Preliminary 3D Modeling of Variably Saturated Flow and Uranium Transport in the 300 Area

Mark Rockhold, Philip Meyer,
Ming Ye, and Paul Thorne

Project Overview

- Objective: develop, test, and document a methodology for the combined assessment of hydrogeologic uncertainties involved in dose assessment modeling, including uncertainty in
  - the conceptual-mathematical basis of the model,
  - model parameters, and
  - the scenario to which the model is applied.
- Funded by the Nuclear Regulatory Commission, Office of Nuclear Regulatory Research

Methodology Approach

- Conceptual model uncertainty is represented by a set of plausible alternative conceptual models supported by the available data.
- Each alternative model is calibrated to assess parameter uncertainty and estimate the relative model probability.
- A weighted average model prediction is computed, with each model's result weighted by that model's probability.
- Scenario uncertainty is incorporated using a similar weighted approach combined with sensitivity analysis.

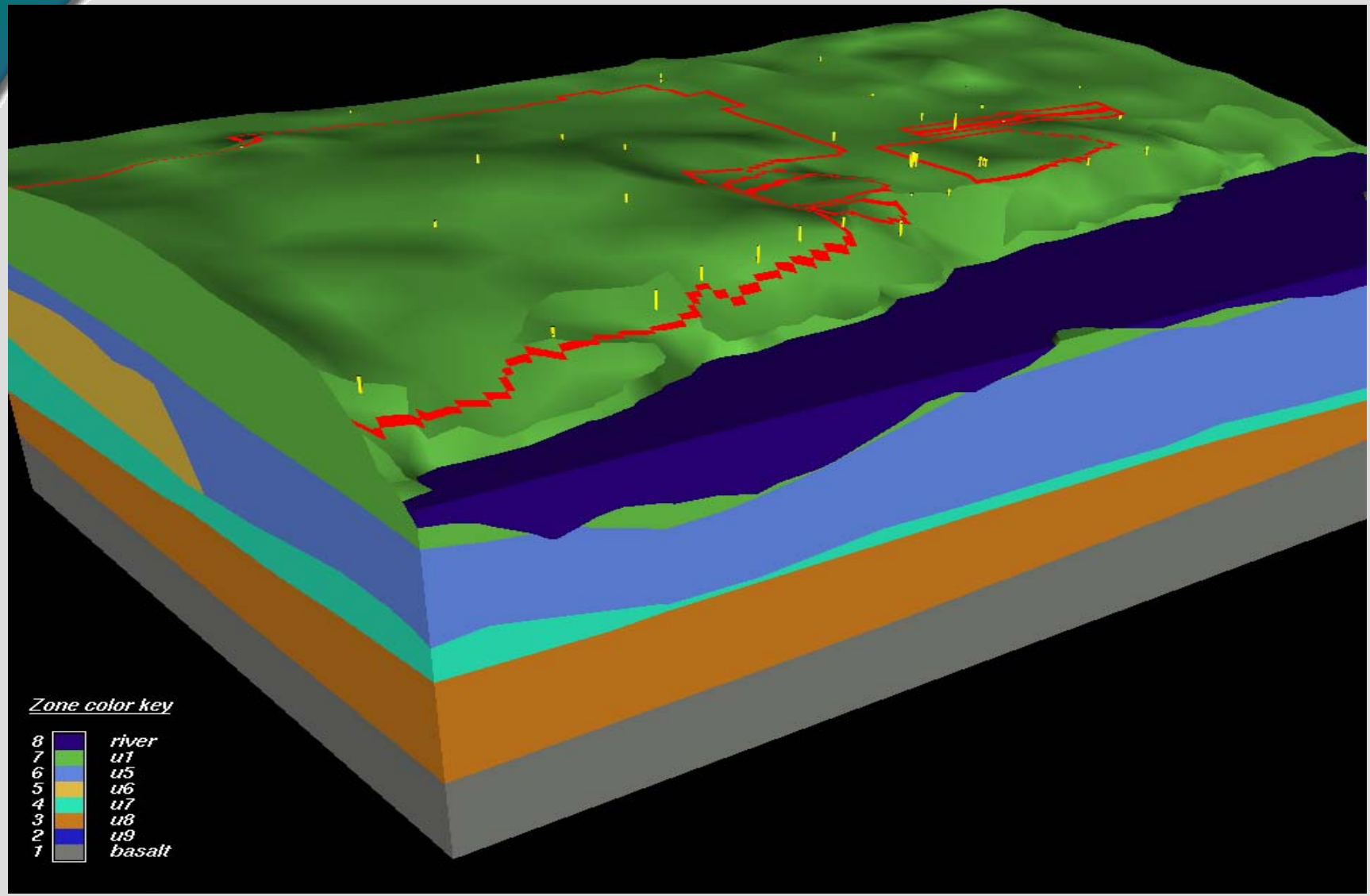
300 Area Uranium Transport Modeling

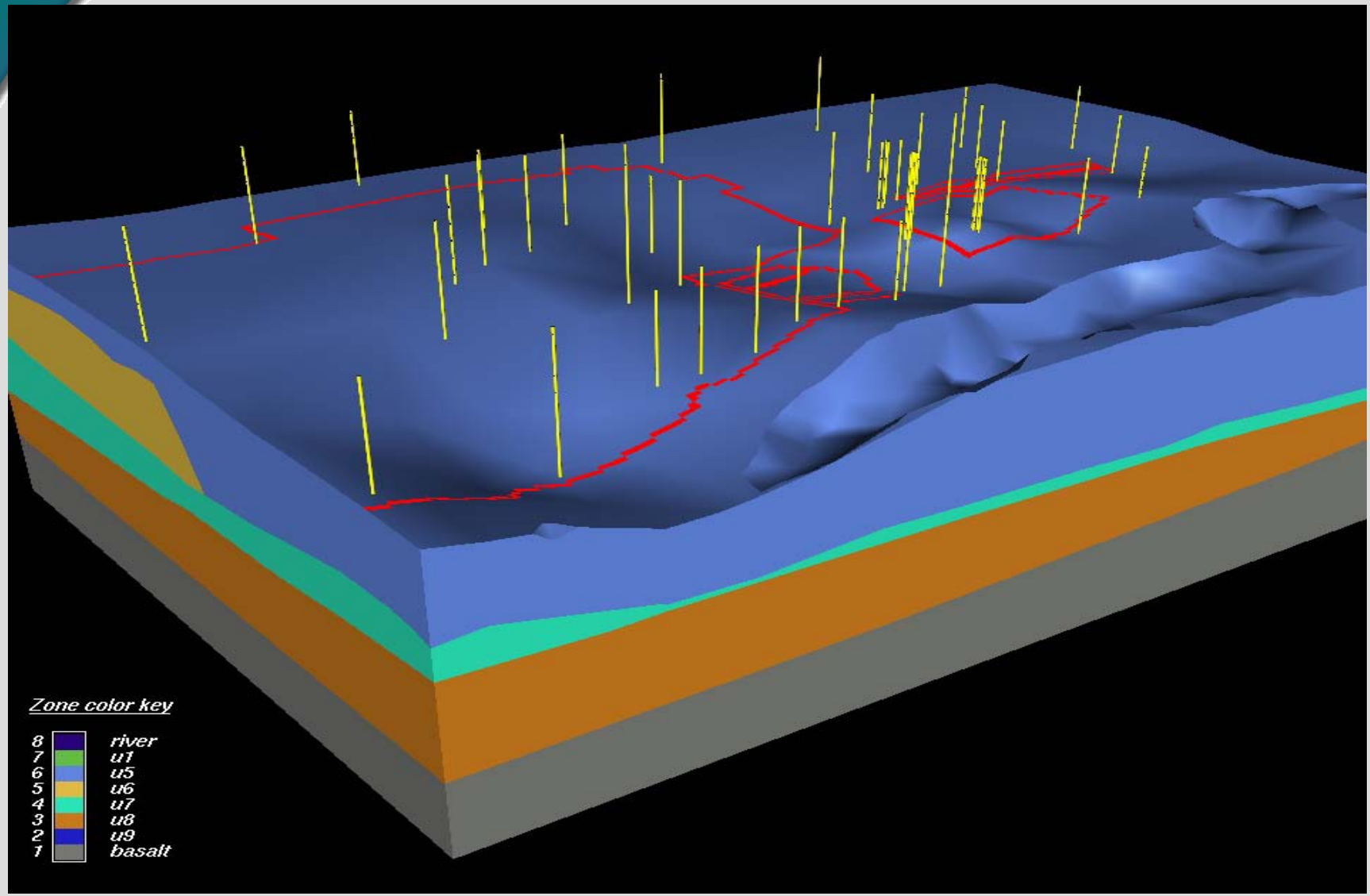
- 300 Area Uranium transport is being modeled as part of a test case application of the uncertainty assessment methodology
- Model described here is a nominal model: it will ultimately include the greatest amount of detail about the system we intend to consider
- Alternative conceptual models will be simplifications (abstractions) of the nominal model

