

# Advanced Simulation Capability for Environmental Management (ASCEM) Overview and Example Application

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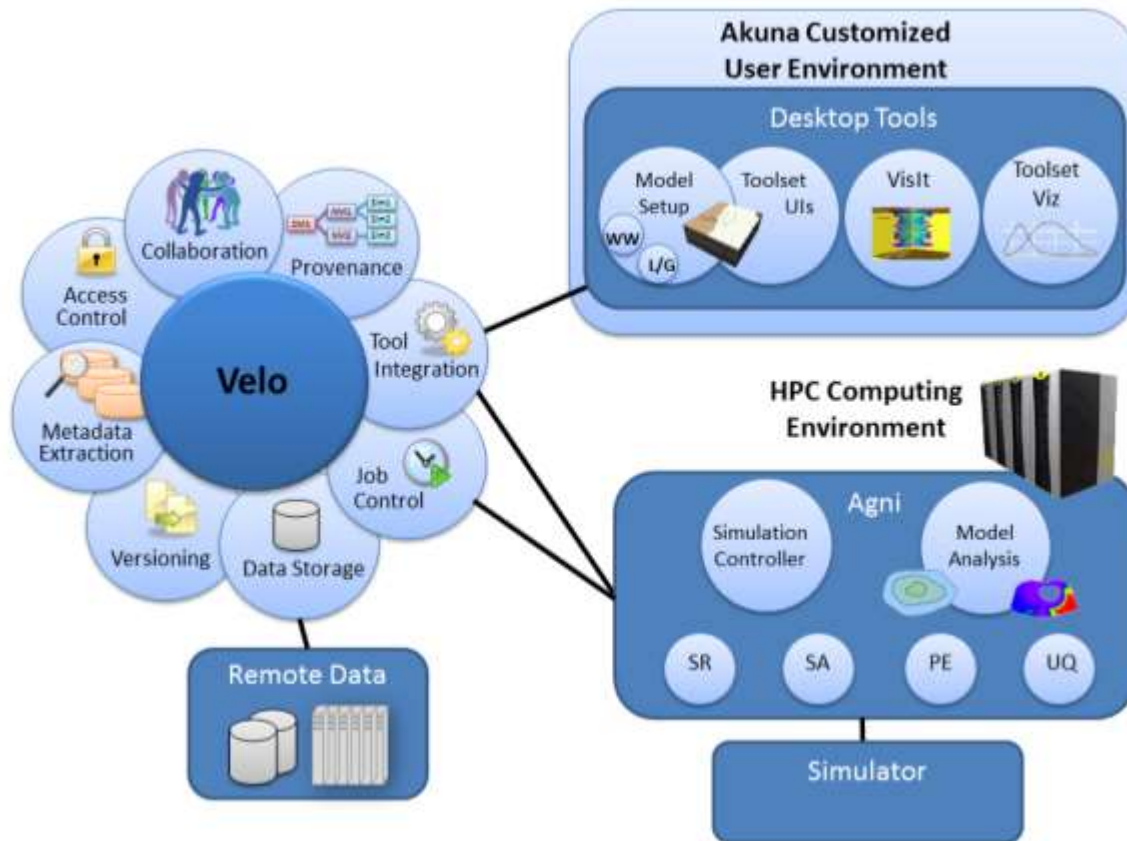
<sup>1</sup>Pacific Northwest National Laboratory

<sup>2</sup>Los Alamos National Laboratory

<sup>3</sup>U.S. Department of Energy, Office of Environmental Management

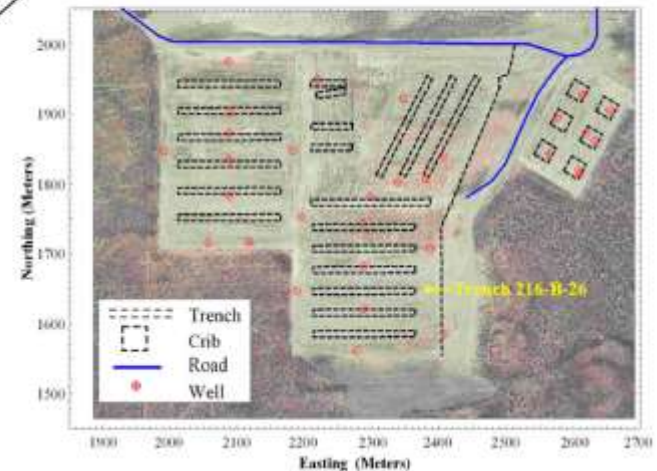
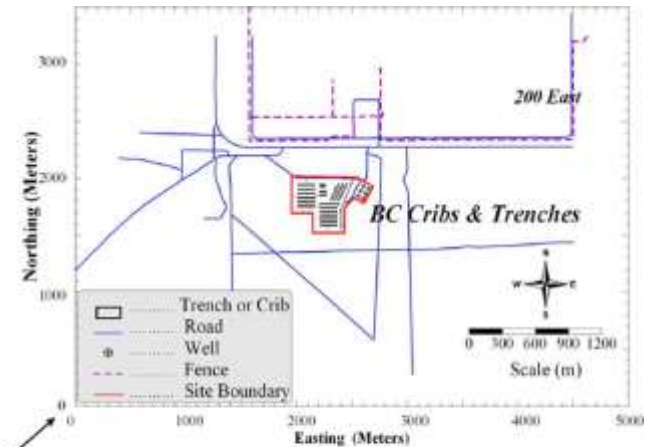
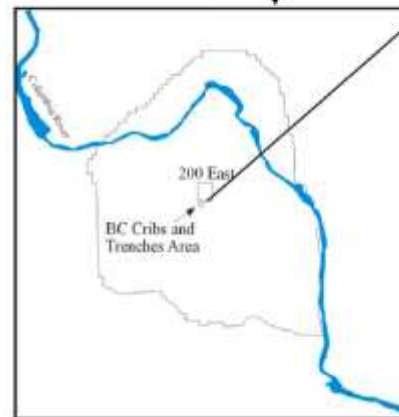


# User Environment



# Application to Hanford BC Cribs

- Former plutonium production site
  - Waste disposed from 1956 to 1958 to 6 cribs
  - Funnel-shaped with sloping sides (~3 x 3 m wide)
- Located a few meters bgs
- Thick vadose zone (~107 m)
- Primary contaminant of concern  $^{99}\text{Tc}$
- Traditional remediation technologies are ineffective
- Evaluate uncertainty impact on remediation



(Rucker and Fink 2007)

