

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

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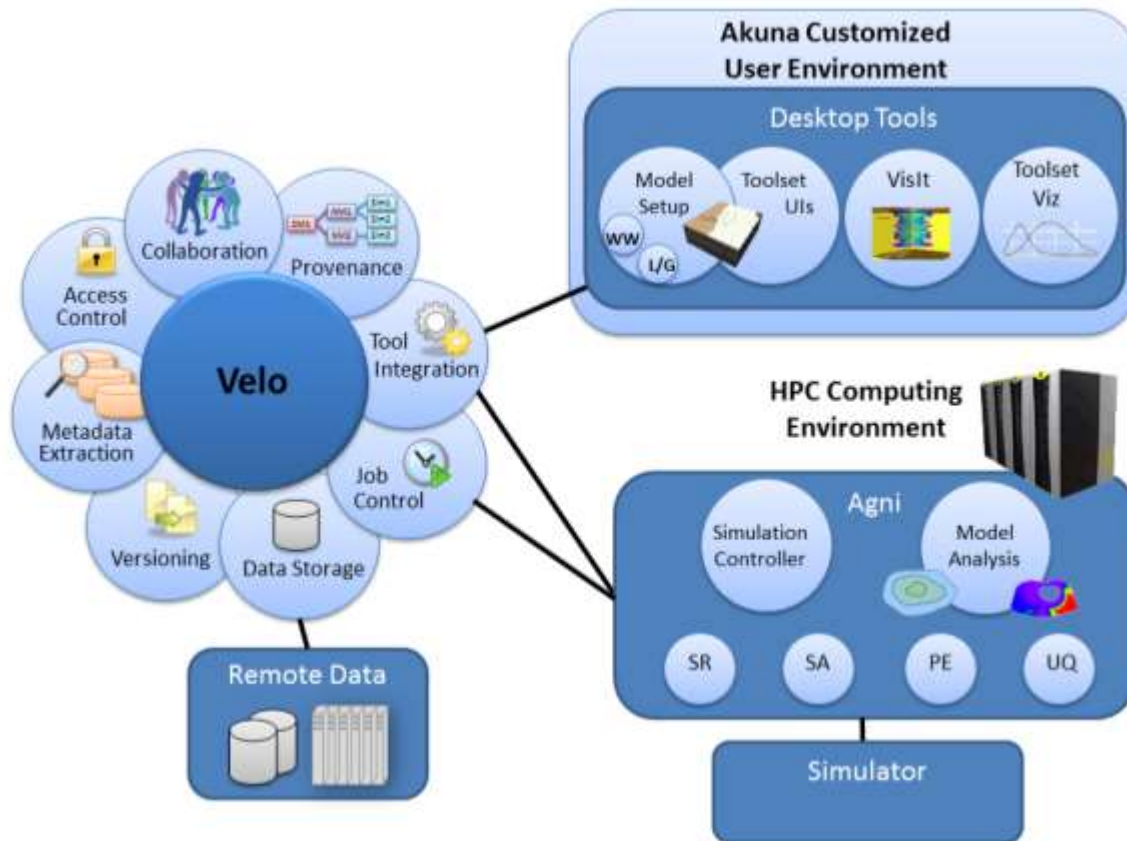
³U.S. Department of Energy, Office of Environmental Management

What is ASCEM?

- Advanced Simulation Capability for Environmental Management
 - Modeling toolset currently under development for understanding and predicting subsurface contaminant fate and transport
- Organized into three thrust areas
 - High Performance Computing – open-source, high performance simulator (Amanzi)
 - Platform – tools that facilitate model setup and simulation execution (Akuna)
 - Applications – demonstrate the tools through applications to real sites
- Completed initial user release of toolset

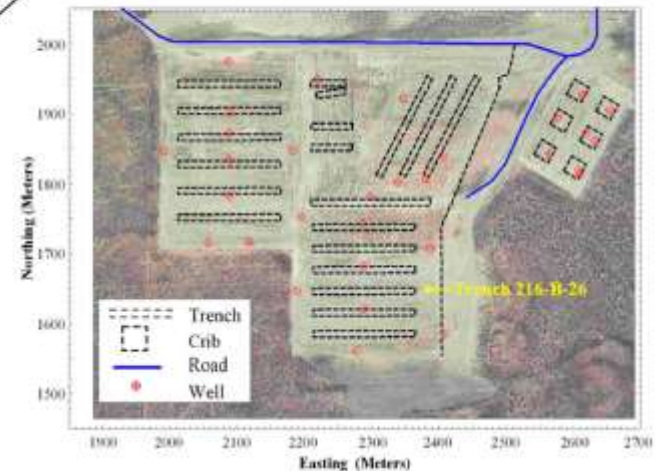
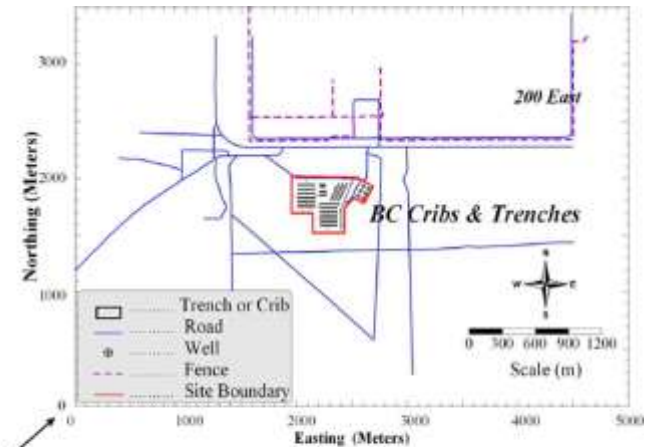
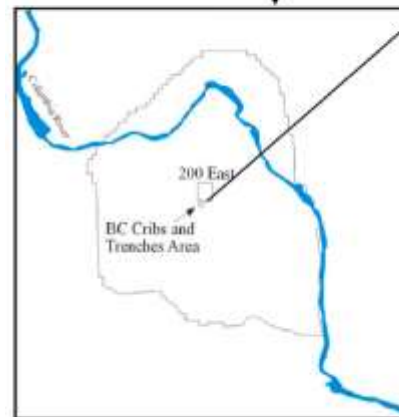