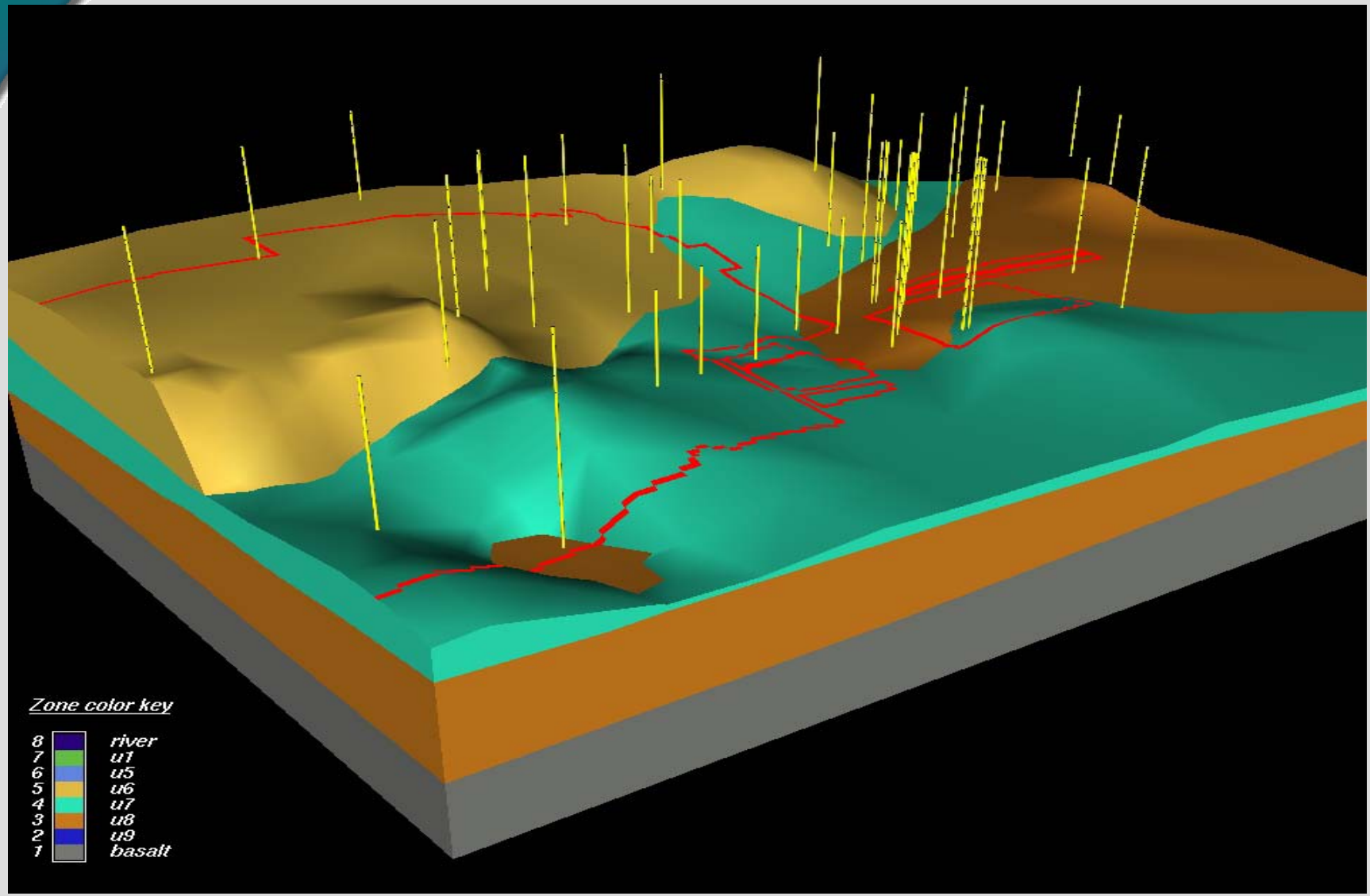
Model Development

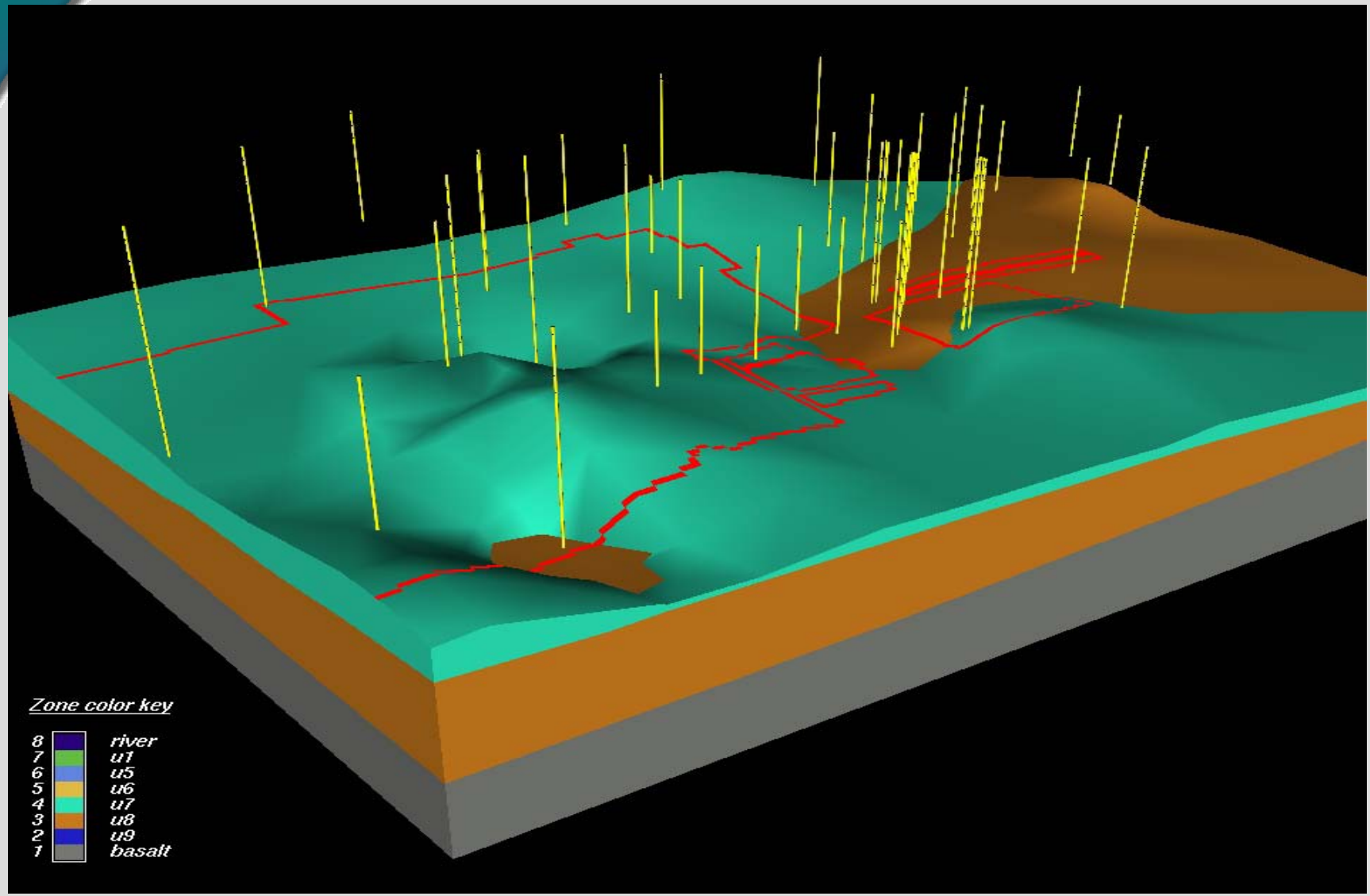
- Available hydrogeologic data were reviewed (eg. Schalla et al., 1988, PNL-6716; Swanson, 1992, WHC-SD-EN-052)
- Existing *earthVision*® model of the 300 Area was updated
- River stage data were compiled and estimates of historical monthly average river stages were generated (1944-present)
- Initial waste-water and uranium source terms and sorption (Kd) parameters from SAC (History 5, median case)
- Preliminary 3D flow and transport model developed using STOMP (**http://www.pnl.gov/etd/stomp/**)