# Problem Description

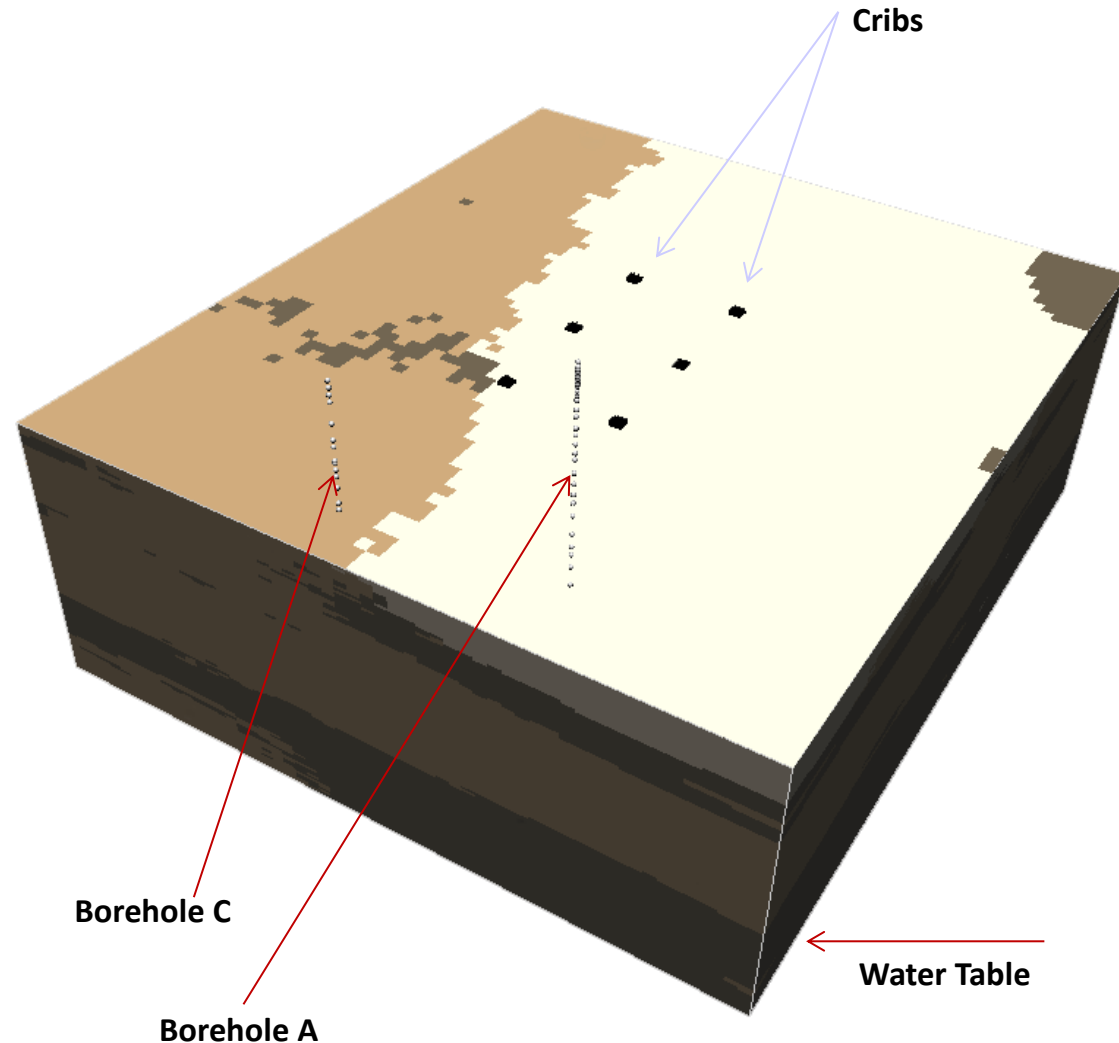
## ➤ Boundary Conditions

- > 10 million gallons liquid waste released at 6 cribs
  - 1956 – 1958
  - $^{99}\text{Tc}$  primary contaminant
  - Source concentrations  $\sim 10^6$  pCi/L
- Recharge at surface
- Water table boundary at the bottom of the domain

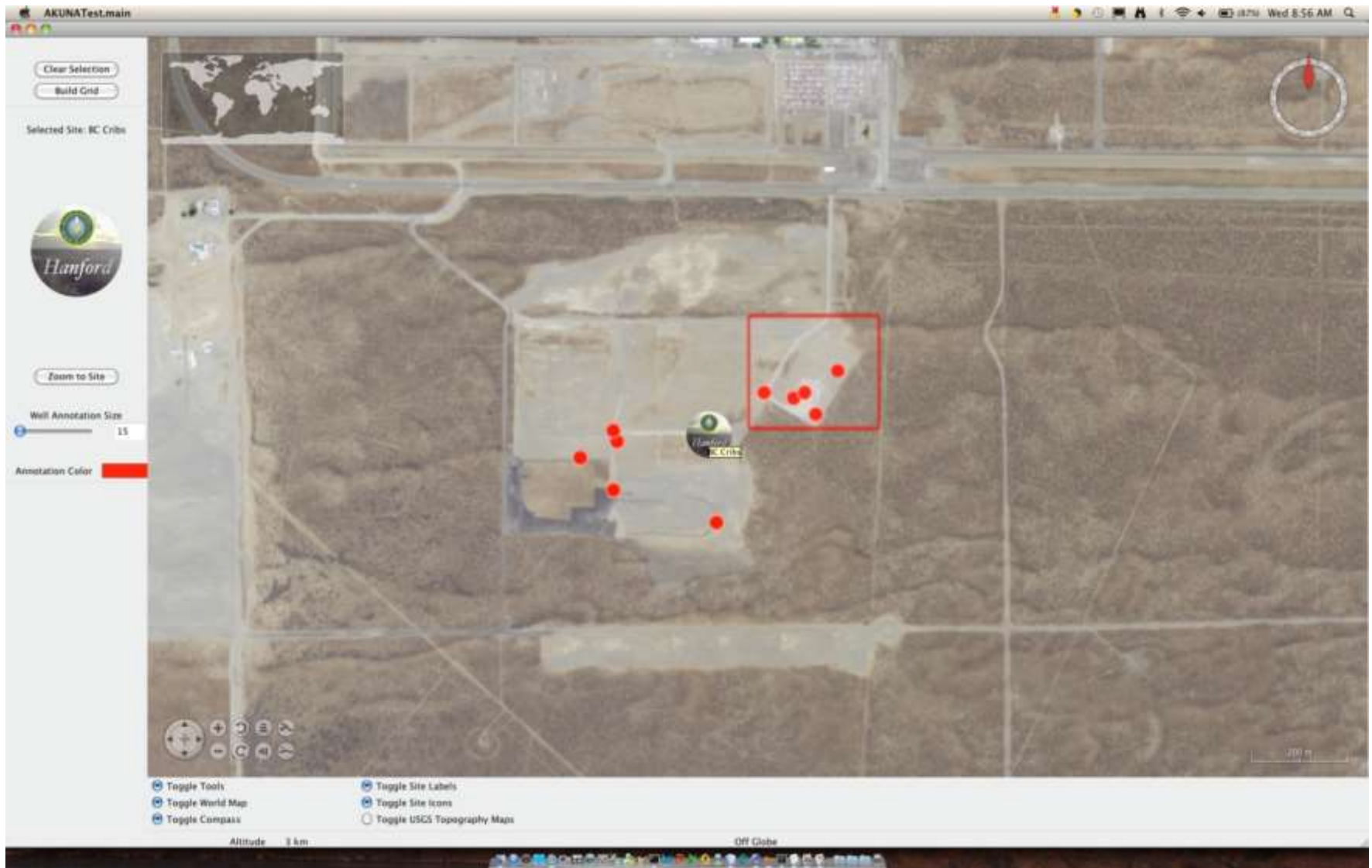
## ➤ 320 m x 280 m x 107 m (~455K grid blocks)

