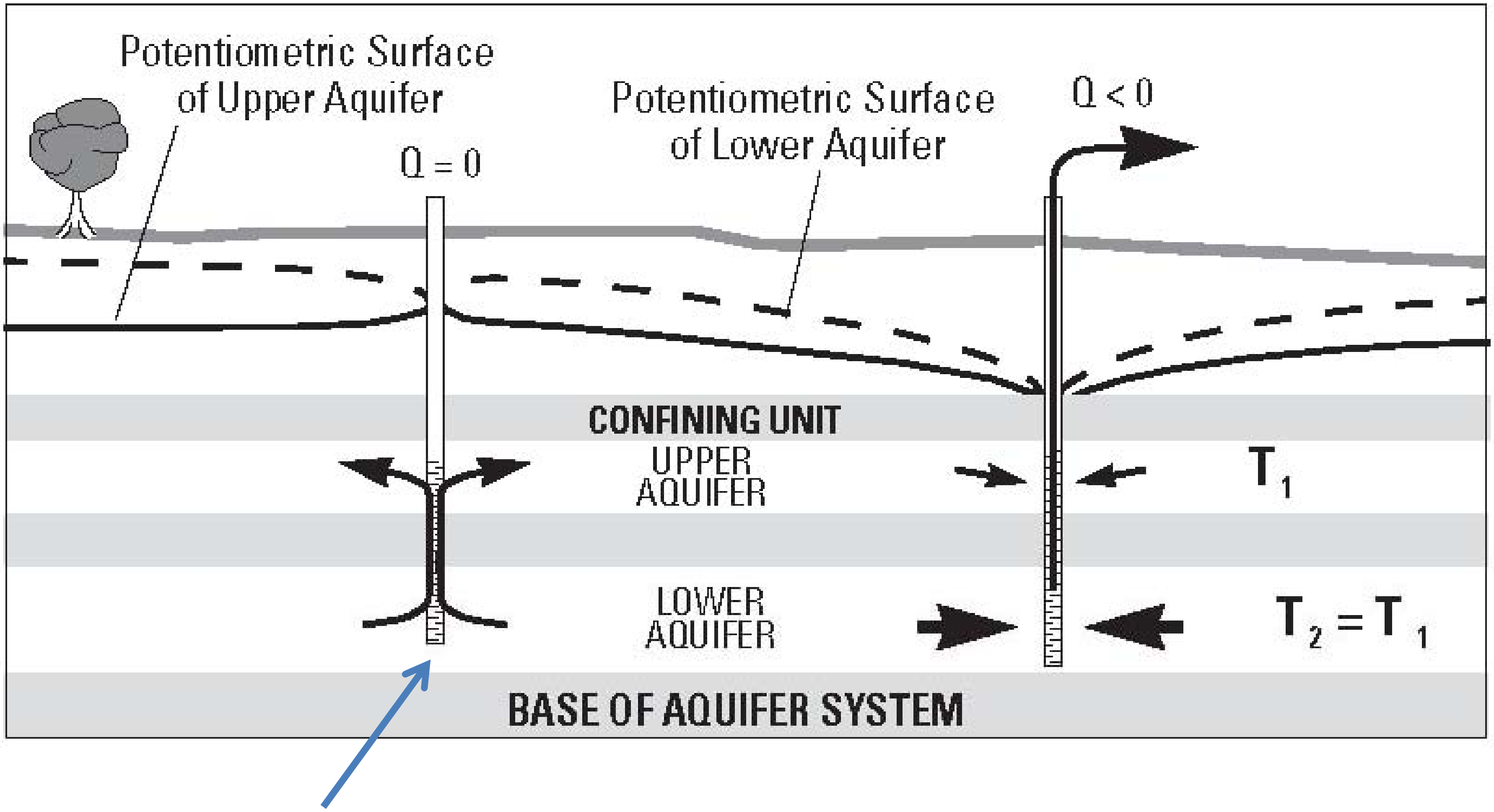


Br and Heat Tracer Experiment in March 2009



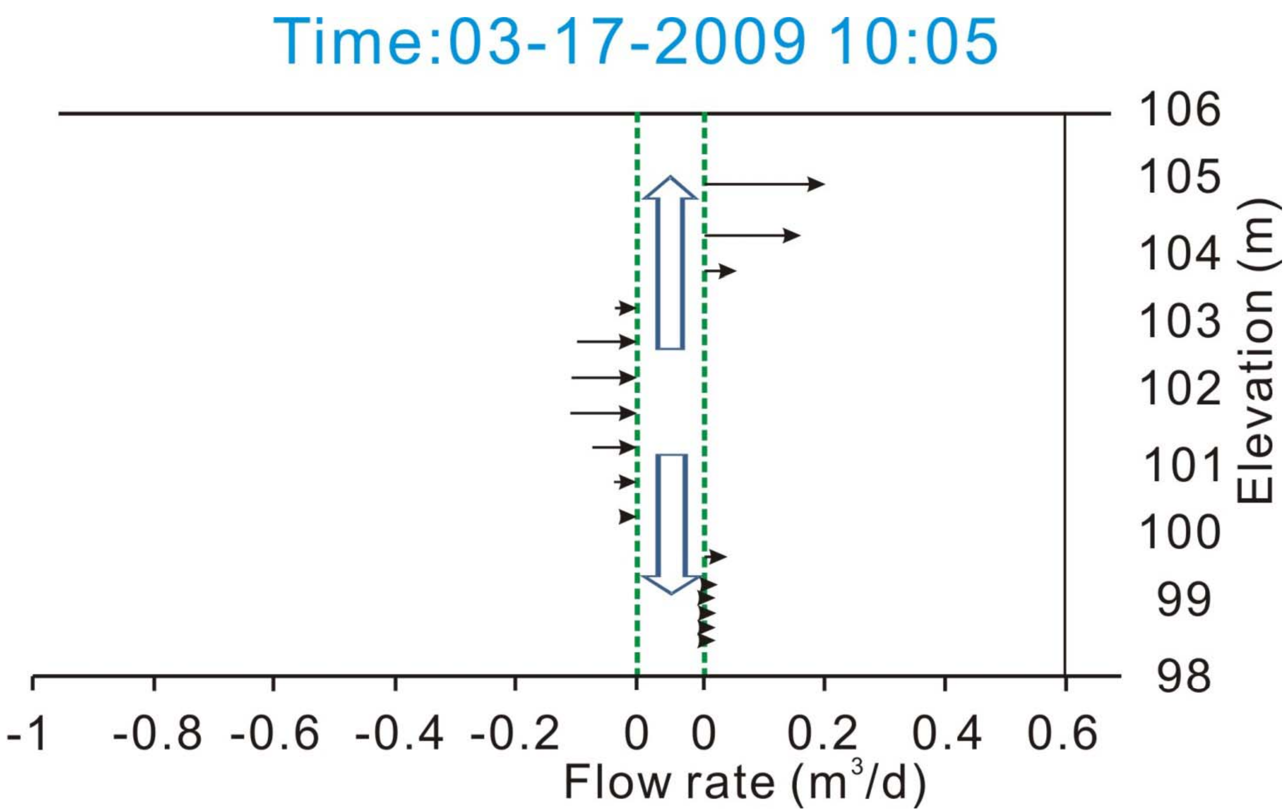

Well 399-2-13
y = 1x
R² = 0.9983
Well 399-2-9
y = 1.0001x
R² = 0.9963
Well 399-2-16
y = 1.0001x
R² = 0.9966
Well 399-2-18
y = 0.9999x
R² = 0.9962
Simulated head (m)
Observed head (m)
Boundary
Effect
37.6
25.3
12.9
Well 399-3-24
y = 1x
R² = 0.9982
Well 399-3-29
y = 1x
R² = 0.9953
Well 399-2-5
y = 0.9999x
R² = 0.9993
Well 399-2-22
y = 1x
R² = 0.9981