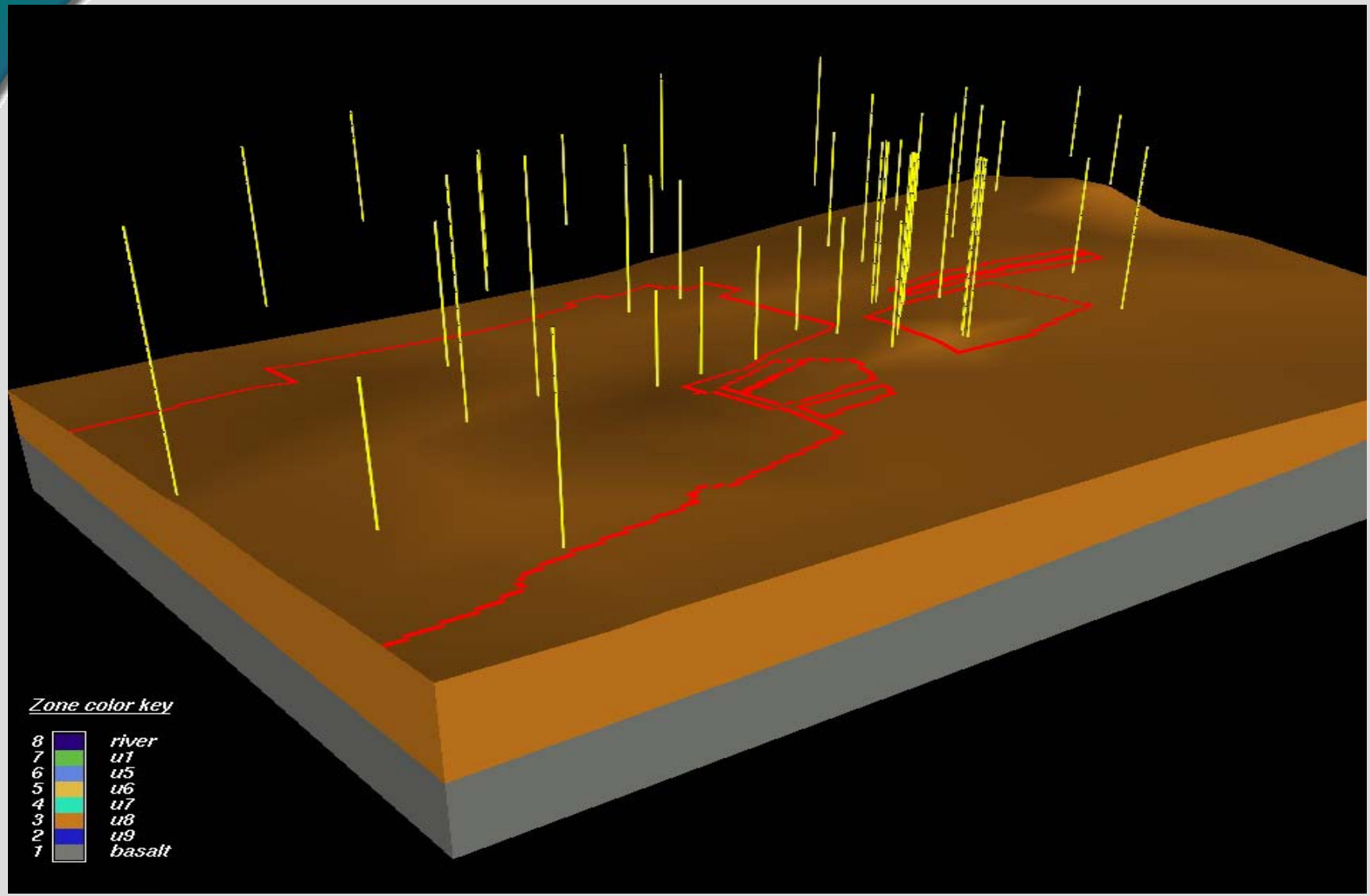
earthVision® 300 Area Update

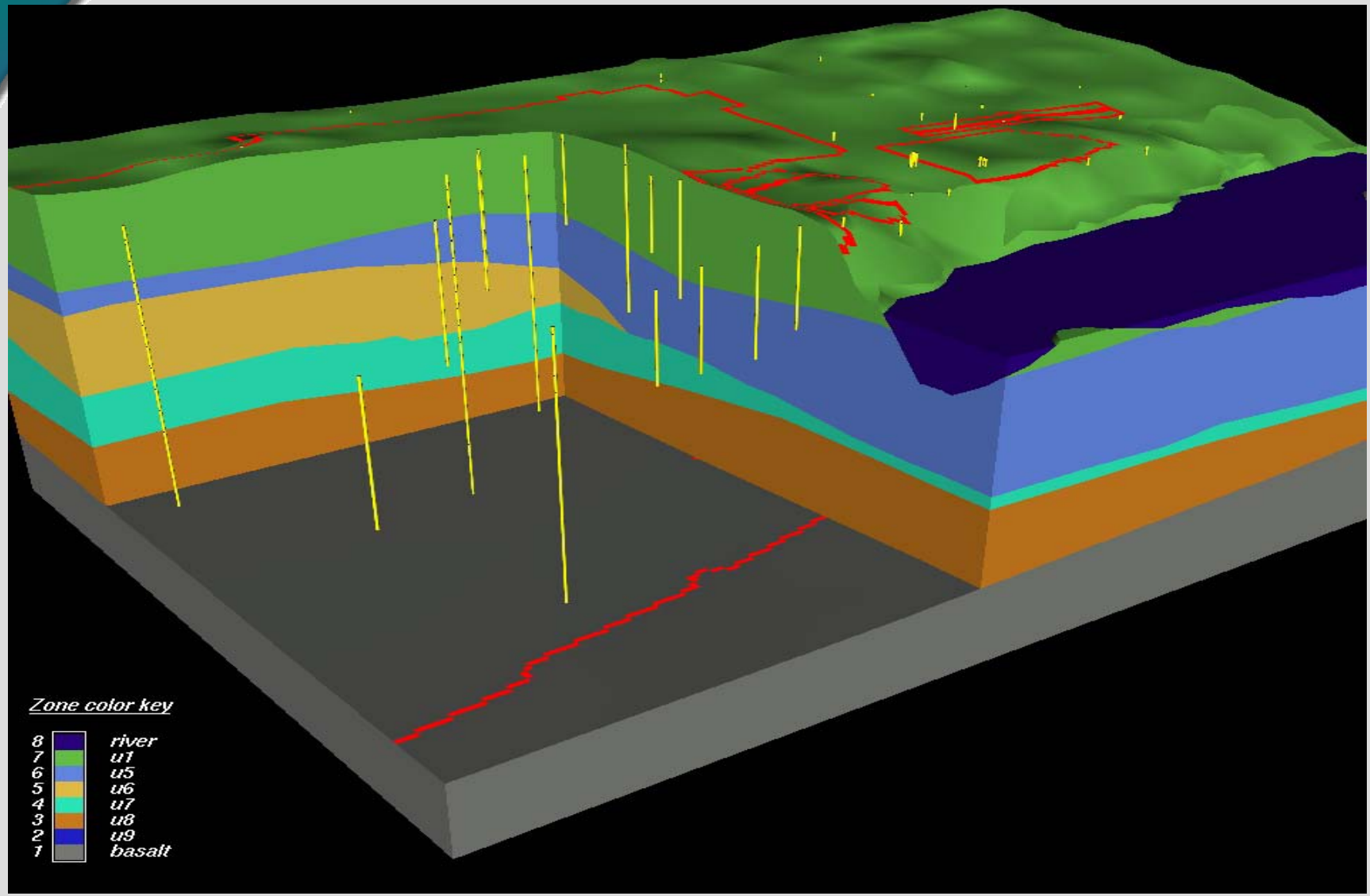


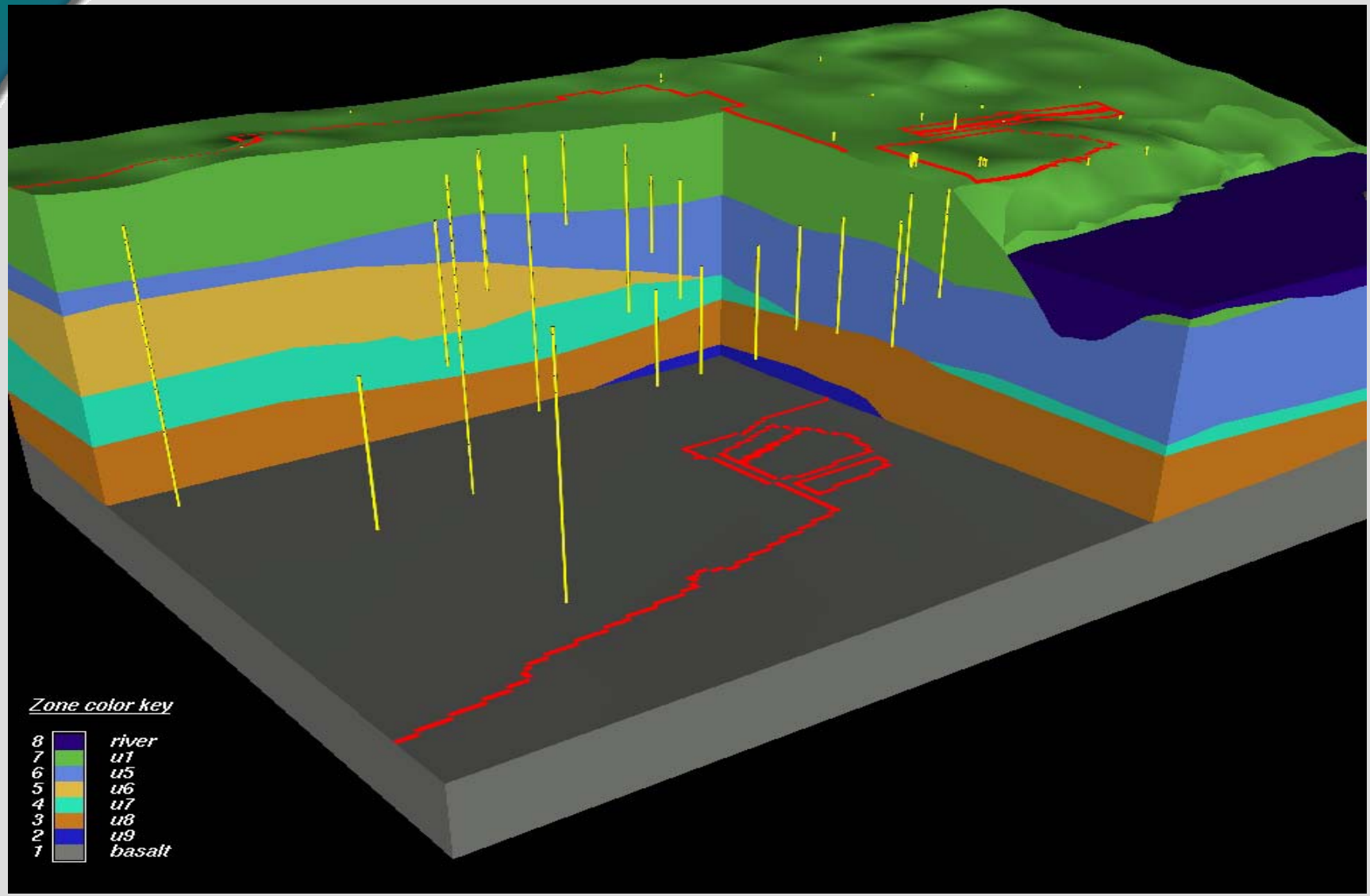

Zone color key
8 river
7 u1
6 u5
5 u6
4 u7
3 u8
2 u9
1 basalt

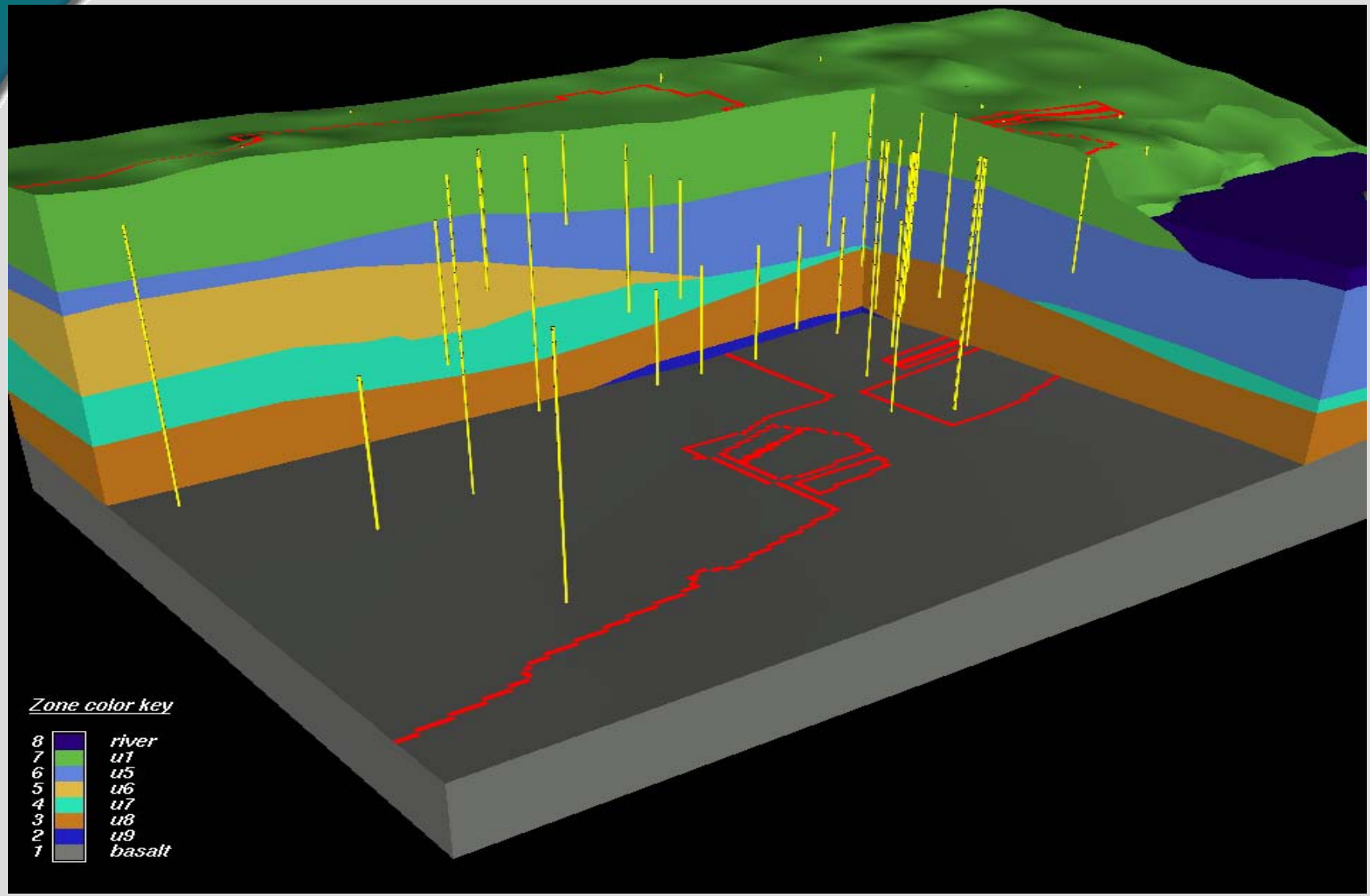

Zone color key
8 river
7 u1
6 u5
5 u6
4 u7
3 u8
2 u9
1 basalt


Zone color key
8 river
7 u1
6 u5
5 u6
4 u7
3 u8
2 u9
1 basalt


Zone color key
8 river
7 u1
6 u5
5 u6
4 u7
3 u8
2 u9
1 basalt


Zone color key
8 river
7 u1
6 u5
5 u6
4 u7
3 u8
2 u9
1 basalt

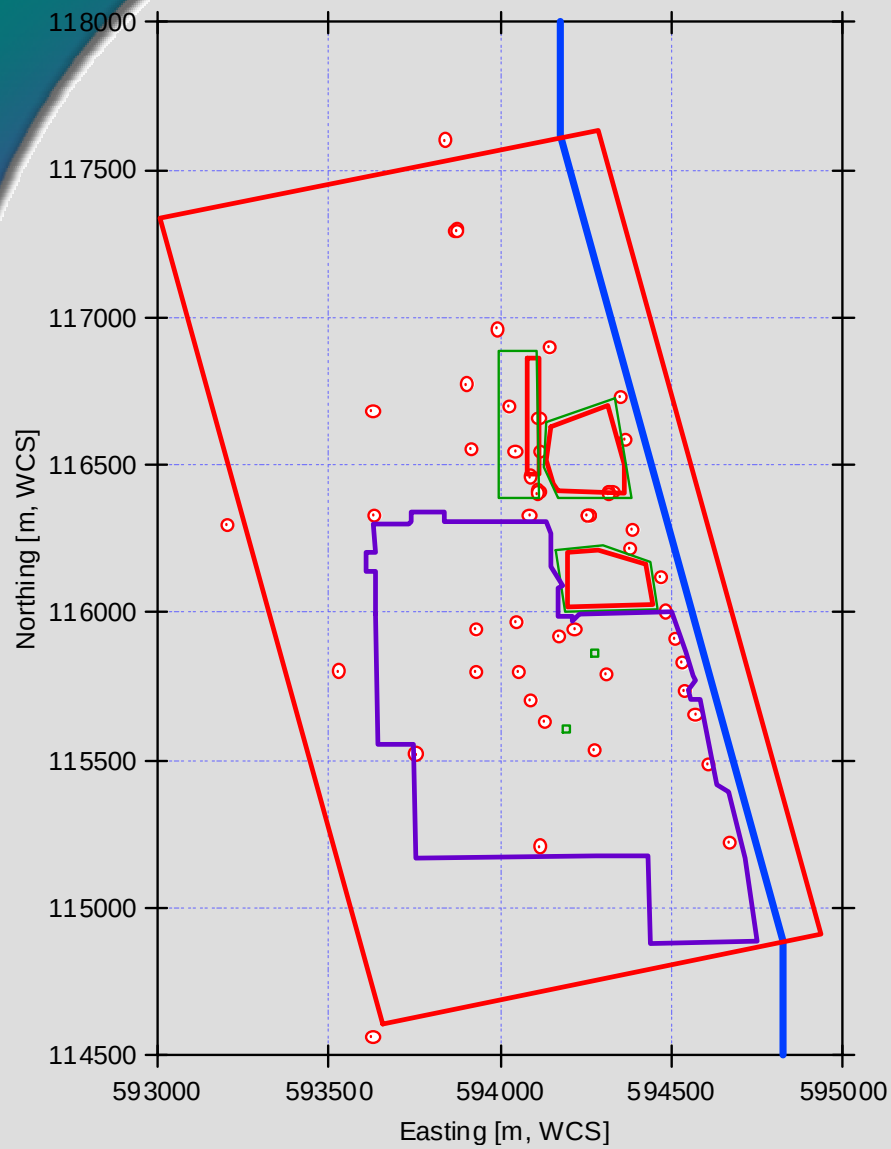

Zone color key