## ➤ Executed simulation from 0 – 2008

- 0 – 1956 period to attain steady state flow field
- 1956 – 2008 transient

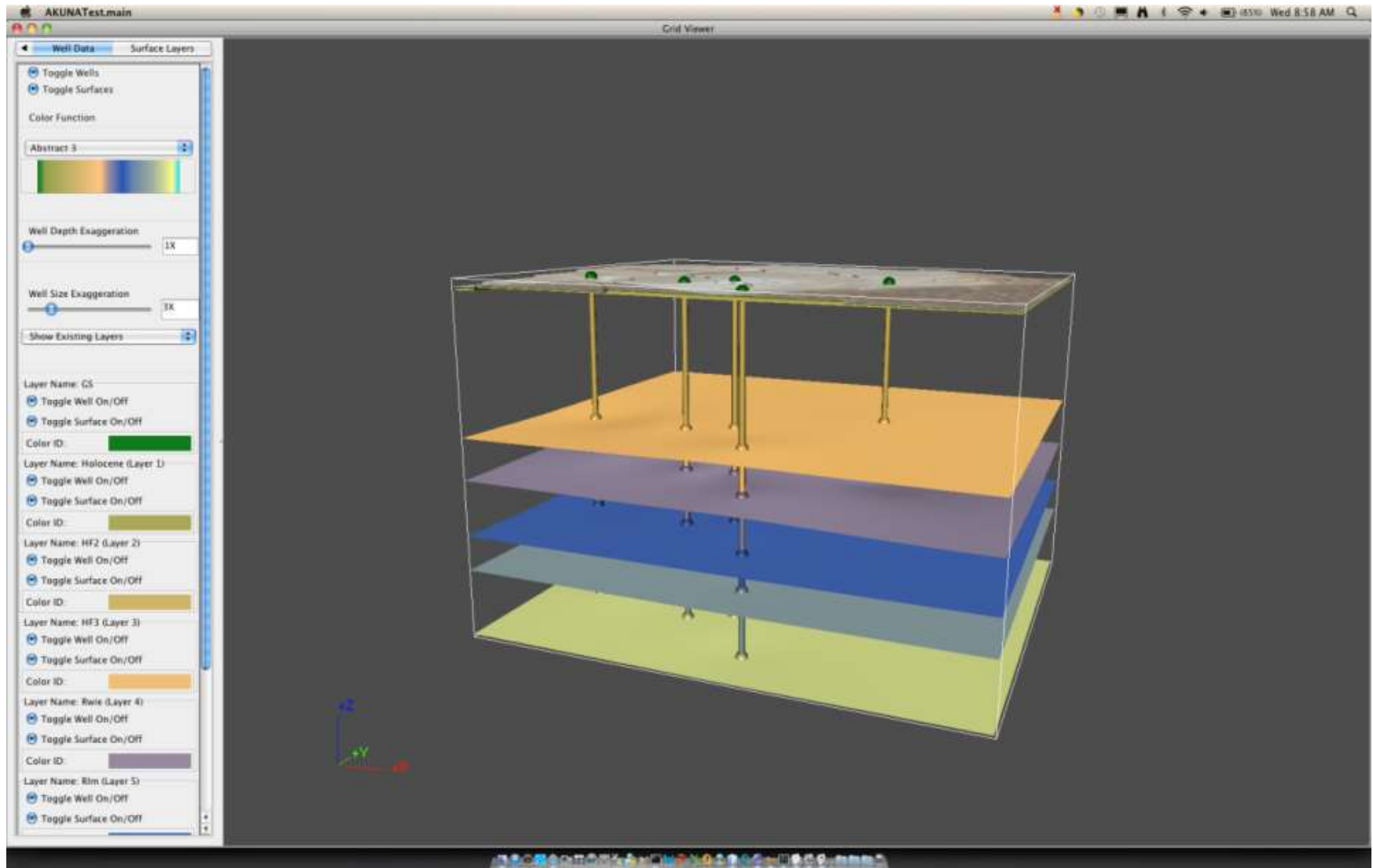


# Model Setup



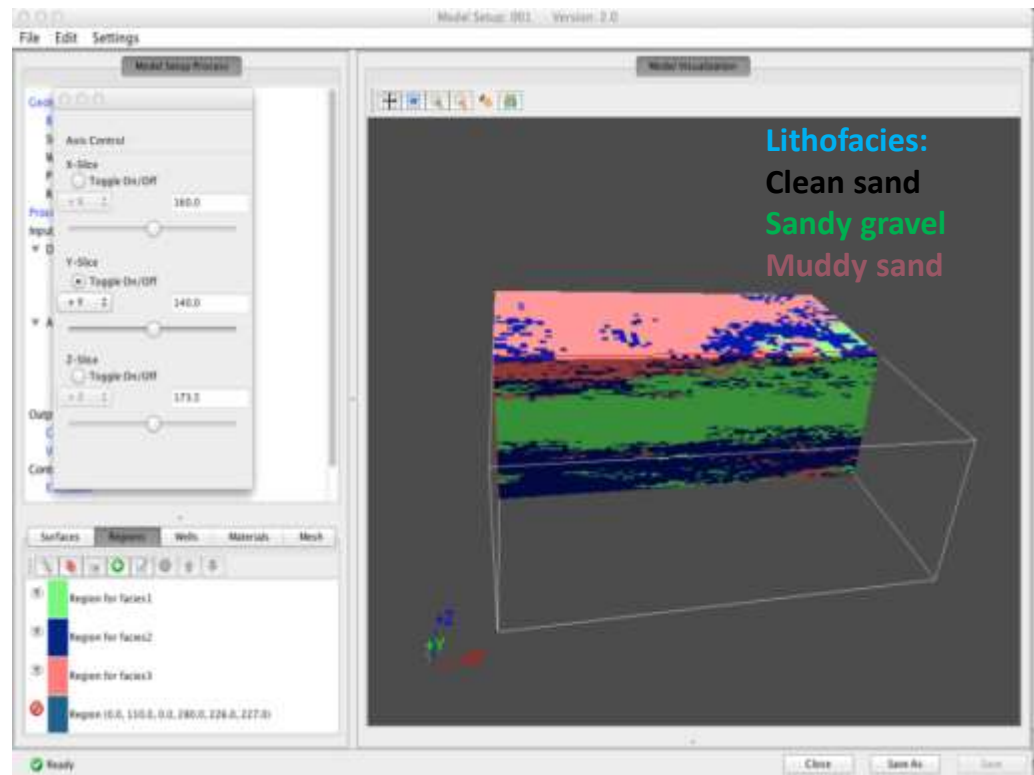


# Major Stratigraphy



# Incorporation of Heterogeneity

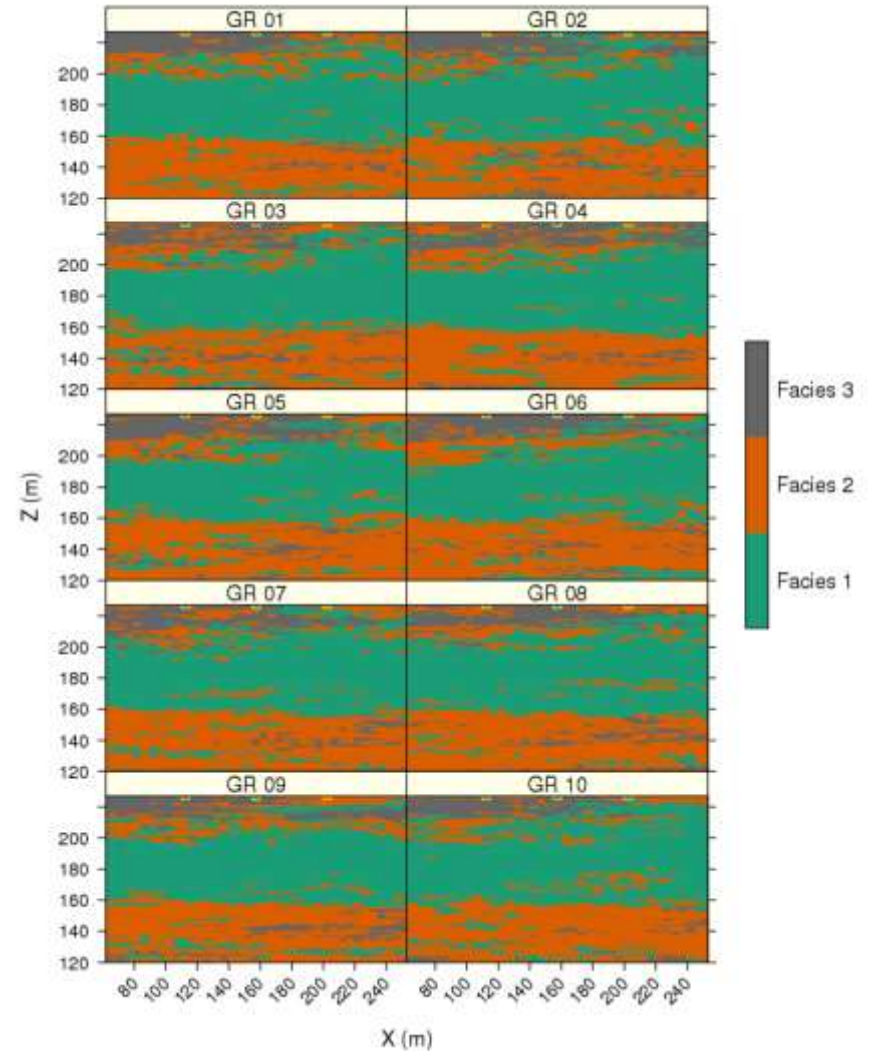