Intra-Borehole Flow

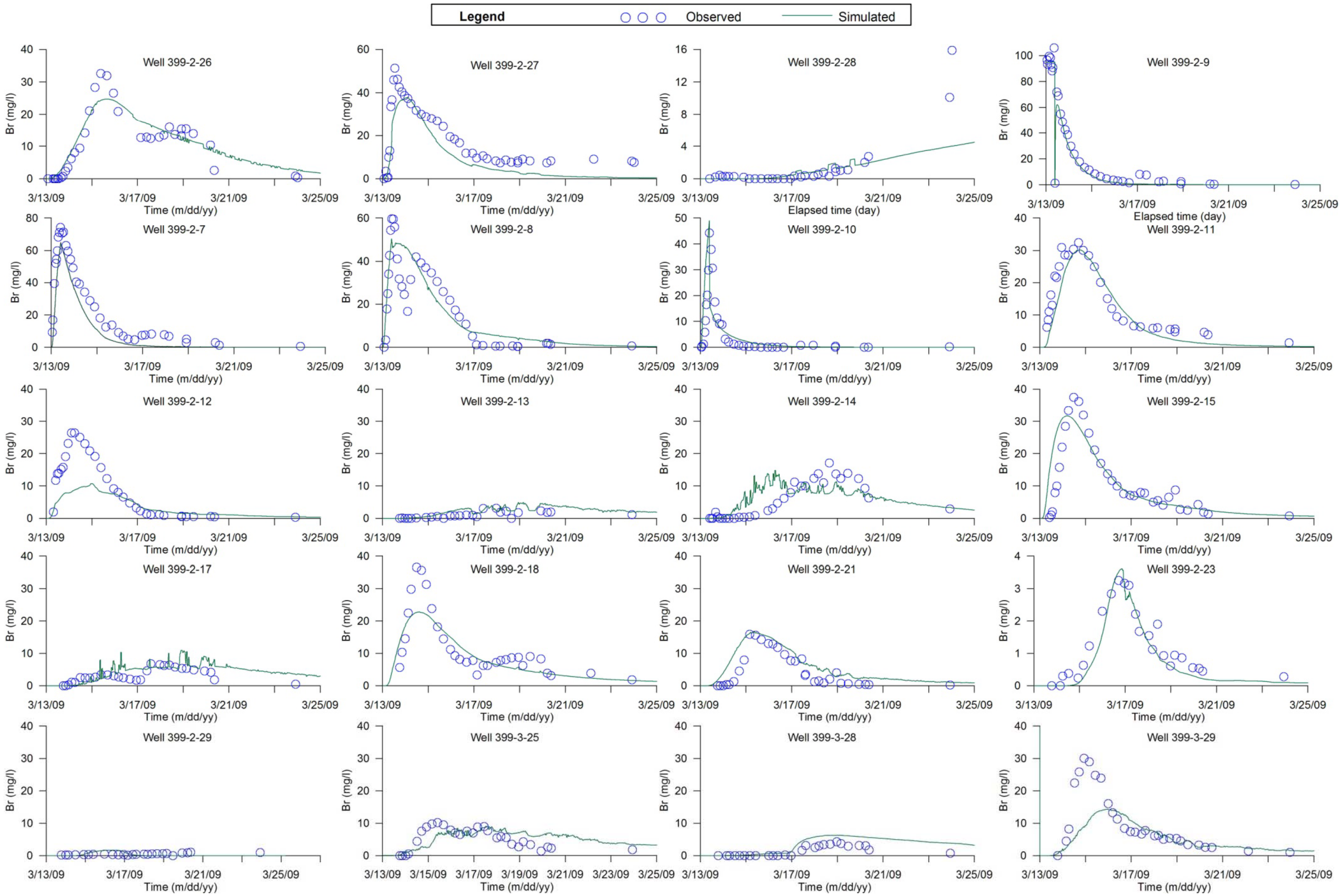


This intra-borehole flow can occur even when the pumping/injection rate is zero… The flow direction can alternate due to highly dynamic nature of the flow field at IFRC 300A in response to Columbia River

Intra-Borehole Flow



Flows in Well 399-2-7 calculated with MODFLOW Multi-node-well Package



Comparison between observed and simulated concentration breakthrough curves with Multi-node Well Package at observation well locations

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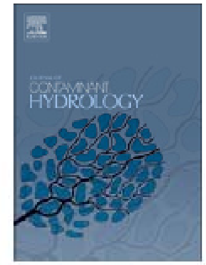

Importance of considering intraborehole flow in solute transport modeling under highly dynamic flow conditions