User Environment



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}Tc
- Traditional remediation technologies are ineffective
- Evaluate uncertainty impact on remediation



(Rucker and Fink 2007)

Problem Description

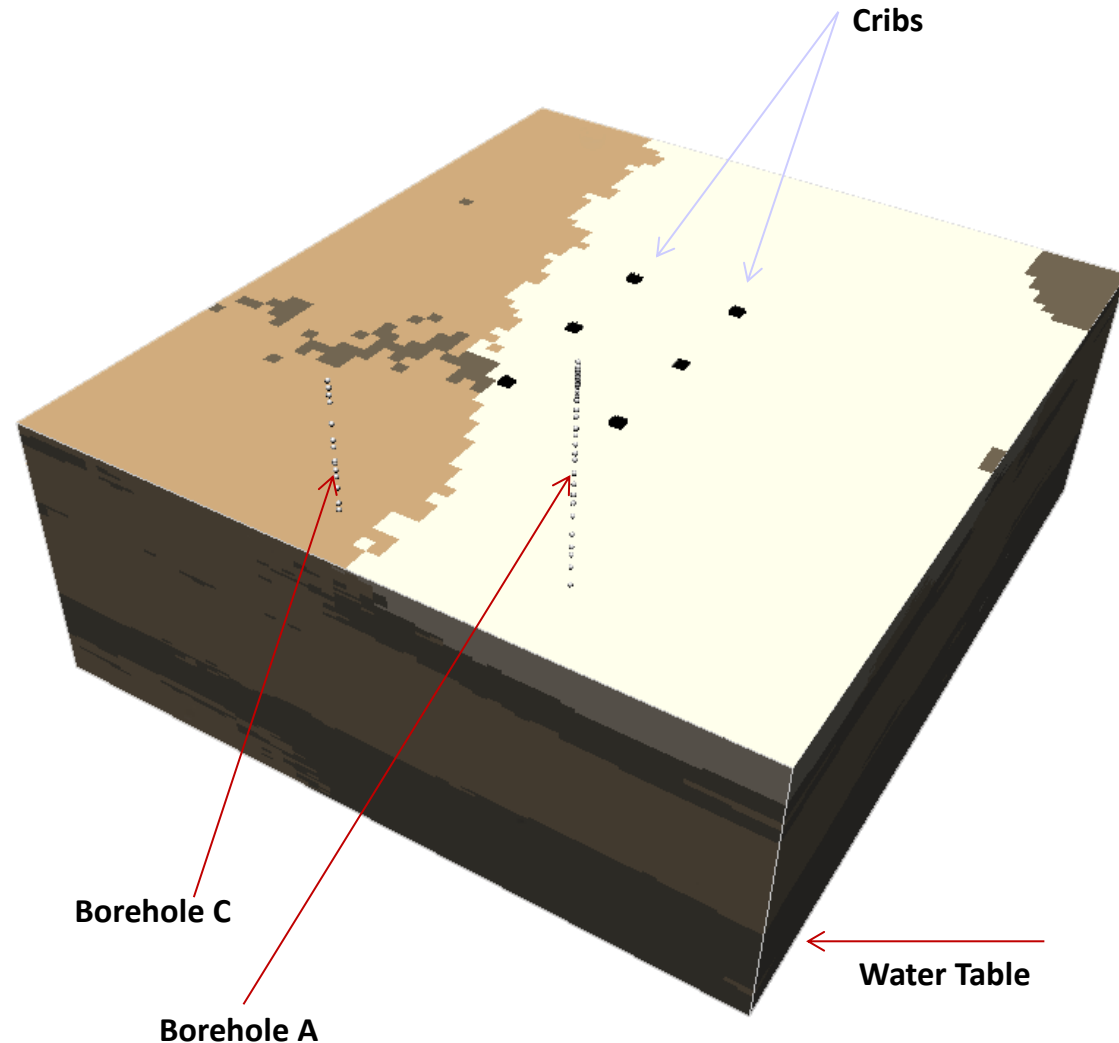
➤ Boundary Conditions