- Generated 100 realizations of three-dimensional lithofacies distributions using geostatistical model
  - Identified by k-means cluster analysis of  $^{232}\text{Th}$  and  $^{40}\text{K}$  data (spectral gamma log data)
  - Three lithofacies identified, log data from 5 wells





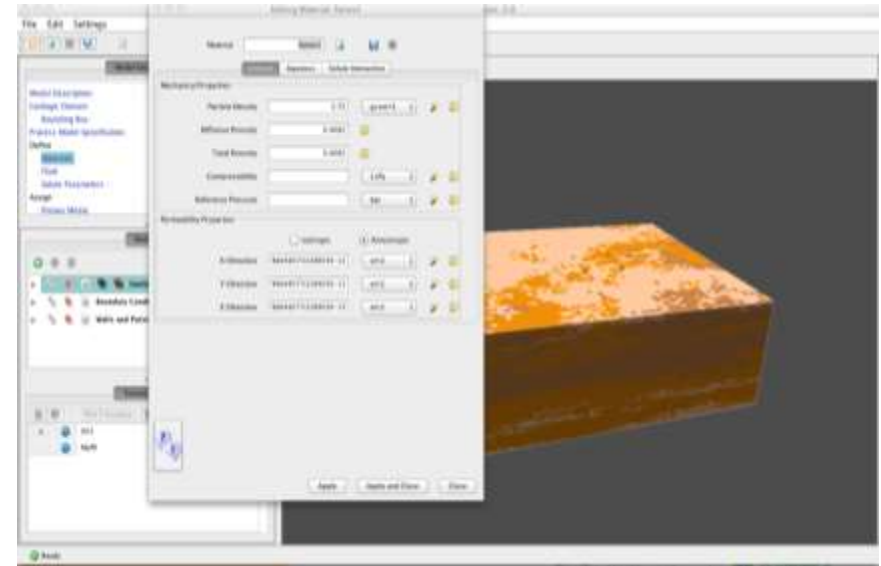
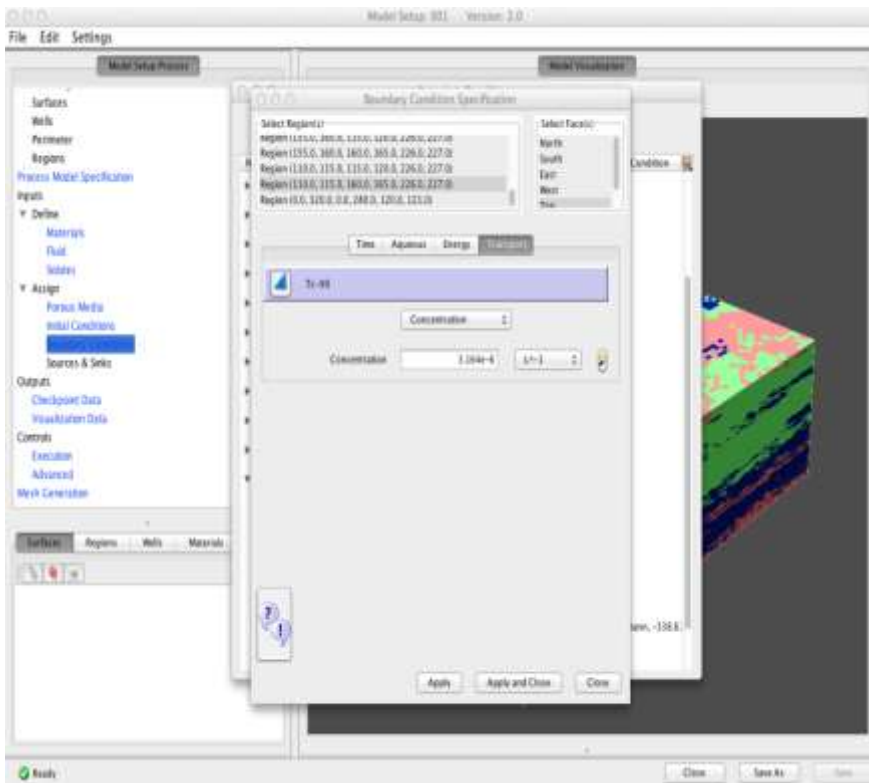
# Geologic Realizations