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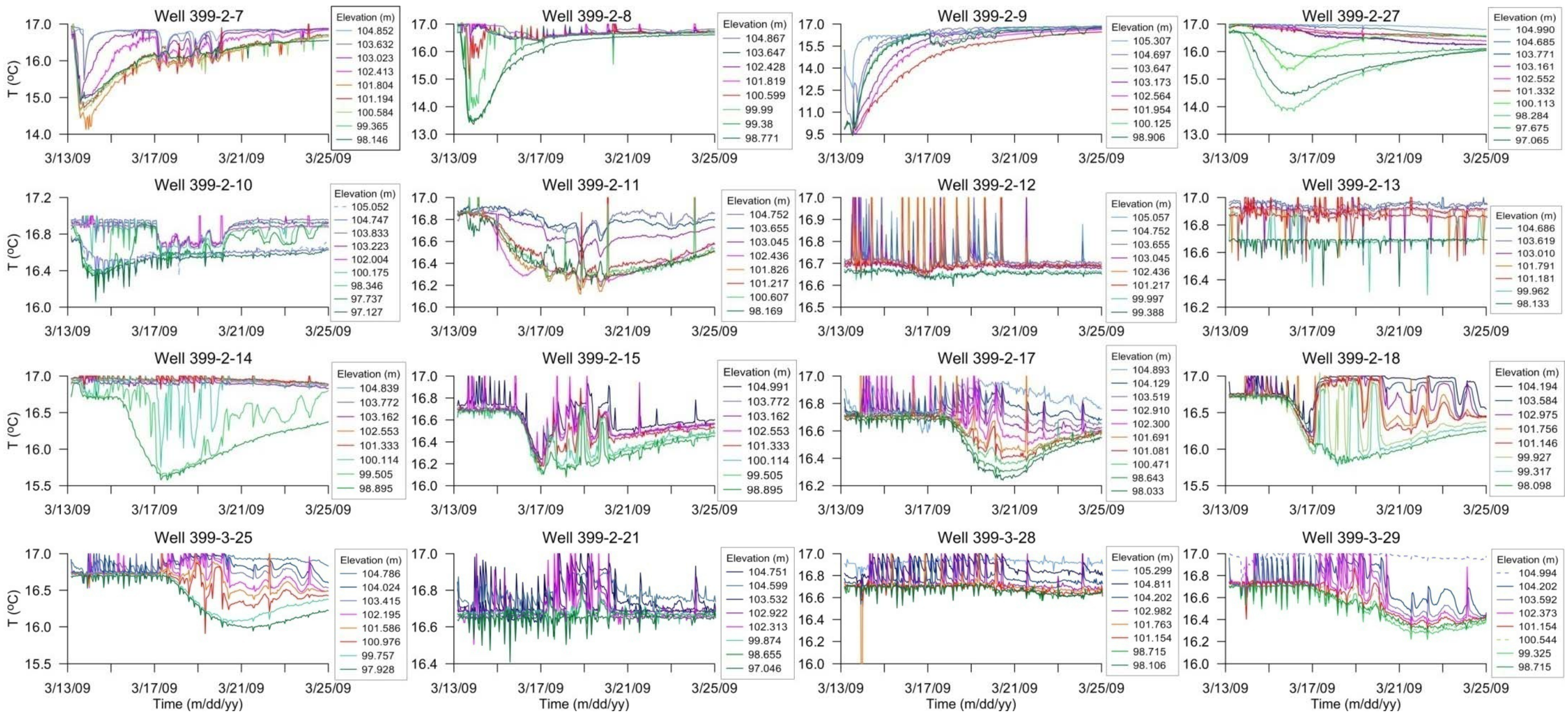
Measured temperature breakthrough curves



- heating effect of the sampling pumps
- mixing caused by intraborehole vertical flow
- aquifer heterogeneity in vertical direction vs. density effect

Blue: shallow
Pink/red: middle
Green: Deep

Heat Transport Simulation
— Thermal parameters

In MT3DMS and SEAWAT:

$$K_d = \frac{c_s}{c_w \rho_w}$$

Hydraulic parameters are same as calibrated from Br tracer transport.

The final calibrated thermal distribution coefficient value of 10^{-1} m^3/kg was found to be the best estimate of the arrival time of temperature change. This calibrated K_d value is about 3 orders greater than the initial value ($1.7081\times10^{-4} m^3/kg$) obtained from literatures according to the type of sediments.