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

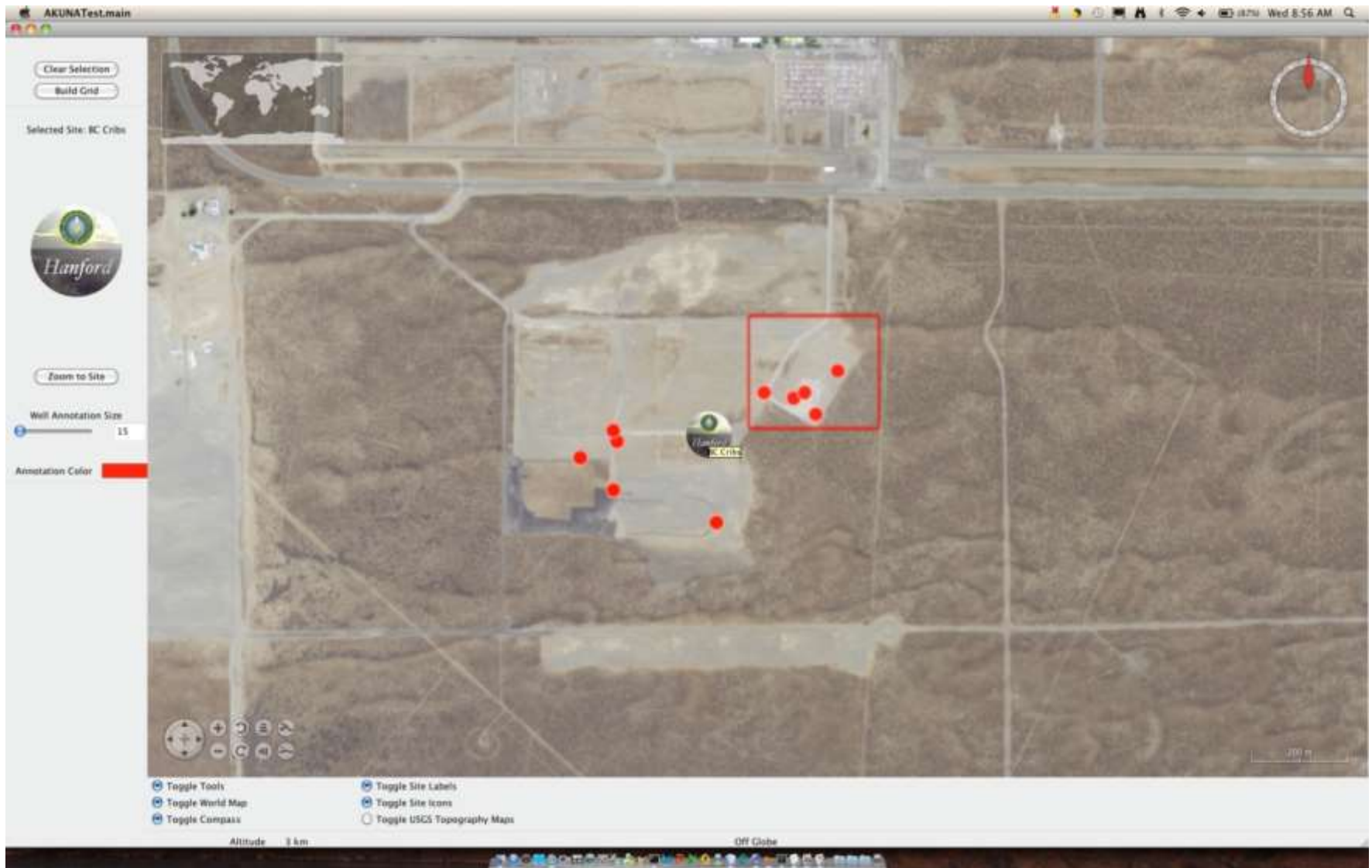
➤ 320 m x 280 m x 107 m (~455K grid blocks)

➤ Executed simulation from 0 – 2008

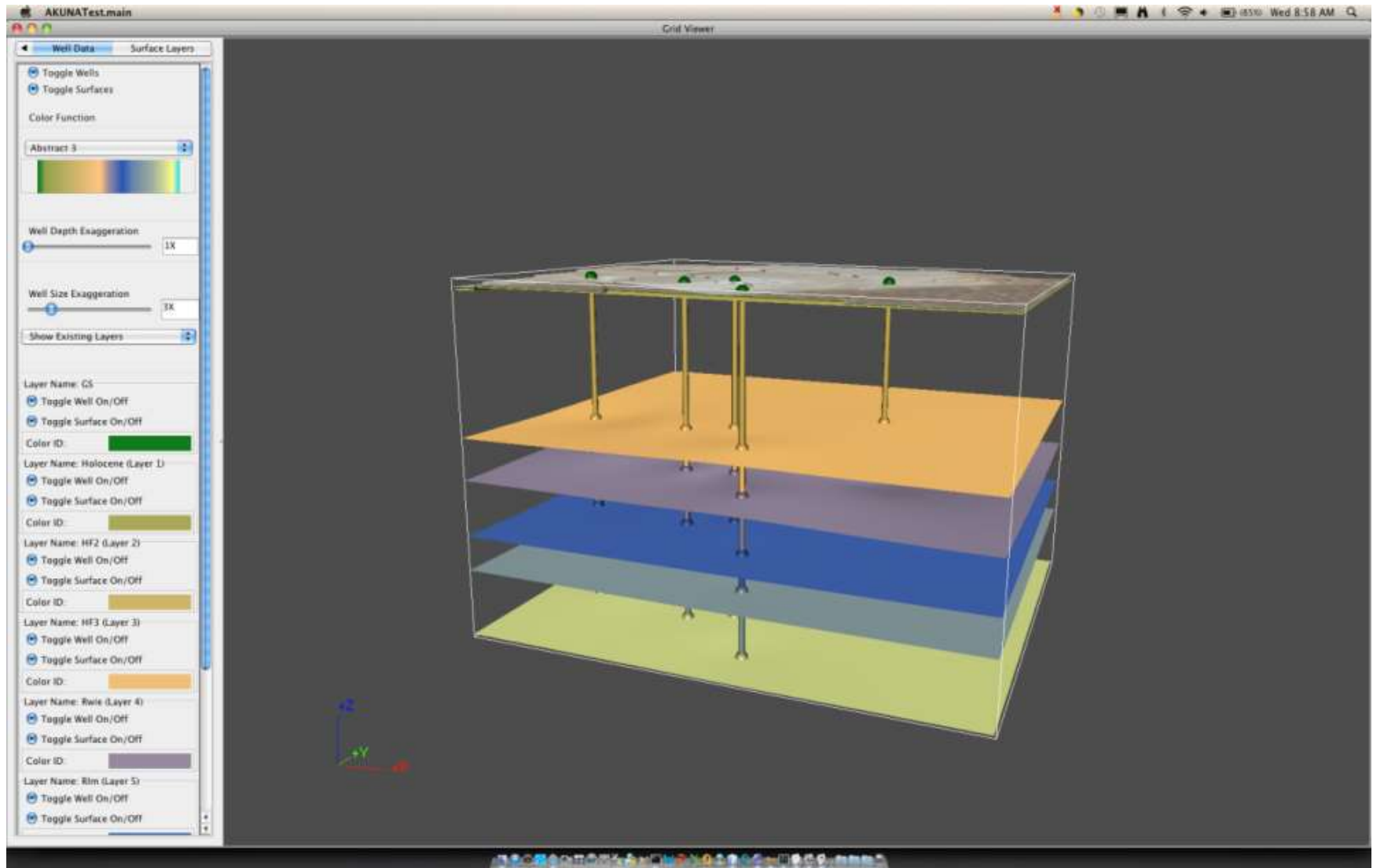
- 0 – 1956 period to attain steady state flow field
- 1956 – 2008 transient