- Selected 10 realizations for demonstration
- Layering is the same, but small-scale variability in heterogeneities captured



# Property Assignments and Boundary Conditions

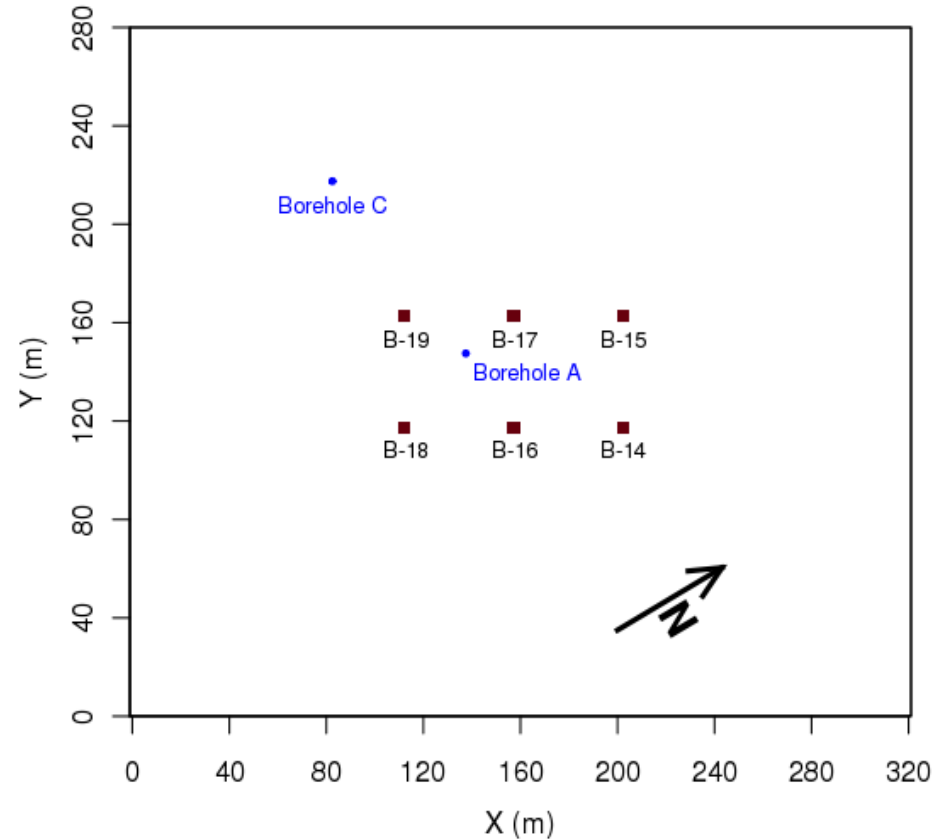
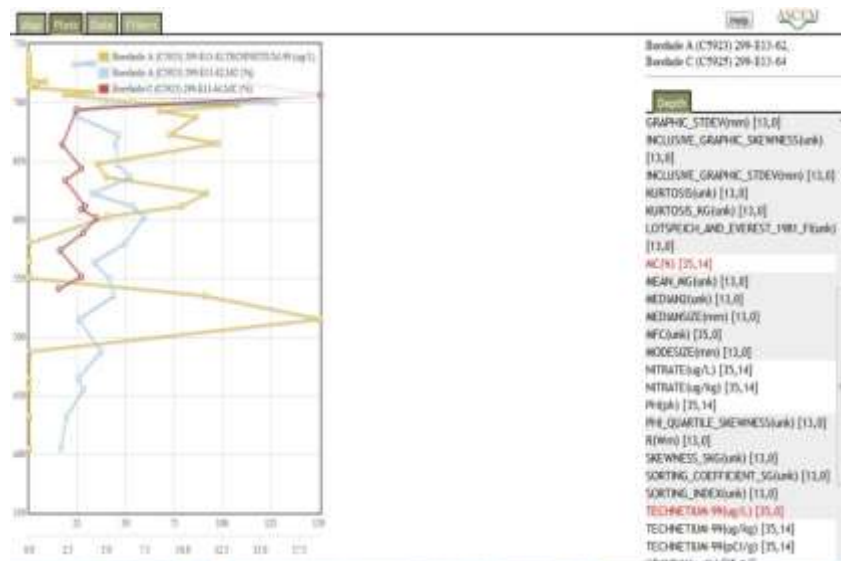
Hydraulic Property  
Input