8 river
7 u1
6 u5
5 u6
4 u7
3 u8
2 u9
1 basalt

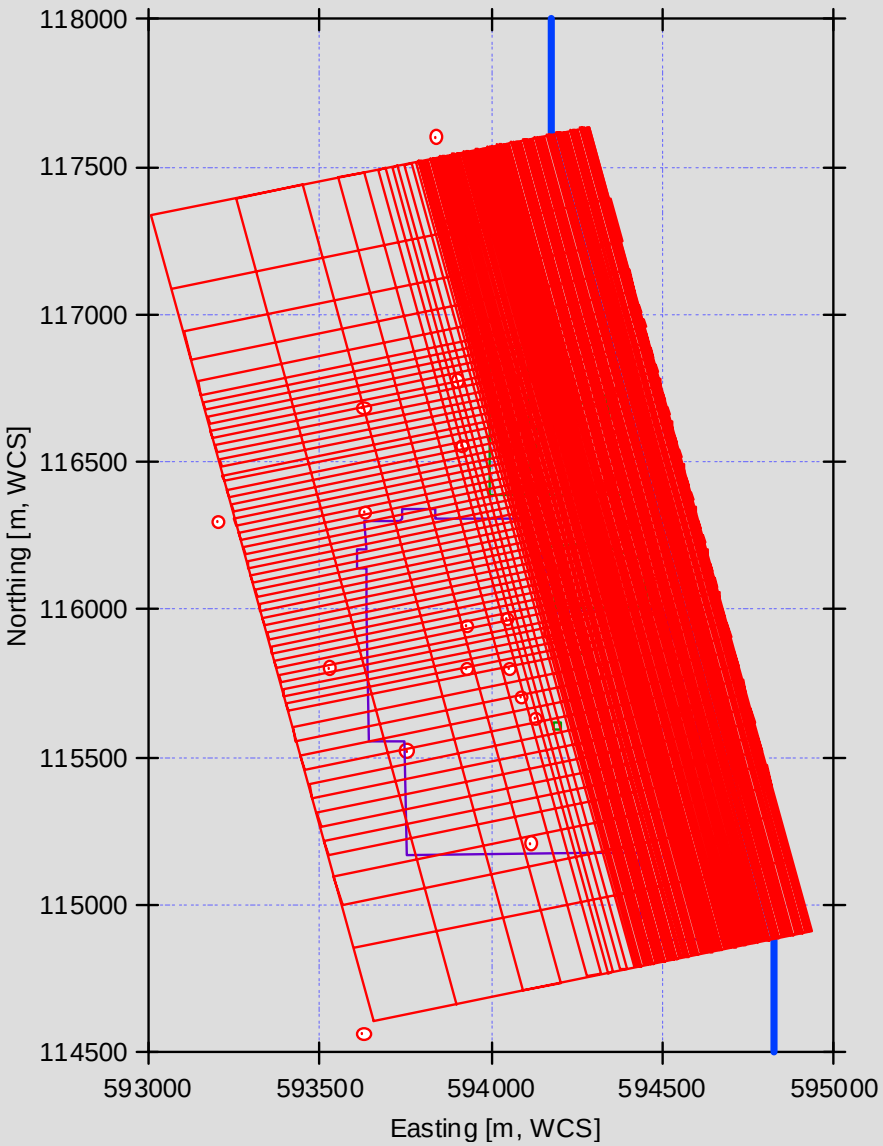

Zone color key
8 river
7 u1
6 u5
5 u6
4 u7
3 u8
2 u9
1 basalt

Preliminary 300 Area STOMP Model

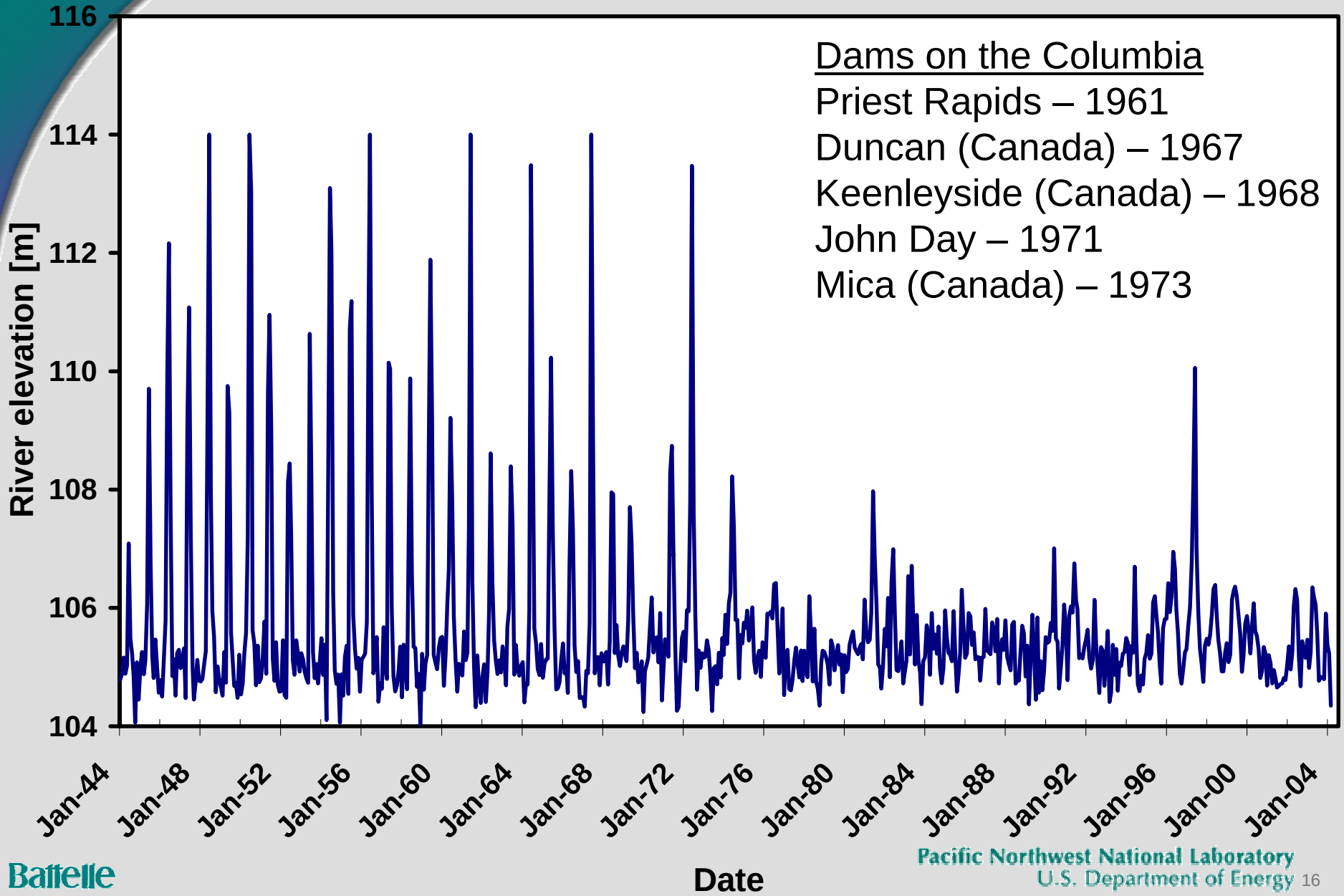
- Spatial domain
  - 2800 m (N-S) x 1300 m (E-W) x 45 m (vertical)
  - 7 material types:
    - U9 - Ringold unit A, U8 - Ringold lower mud, U7 – Ringold unit B, U6 – overbank deposits, U5 – Ringold unit E, U1 – Hanford fm (undifferentiated), Fines
- Discretization
  - 63 x 63 x 45 = 178,605 nodes (~132,000 active)
  - Minimum grid spacings [m]: dx=10, dy=25, dz=1 (constant)
  - Time step size = 1 day
- Boundary conditions
  - Natural groundwater recharge at upper surface
  - Artificial recharge and uranium loading from SAC (History 5, Median case) for 316-1 (N. pond), 316-2 (S. pond), 316-3 (324 Bldg.), 316-5 (N. trench)
  - Inland – Dirichlet (fixed head) boundary conditions with N-S gradient
  - River – Dynamic, Dirichlet and seepage faces with monthly avg. river stages
- Transport
  - TVD numerical scheme
  - Linear Kd model for uranium sorption
    - Kd = 0.8 mL/g for sediments, Kd = 4 mL/g for fines