Model Setup

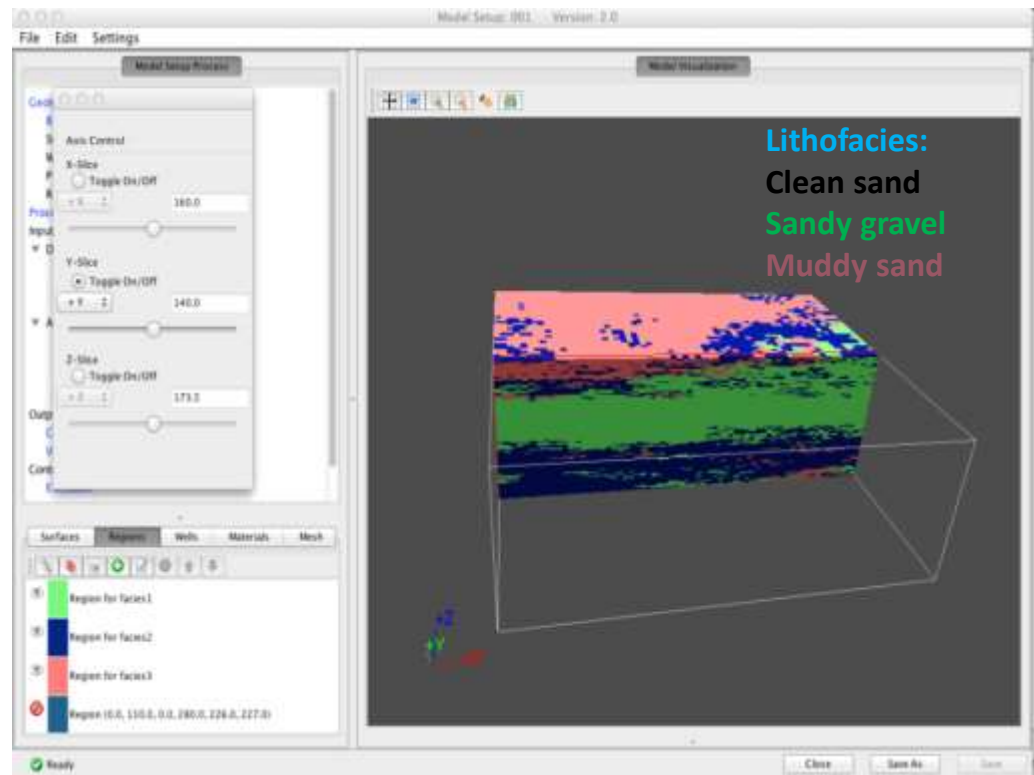


Major Stratigraphy



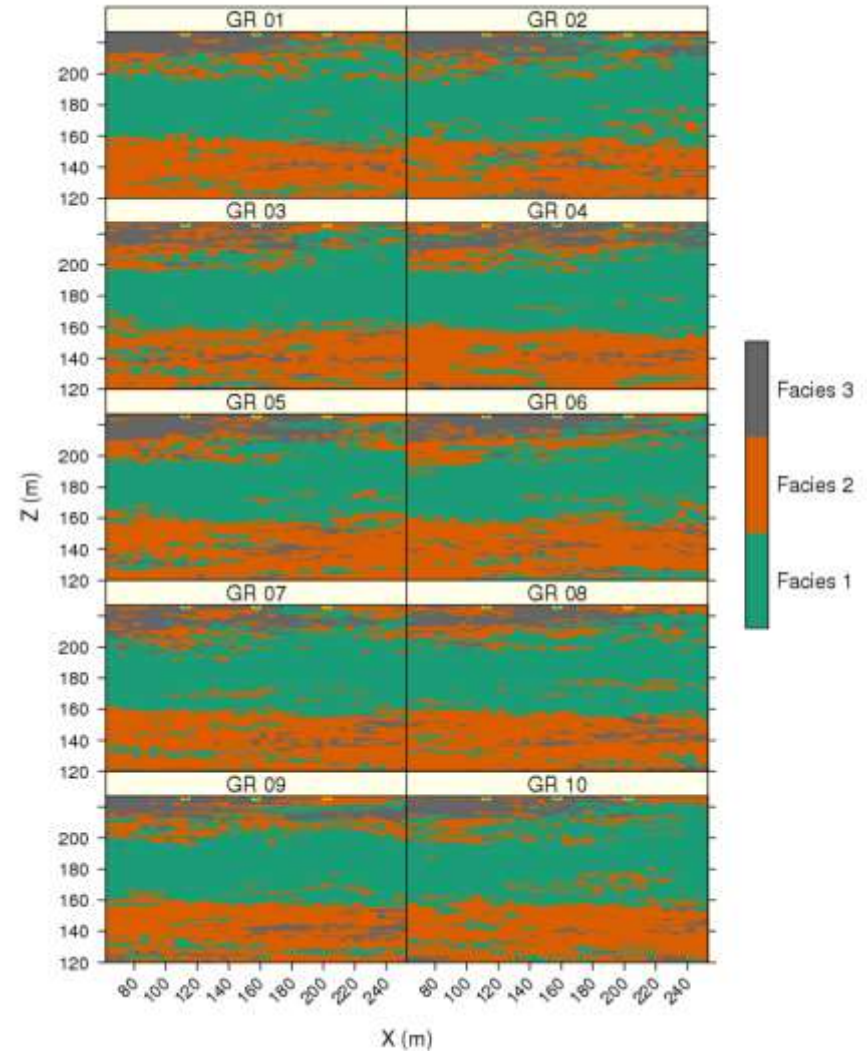
Incorporation of Heterogeneity