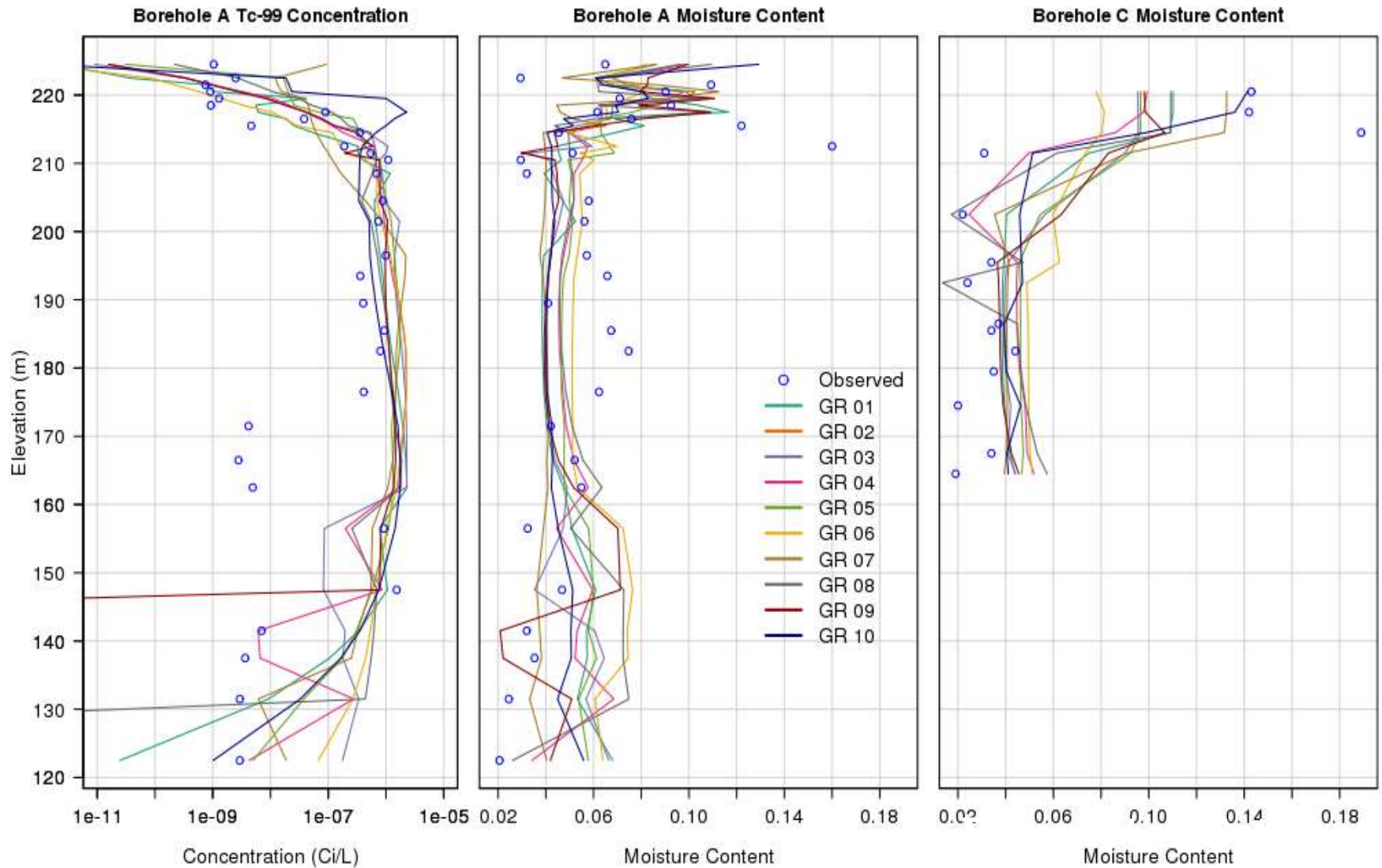
Boundary Condition  
Input

# Parameter Estimation

- Permeability and porosity estimation
- Moisture content and  $^{99}\text{Tc}$  measured in 2008 at Boreholes A & C
- Data obtained from database, accessed through web interface, and exported to Akuna



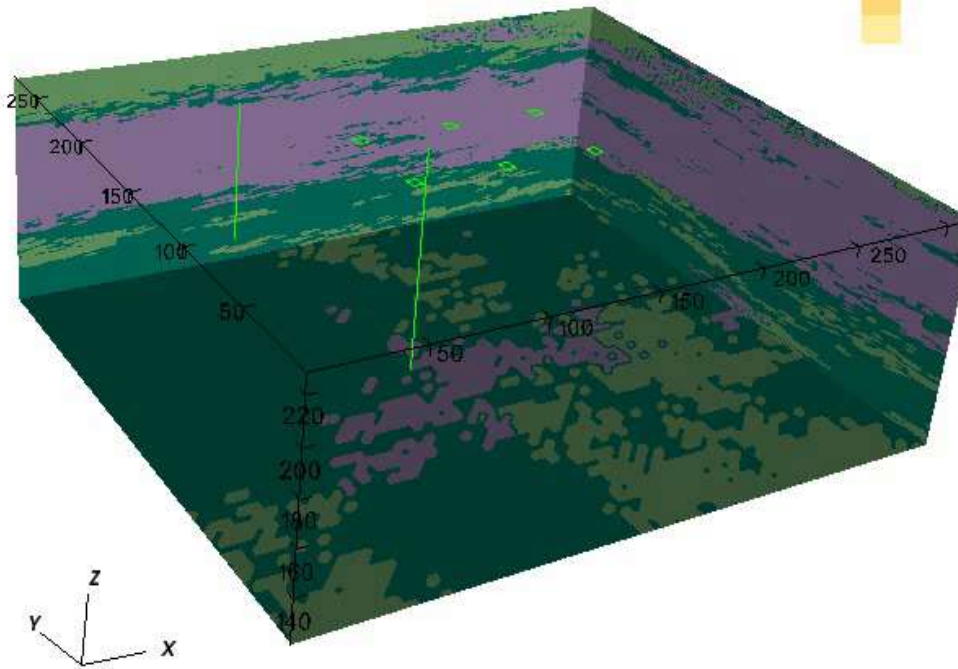
# Parameter Estimation



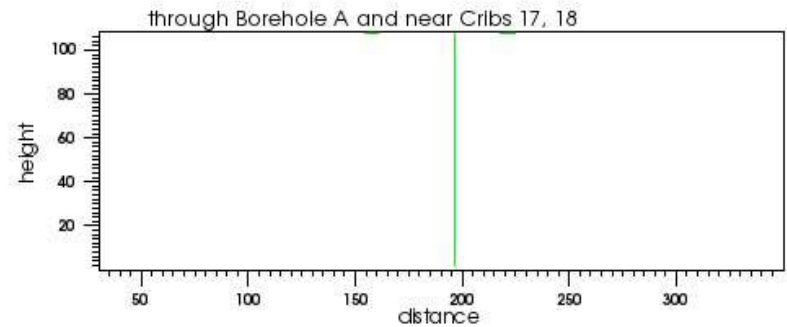
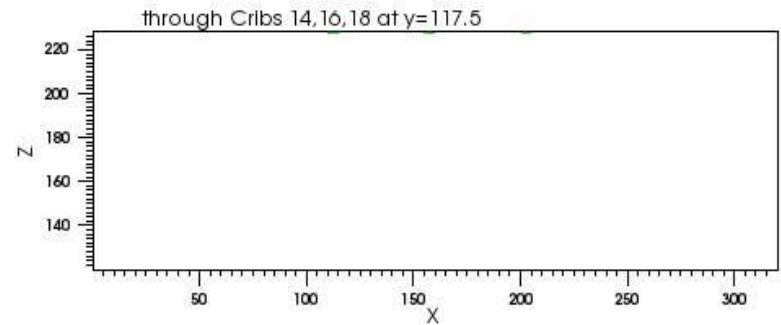
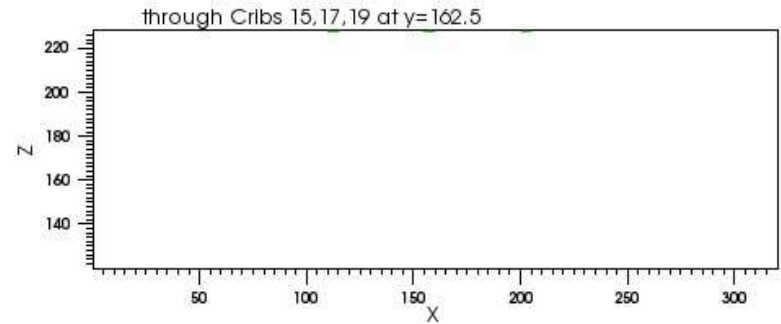
# Simulation 1956 – 2008