Plan Views of STOMP Model Domain

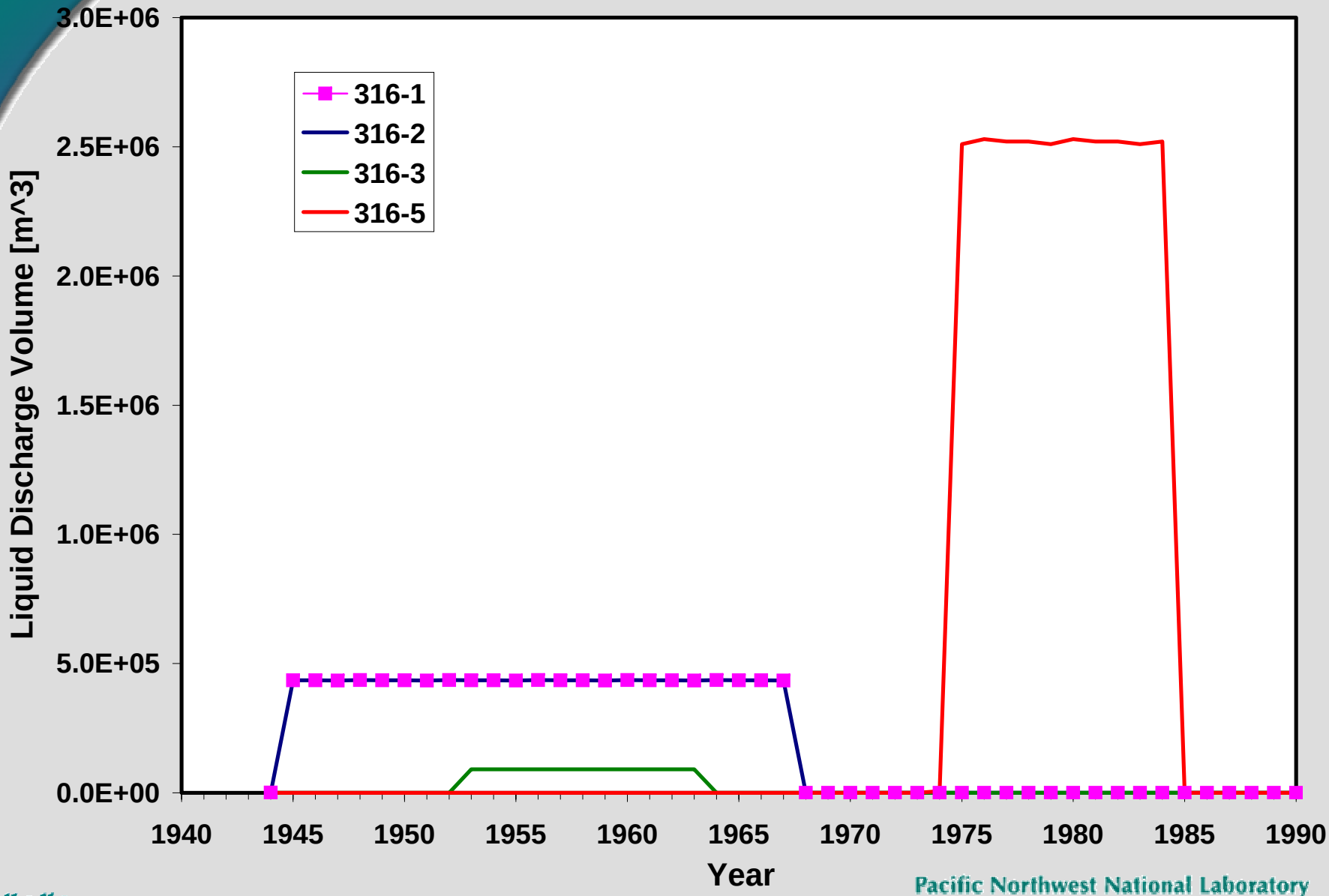




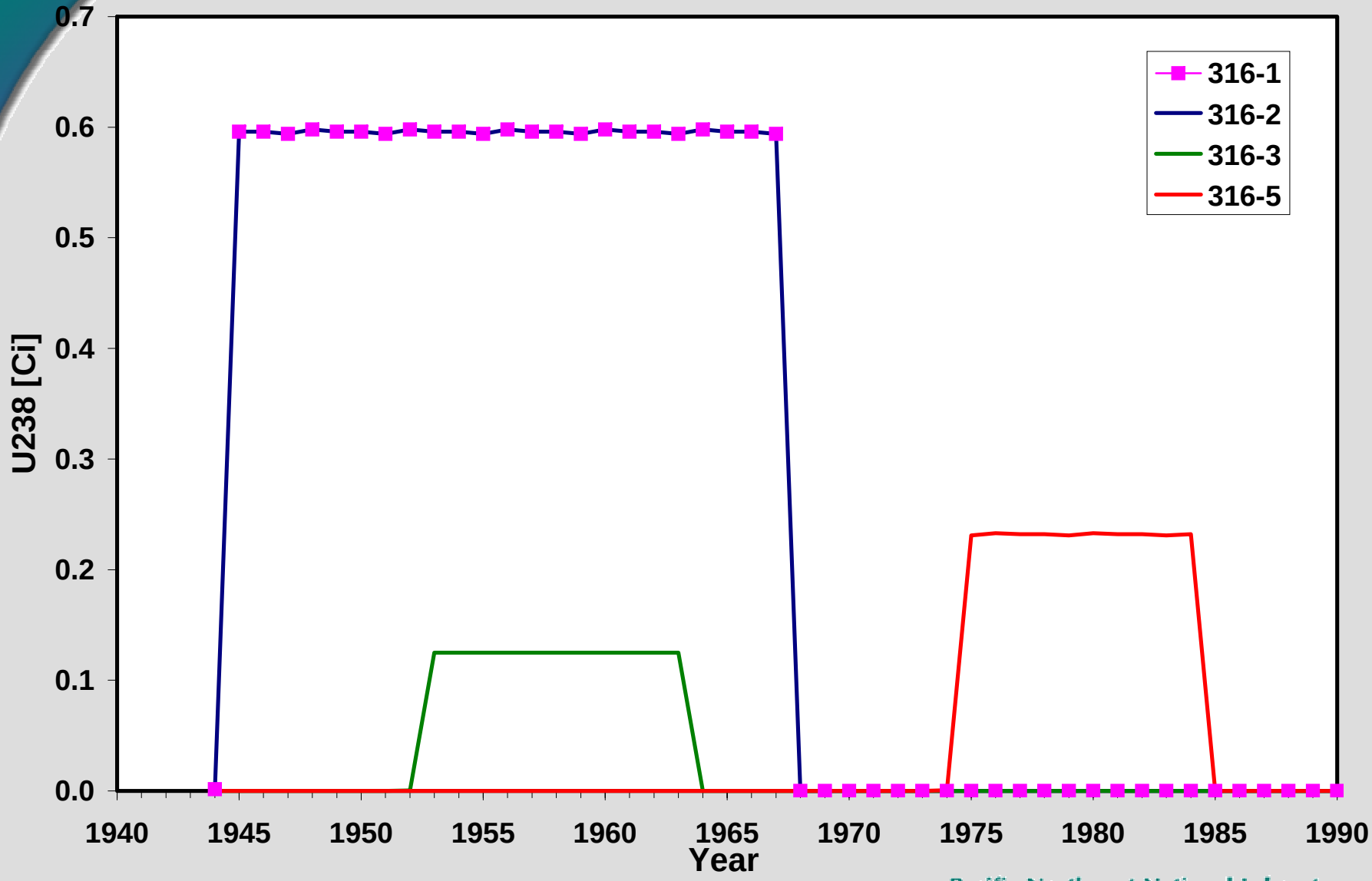
Reconstruction of Historical River Stages



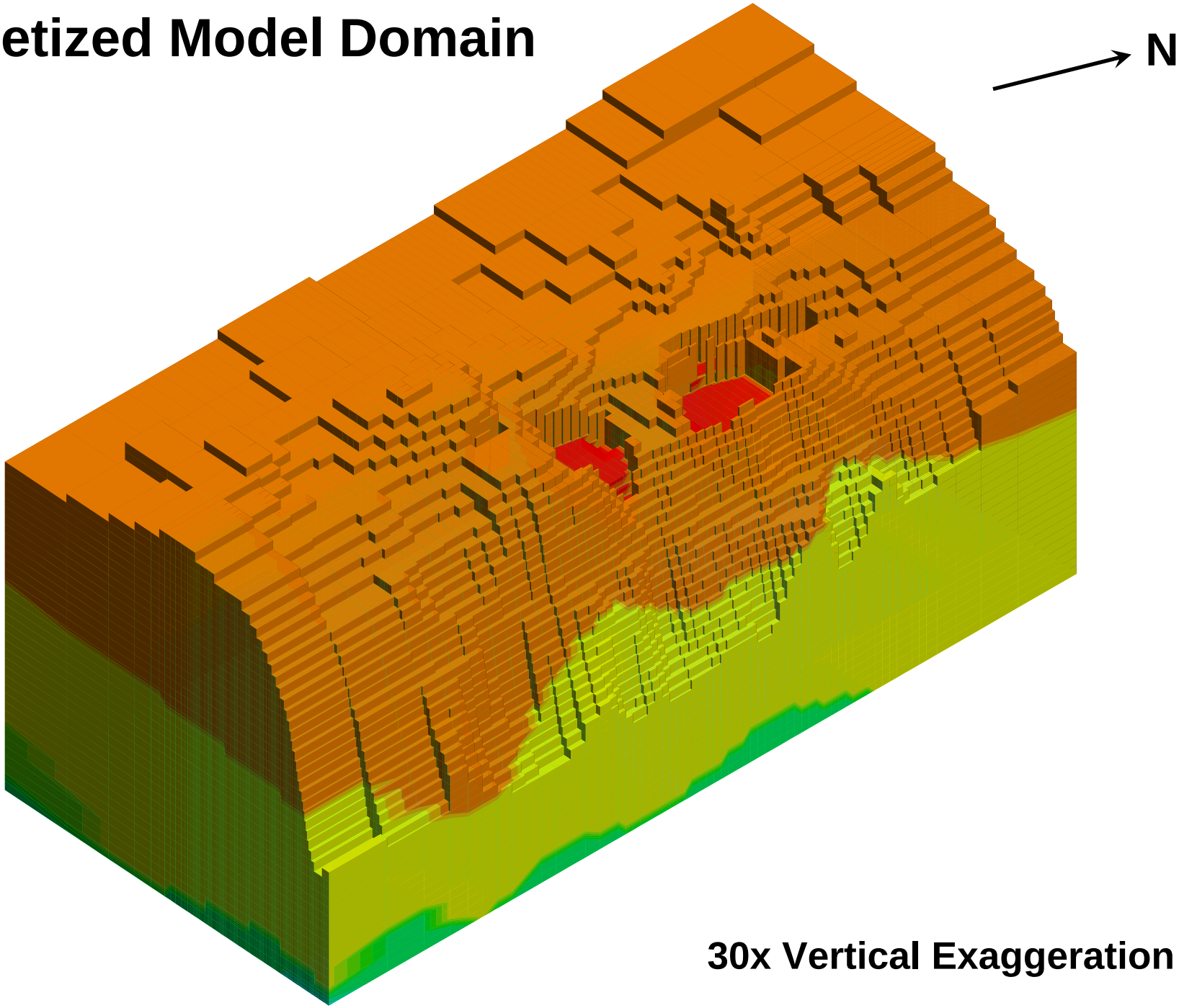
SAC Liquid Discharges (History 5, Median)