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



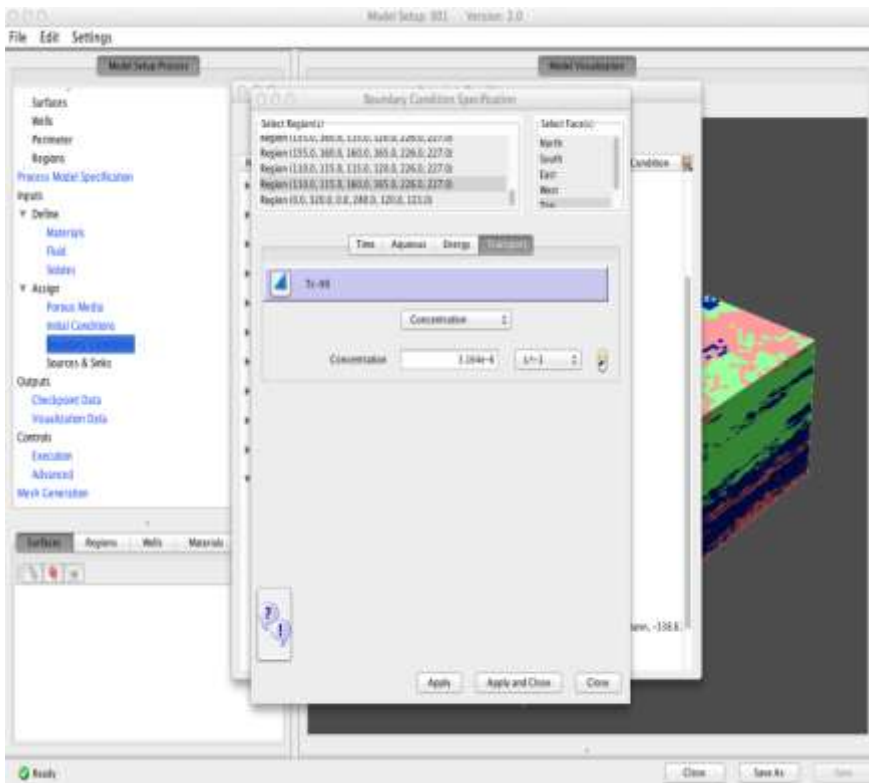
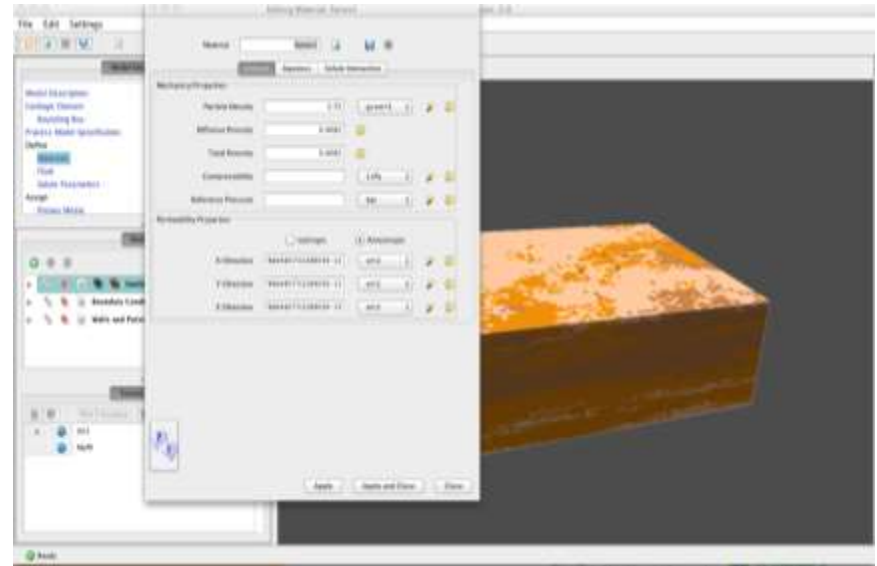
Geologic Realizations