Tc-99 (pCi/L)

Facies 1   Facies 2   Facies 3

A horizontal bar legend with three colored segments: purple for Facies 1, teal for Facies 2, and light green for Facies 3.

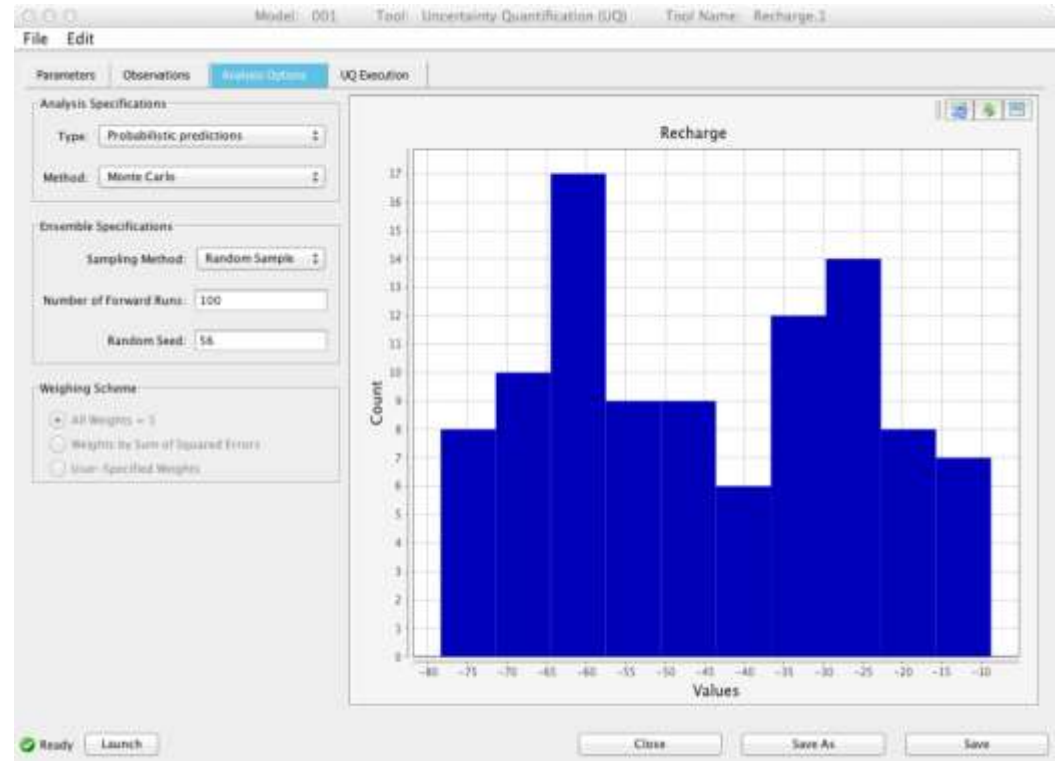
Year = 1956





# Uncertainty Quantification

- Varied recharge rate for 100 simulations for 2012 – 3000
  - Rates represent management actions (1 – 75 mm/yr)
    - Soil desiccation
    - Surface barriers
    - No-action
    - Soil flushing
- Metrics
  - Peak concentration and arrival time at water table
  - Time at which a threshold concentration is exceeded
- Launched on 9600 processor cores, 96 per simulation



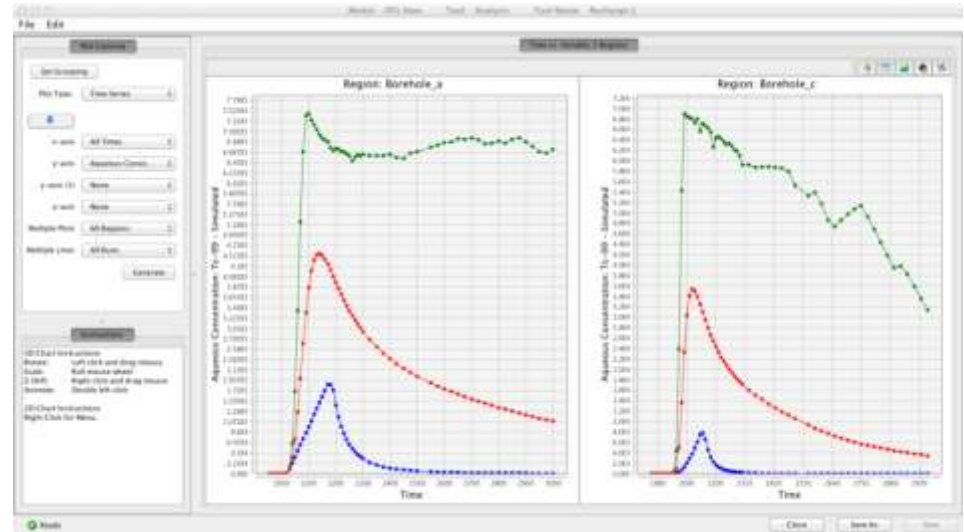
Screenshot from UQ Toolset:  
Histogram of Recharge Rates