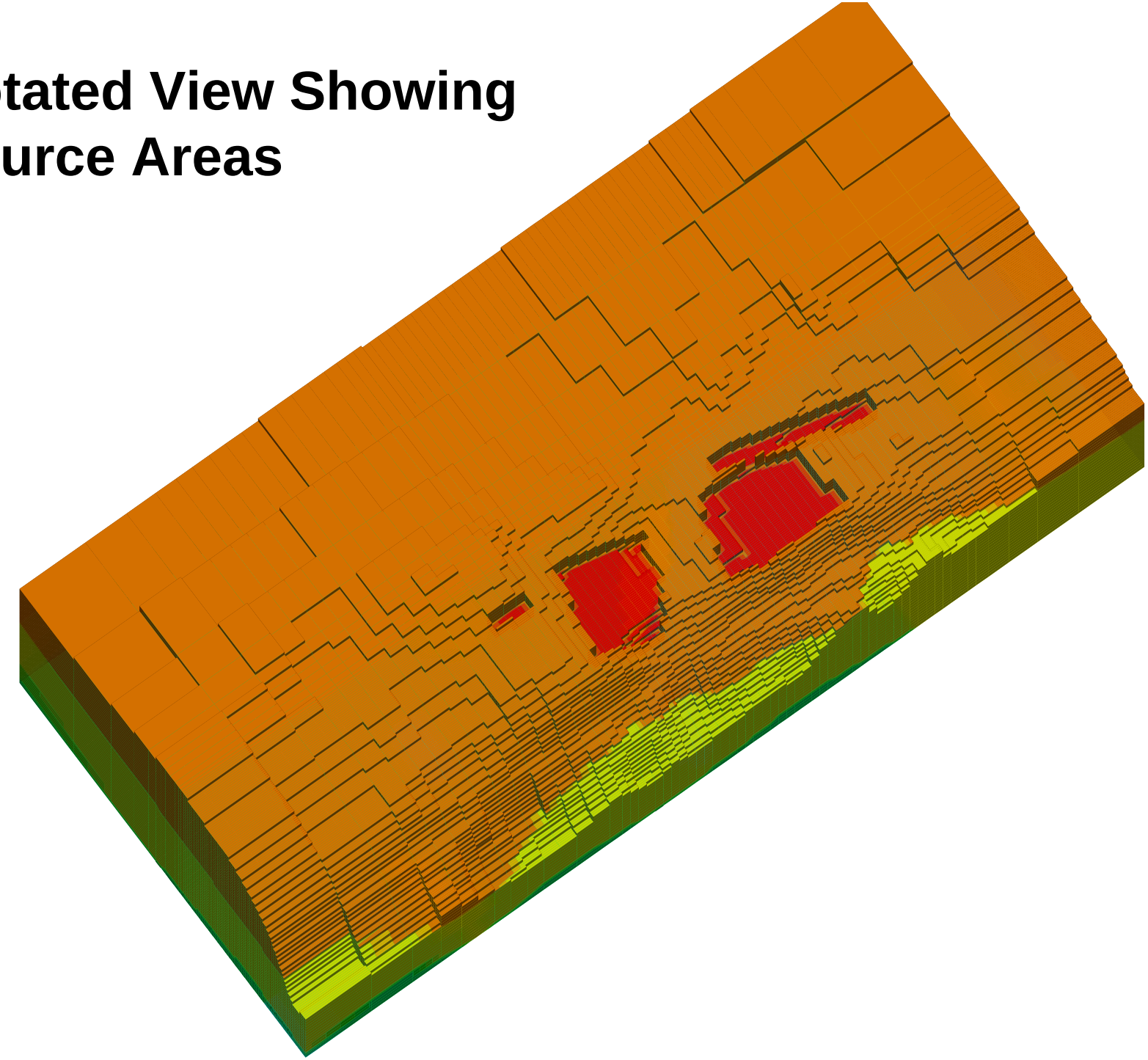
SAC Uranium Loading (History 5, Median)