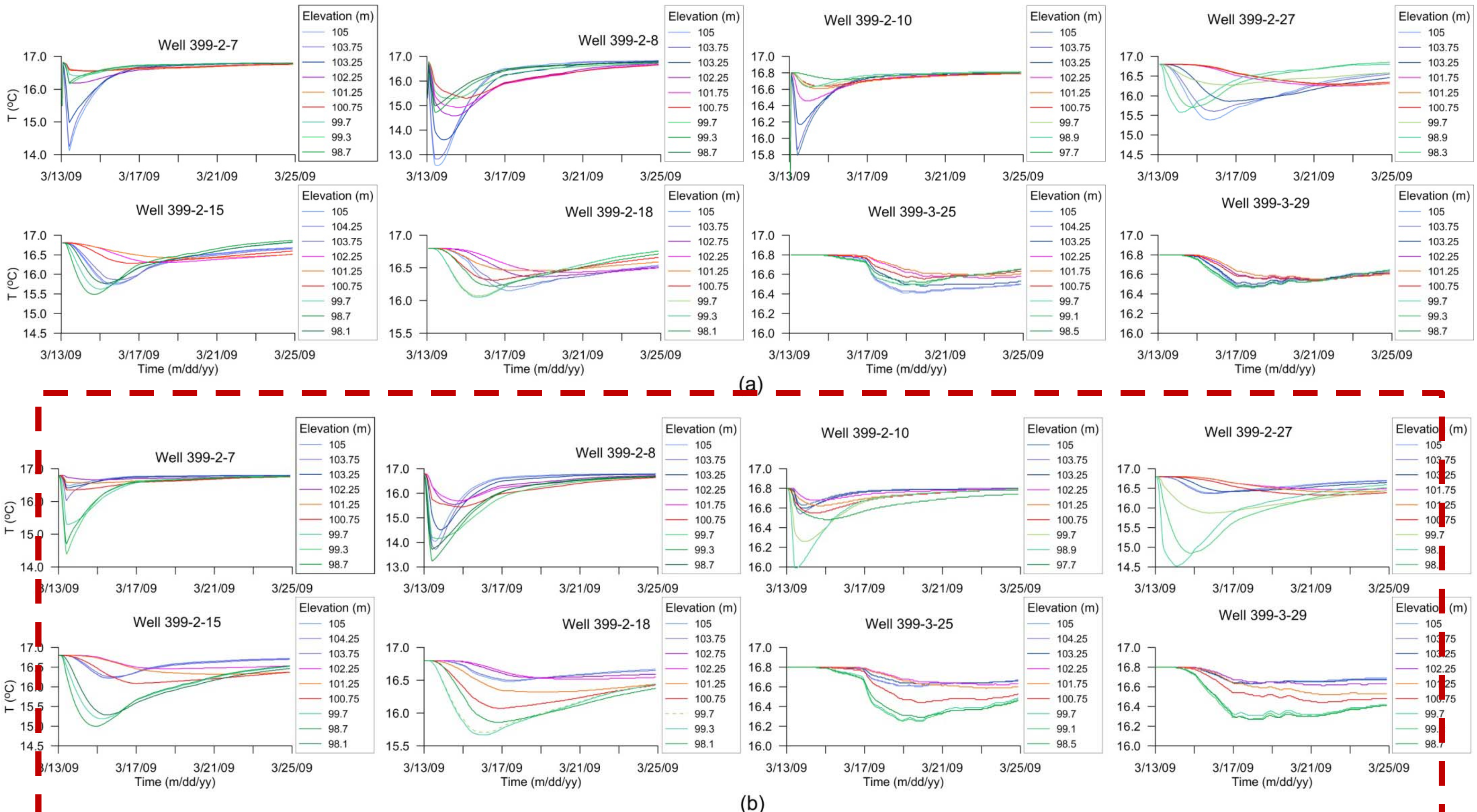
Blue: shallow

Pink/red: middle

Green: Deep

Heat Transport Simulation

— Density Effect



The simulated temperature breakthrough curves along the depth without (a) and with (b) considering the density and viscosity effect.