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



Property Assignments and Boundary Conditions

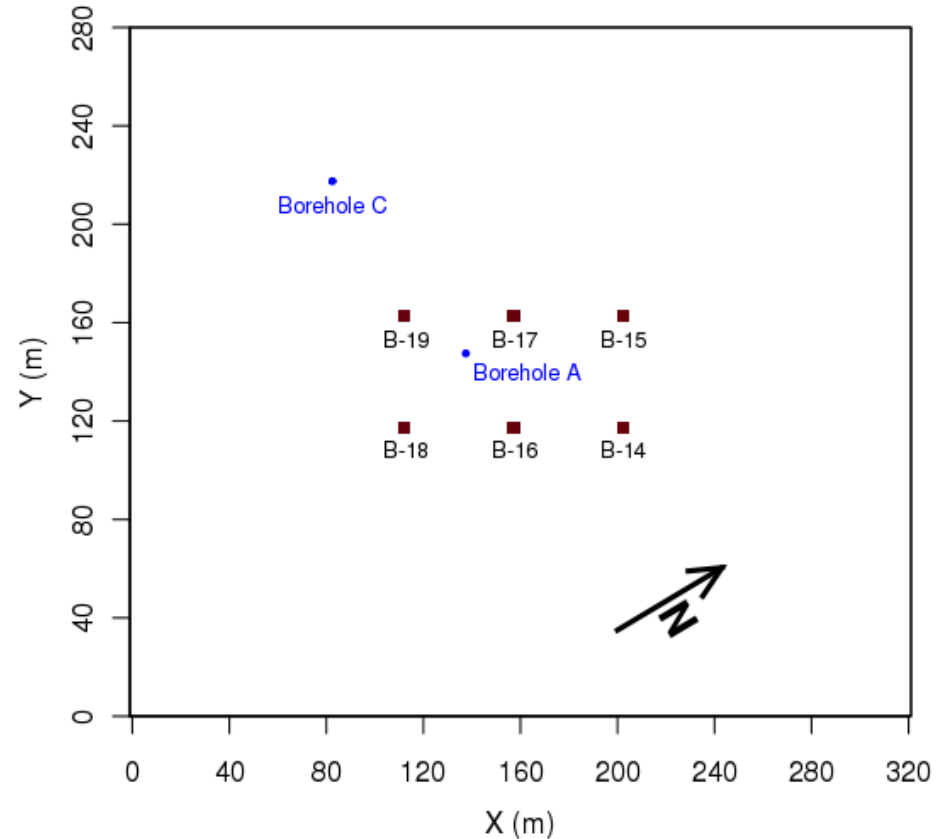
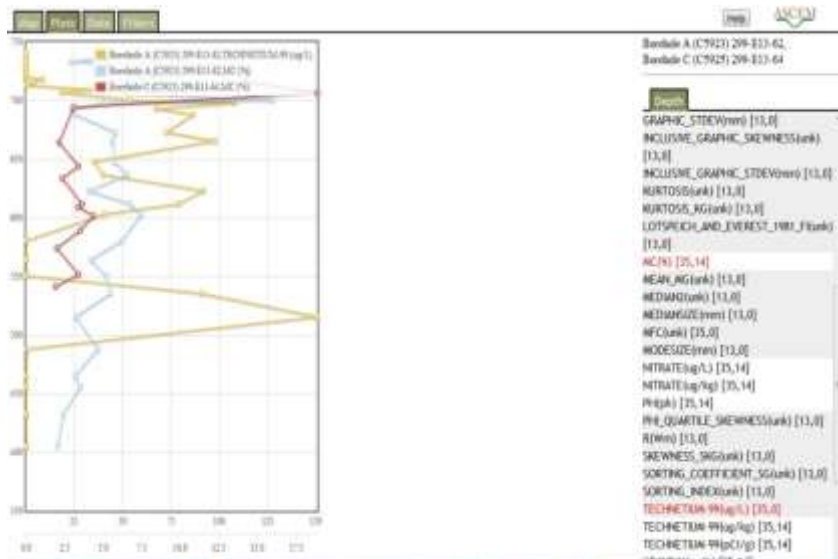
Hydraulic Property
Input