Discretized Model Domain

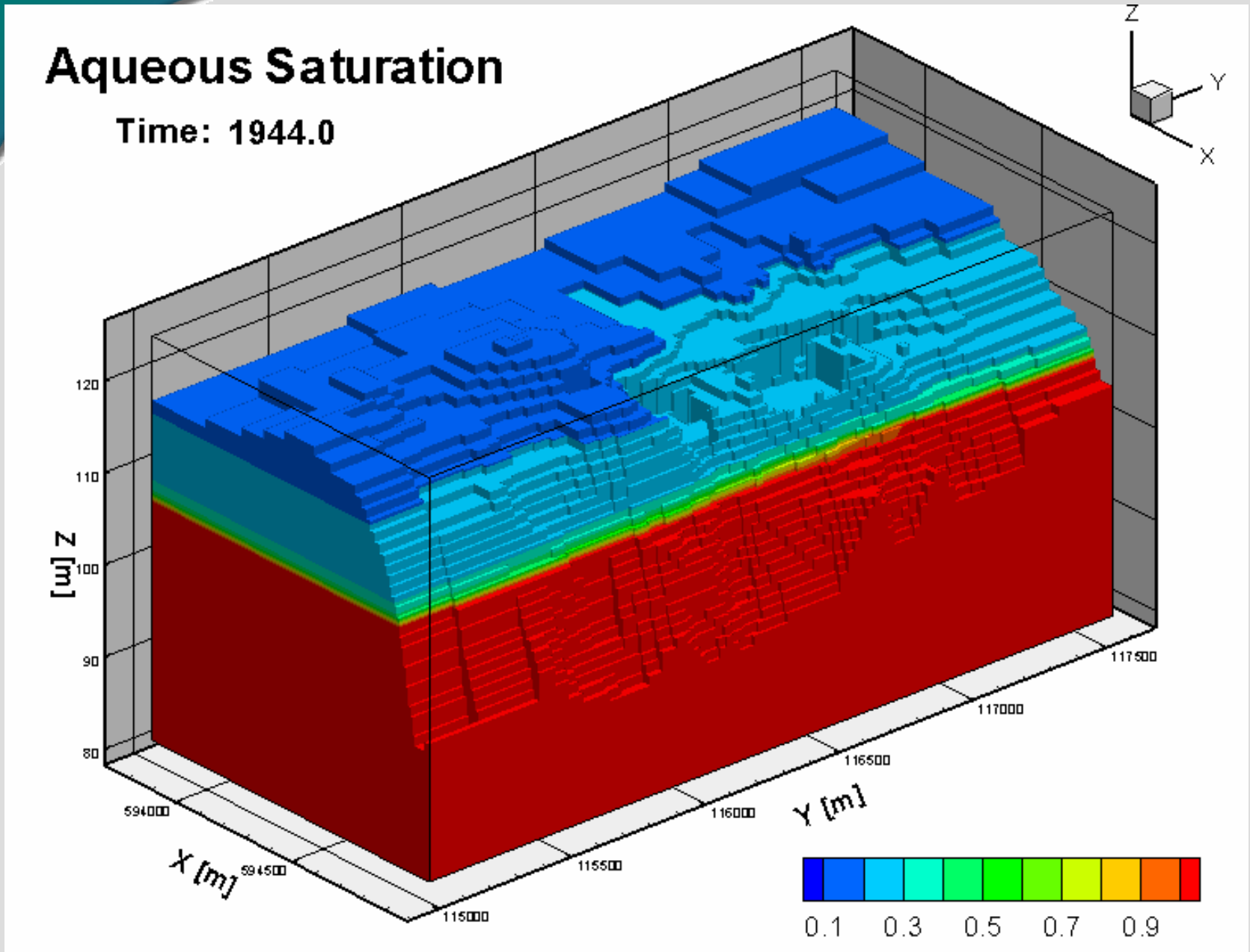


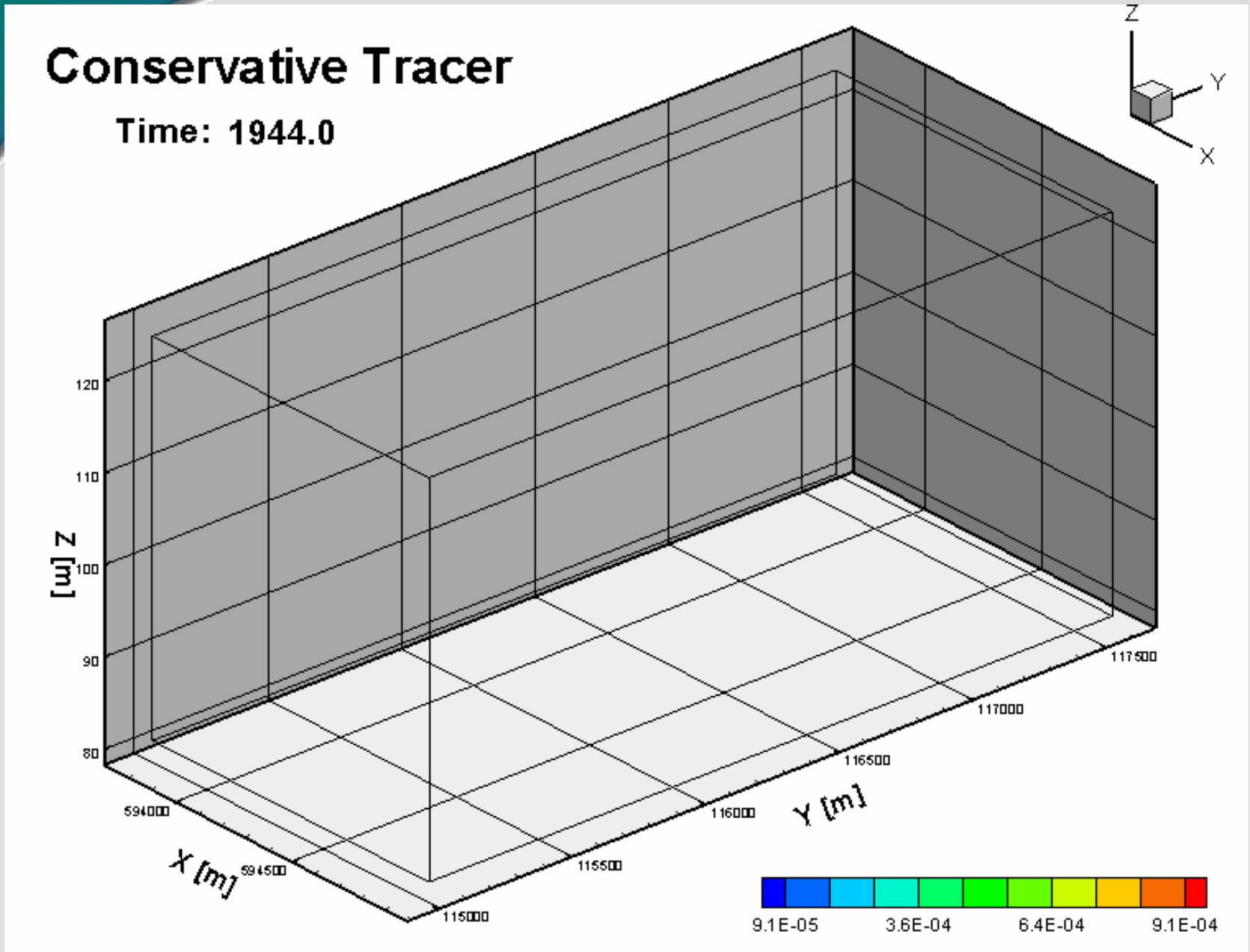
Rotated View Showing Source Areas

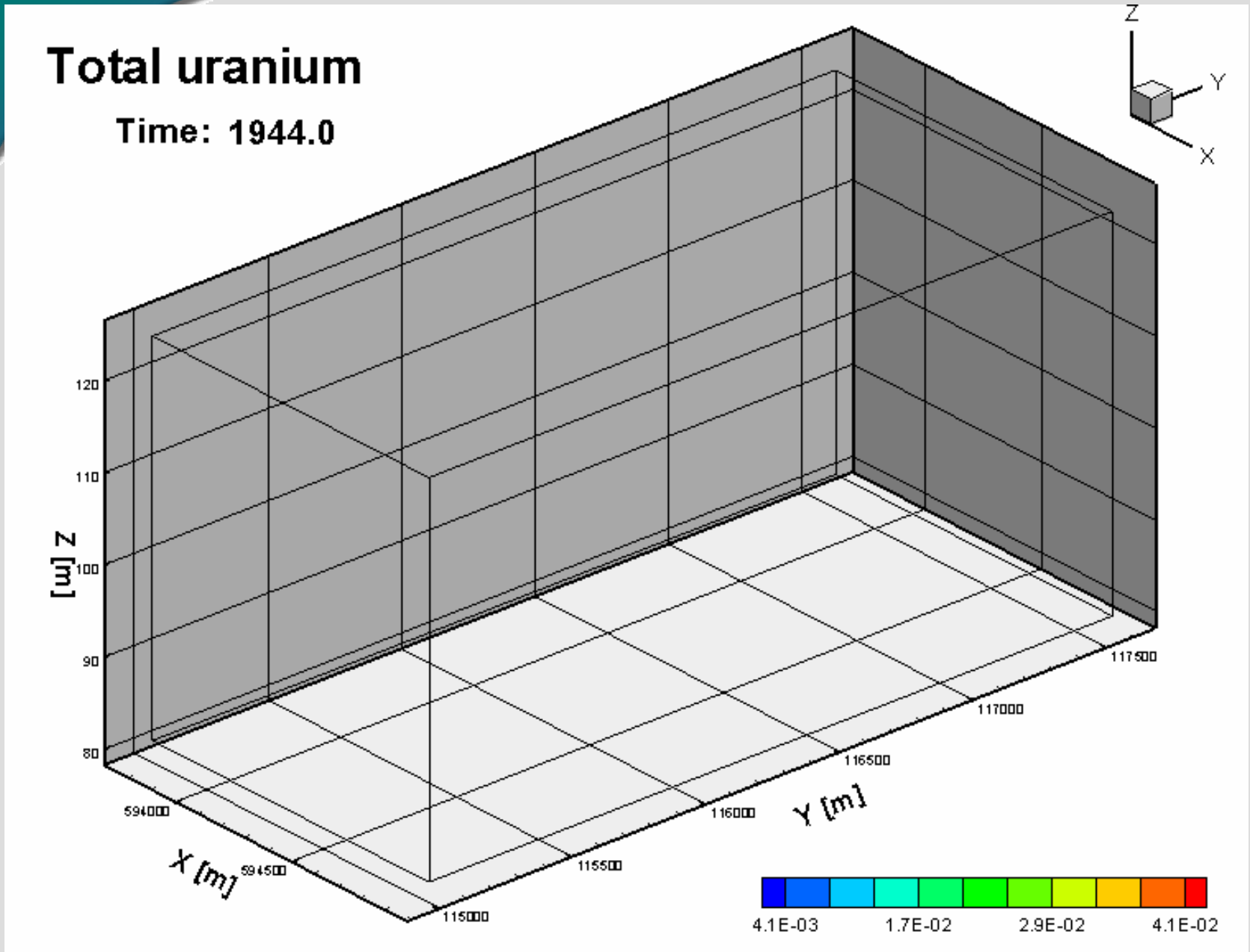


Animations

- 1944 – 1950
  - Aqueous saturation
  - Conservative tracer
  - Total uranium


Aqueous Saturation
Time: 1944.0
Z
Y
X
120
110
100
90
80
Z [m]
594000
594500
X [m]
115000
115500
116000
116500
117000
117500
Y [m]
0.1
0.3
0.5
0.7
0.9


Conservative Tracer
Time: 1944.0
Z
Y
X
120
110
100
90
80
Z [m]
594000
594500
X [m]
115000
115500
116000
116500
117000
117500
Y [m]
9.1E-05
3.6E-04
6.4E-04
9.1E-04


Total uranium
Time: 1944.0
Z
Y
X
120
110
100
90
80
Z [m]
594000
594500
X [m]
115000
115500
116000
116500
117000
117500
Y [m]
4.1E-03
1.7E-02
2.9E-02
4.1E-02

Ongoing and Future Work

- Incorporate physical and hydraulic property data and well log information into parameterization
  - Geostatistics, conditional simulation, upscaling
- Add parsimonious sub-model for uranium transport (kinetic reactions)
- Develop alternative conceptual models
- Inverse modeling and uncertainty analysis

Additional Information

- NRC Report
  - PD Meyer, M Ye, SP Neuman, and KJ Cantrell, **Combined Estimation of Hydrogeologic Conceptual Model and Parameter Uncertainty,** NUREG/CR-6843, U.S. Nuclear Regulatory Commission. **http://www.nrc.gov/reading-rm/doc-collections/nuregs/contract/cr6843/cr6843.pdf**
- Forthcoming Paper
  - M Ye, SP Neuman, and PD Meyer, **Maximum Likelihood Bayesian Averaging of Spatial Variability Models in Unsaturated Fractured Tuff,** Water Resources Research