Conclusions

- Groundwater head data *alone* were of little value in model calibration.
- Aquifer heterogeneity and dynamic flow field led to significant intraborehole flows in fully-screened wells.
- Density effect occurred during heat experiment due to temperature difference. It was not apparent in fully-screened wells, but obvious from multi-level clusters.
- Results of heat transport model calibration indicated that the thermal distribution coefficient K_d is about 3 orders of magnitude larger than that obtained from the literature for the similar type of sediments.

Research Opportunities: (1)

- Test if we can better explain the principal character of plume behaviour, i.e., high mobility + high (UVI) concentrations + long plume persistence.

Approach:

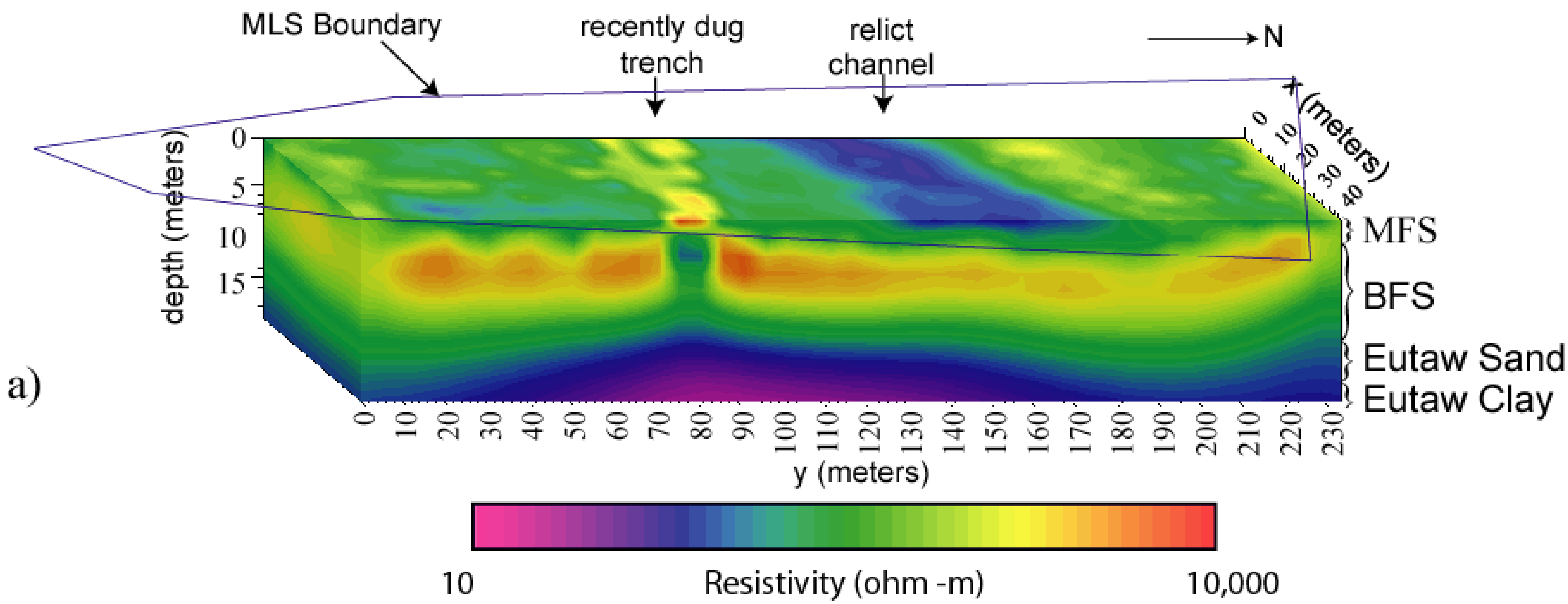
Use 2D cross section model to conceptually explore the effect of:

- different SC models (Doug Kent‘s, Bond et al.) (effective Kd)
- sorption rate-constants
- U(VI) release from the unsaturated zone during times of high water levels

Research Opportunities: (2)

- Based on the previously (separately) developed/tested hydrogeological (heterogeneous K-field) and reaction models, set up and adopt a full 3D model to simulate/interpret the first uranium (desorption) experiment.
- Inclusion of intraborehole flow is thought to be crucial for the interpretation of the experiment – can only be considered by MODFLOW/MT3DMS-based codes