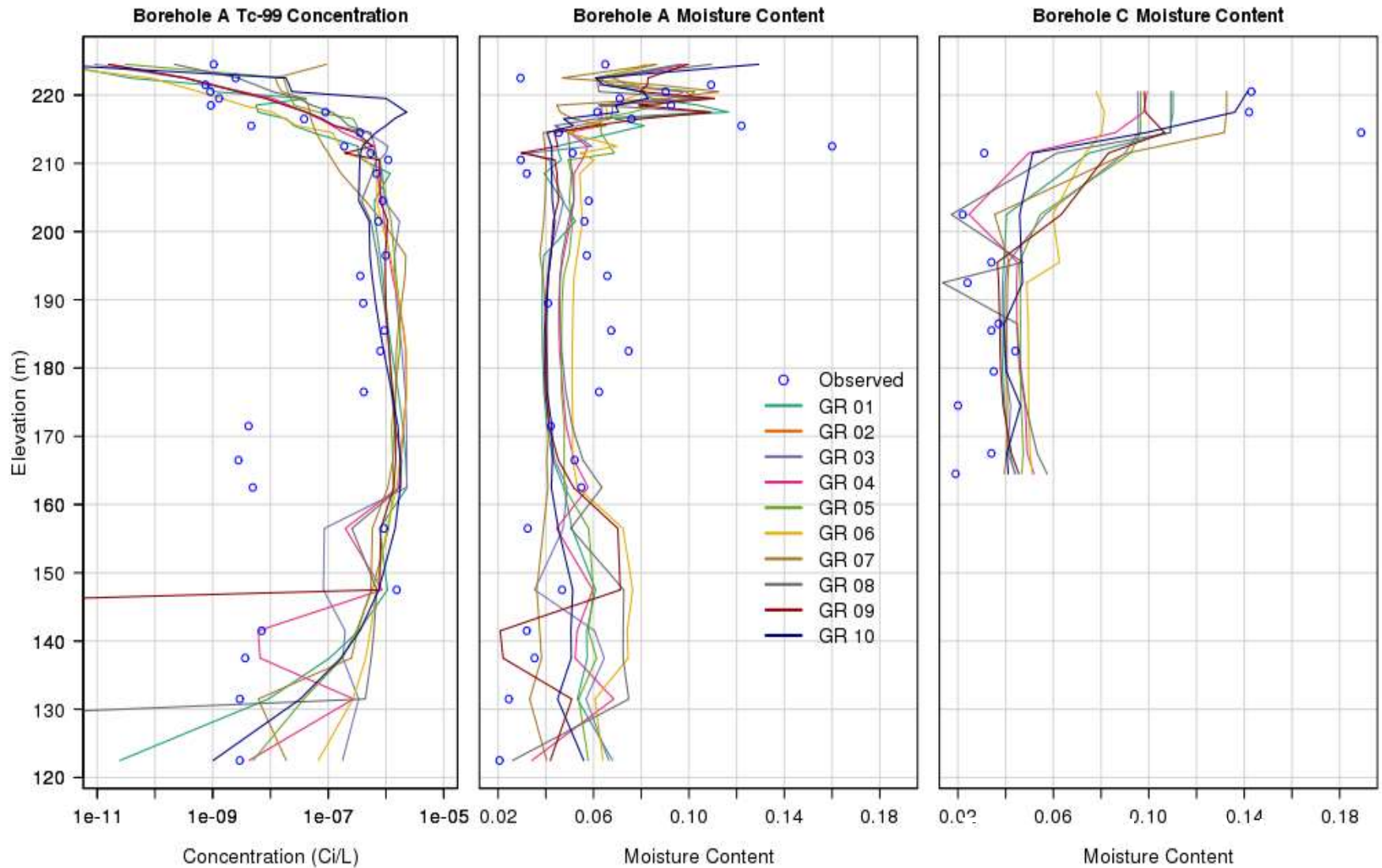
Boundary Condition
Input

Parameter Estimation

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



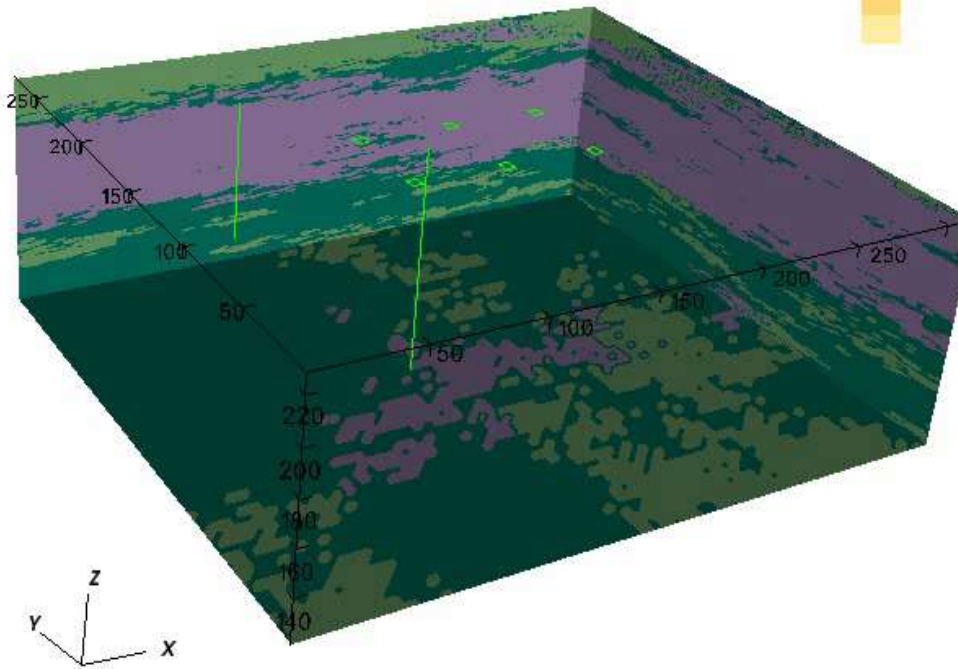
Parameter Estimation



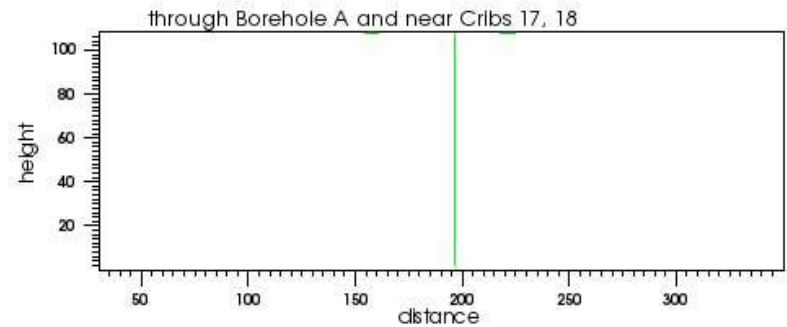
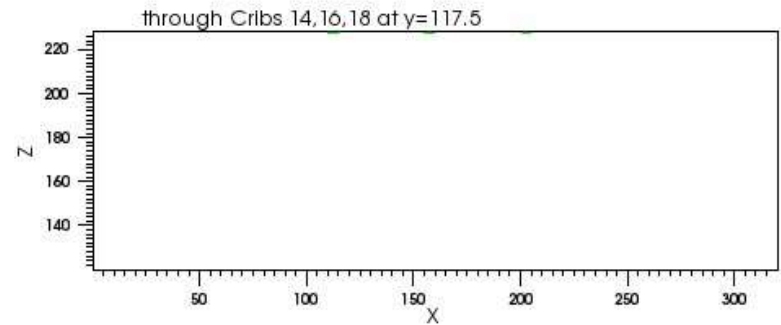
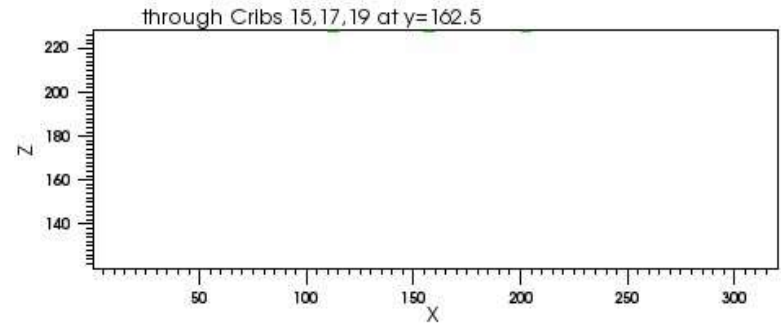
Simulation 1956 – 2008

Tc-99 (pCi/L)