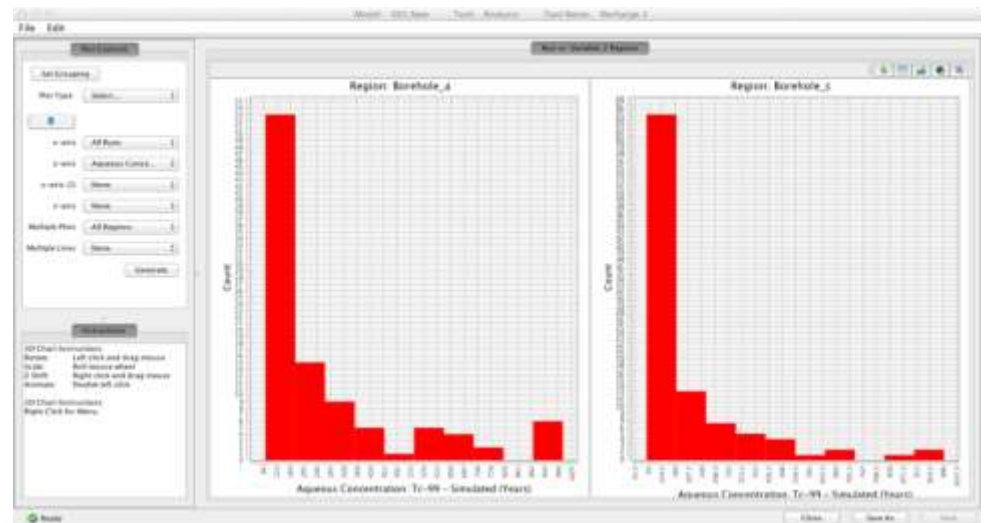
# Uncertainty Quantification

- Time to peak occurs within 200 years, small variation with recharge rate
  - a) Mean and 95% confidence intervals for  $^{99}\text{Tc}$  breakthrough at boreholes A and C
  - b) Histogram of time to reach peak concentration

a)

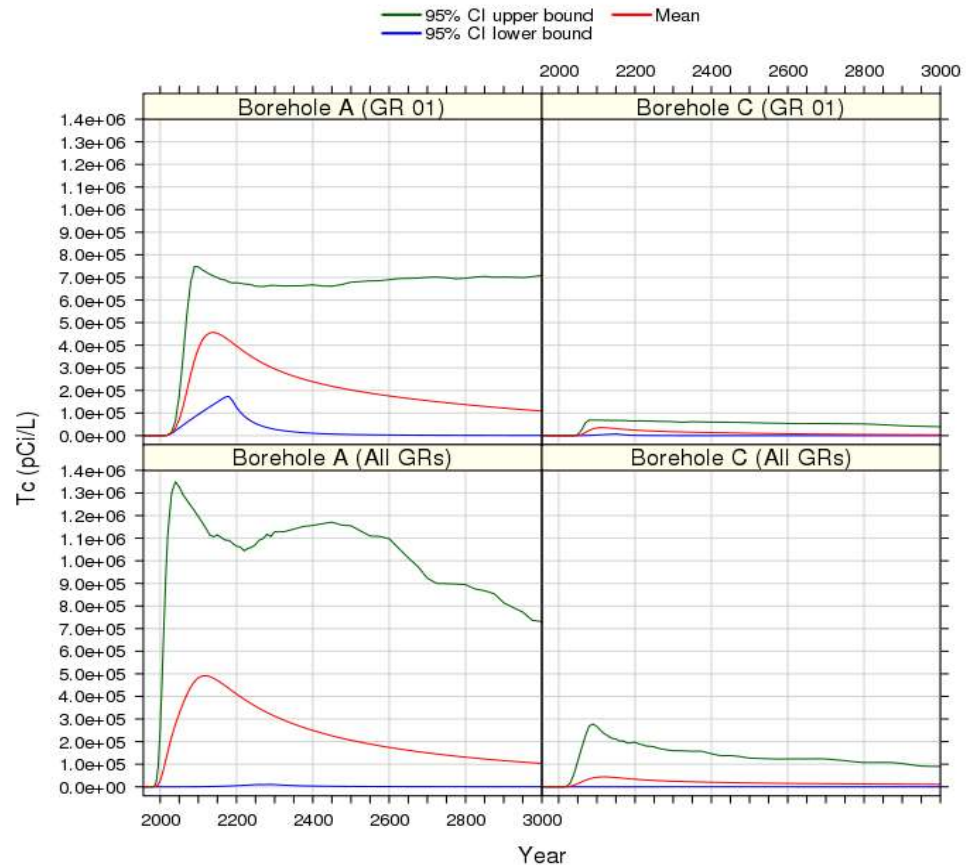


b)



# Uncertainty Quantification

- Compare breakthrough curves for one conceptual model realization to all 10
  - Confidence intervals are wider when 10 realizations of the conceptual model are considered
  - Upper bound is ~85% higher at Borehole A for all ten models than for GR01



Mean and 95% confidence intervals for the  $^{99}\text{Tc}$  breakthrough curve at Boreholes A and C for single and multiple geologic realizations

# Conclusions

- ASCEM facilitates model setup, execution, analysis, and visualization
- High performance computing enables multiple realizations of complex model through reduction in computational time
- Simulations of BC Cribs provides insight on controlling processes and properties for  $^{99}\text{Tc}$  transport in the subsurface
  - Baseline conditions for “no action” alternative
  - Variation in recharge rate from soil desiccation and surface barriers
  - Variability in conceptual models impacted the magnitude of peak concentrations, but had minor impact on arrival times

# Thank You!



The screenshot shows the ASCEM website interface. At the top, there is a navigation menu with links for HOME, ABOUT, THRUST AREAS, CONTACTS, and RESOURCES. Below the menu is a large 3D visualization of a waste site simulation, showing various components like Landfill, In-Situ D&D, Liquid Waste Tank, Disposal Trench, Ruined, and Deep Flush to Receptor. The simulation is labeled 'Engineering Status Degradation (ASCEM)' and 'ASCEM'. Below the simulation, there is a section titled 'THRUST AREAS' which lists three areas: Platform and Integrated Toolsets, Multi-Process HPC Simulator, and Site Application. Each area has a brief description of its role in the ASCEM framework.

**ASCEM**  
U.S. DEPARTMENT OF ENERGY  
HOME ABOUT THRUST AREAS CONTACTS RESOURCES

**ASCEM**  
Advanced Simulation Capabilities for Environmental Management (ASCEM) is a software project that aims at developing next-generation, science-based reactive flow and transport simulation capabilities and supporting modeling toolsets within a high-performance computing framework to address DOE-EM's waste storage and environmental cleanup challenges.

**THRUST AREAS**  
ASCEM is an integrated simulation framework developed along three Thrust Areas:

1. Platform and Integrated Toolsets: Provides the user with toolsets for model development and analysis, visualization, and management of data and simulation results.
2. Multi-Process HPC Simulator: Provides the user with state-of-the-art

**PLATFORM**  
The Platform consists of a set of tools integrated into a consistent user interface that supports a flexible modeling workflow. It includes tools for data management, visualization, model

**HPC SIMULATOR**  
The Multi-Process HPC Simulator, named Amanzi, is a flexible and extensible open-source simulator for coupled flow and reactive transport in geologic media and engineered system components.

**APPLICATION**  
Site Application experts ensure that the HPC simulator and Platform toolsets incorporate the capabilities needed to support DOE-EM's remediation and closure decisions.

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<http://ascemdoe.org/>