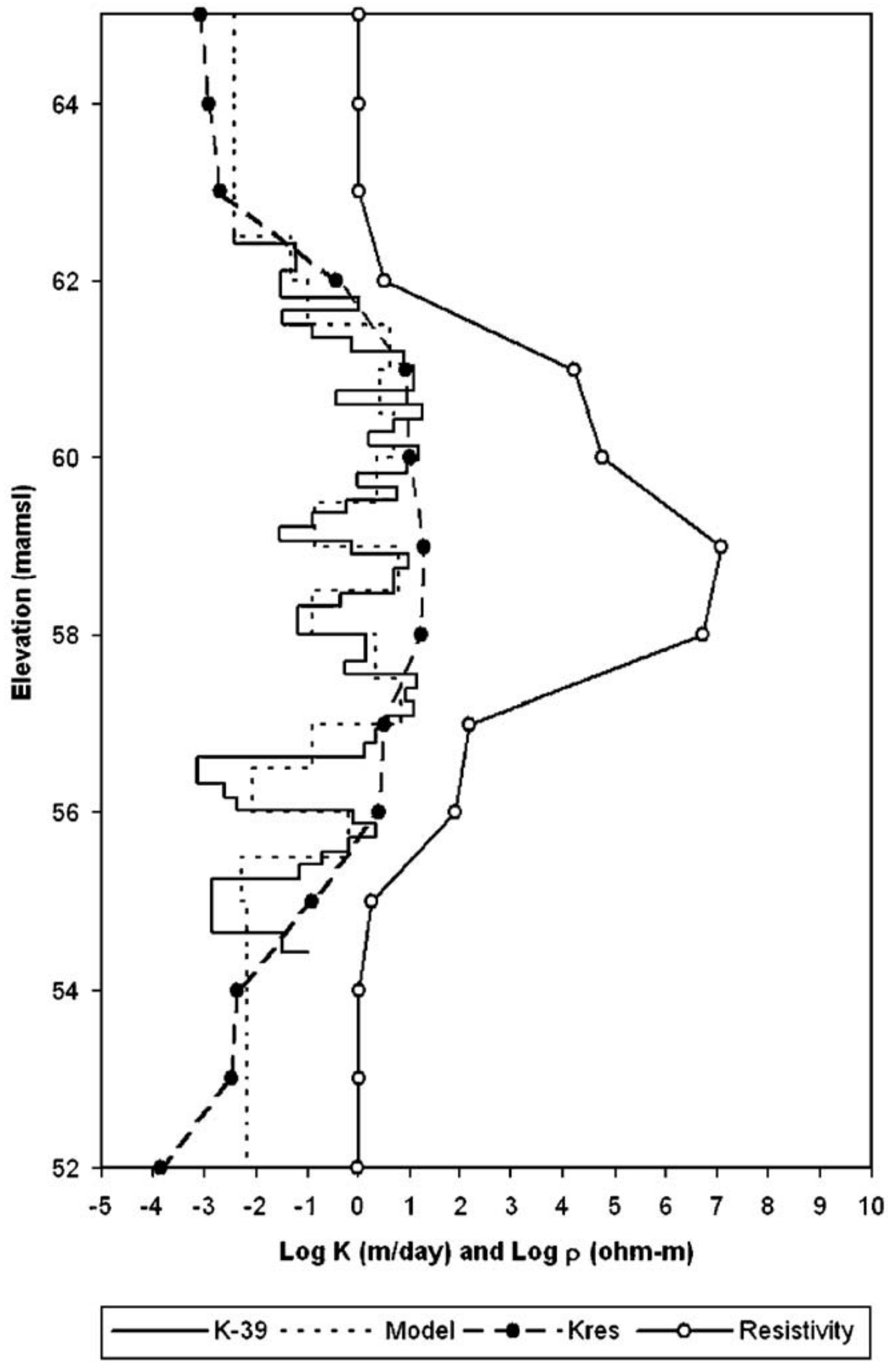
Resistivity Image of the MADE Site



(Bowling et al., 2005, GW)

Correlation between Hydraulic Conductivity (K) and Resistivity (Res)

$$\log(K) = \log(Res)/A+B$$



Elevation (mamsl)
64
62
60
58
56
54
52
-5
-4
-3
-2
-1
0
1
2
3
4
5
6
7
8
9
10
Log K (m/day) and Log ρ (ohm-m)
K-39
Model
Kres
Resistivity