Facies 1 Facies 2 Facies 3

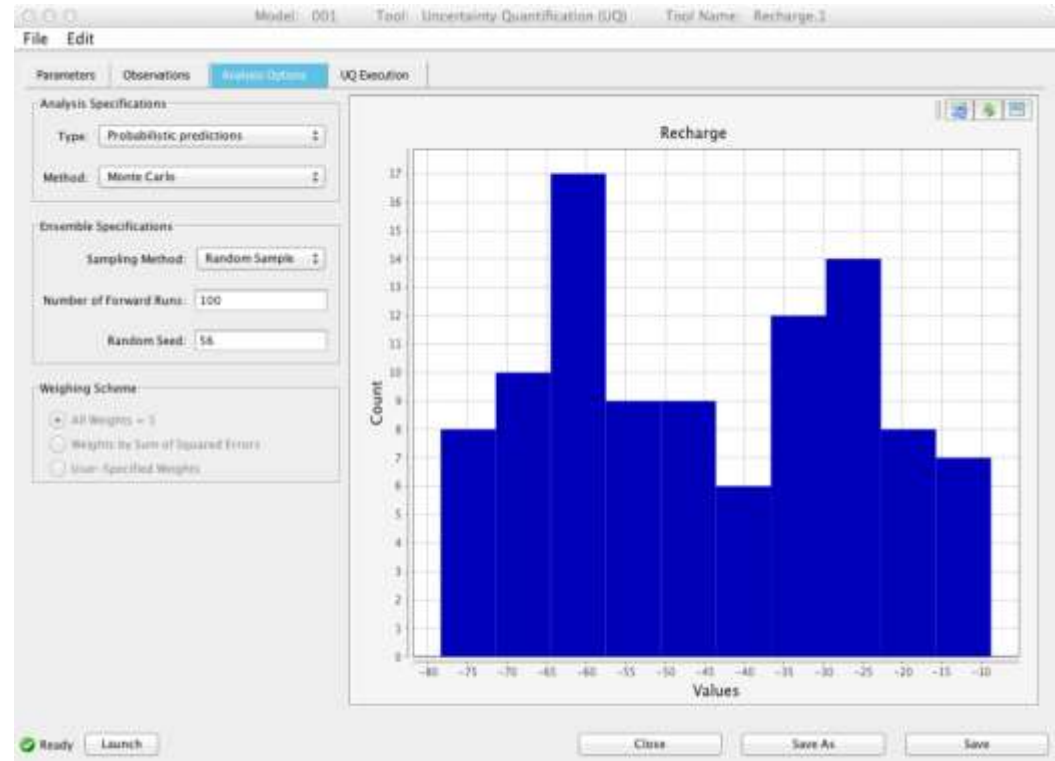


Year = 1956



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

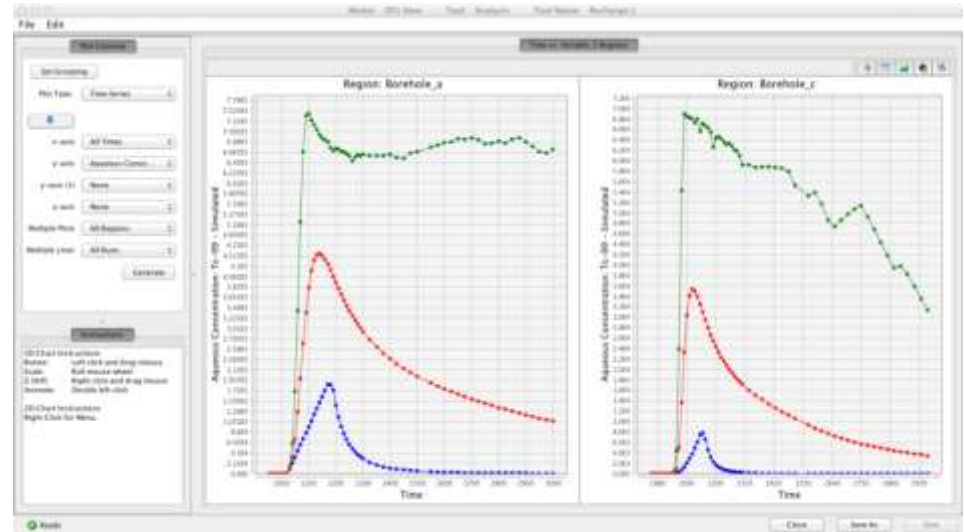


Screenshot from UQ Toolset:
Histogram of Recharge Rates

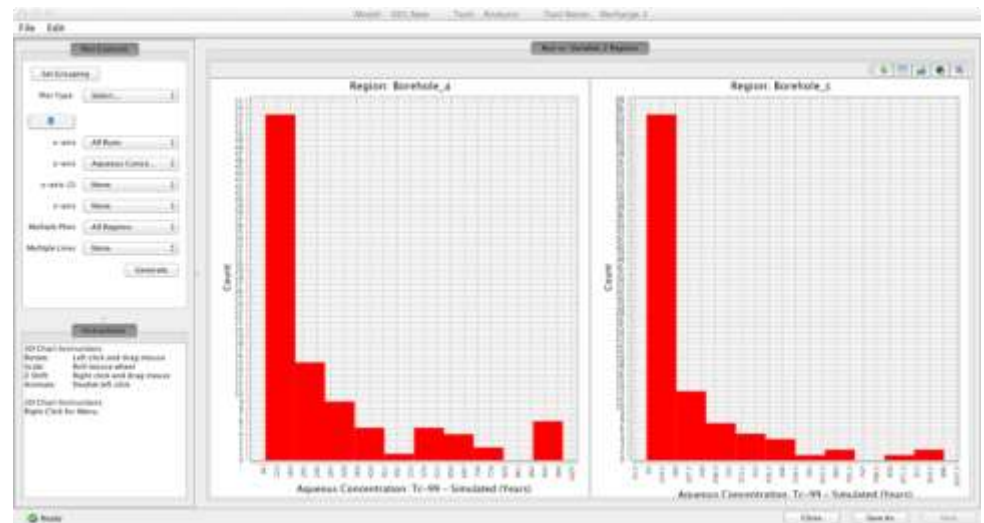
Uncertainty Quantification

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

a)

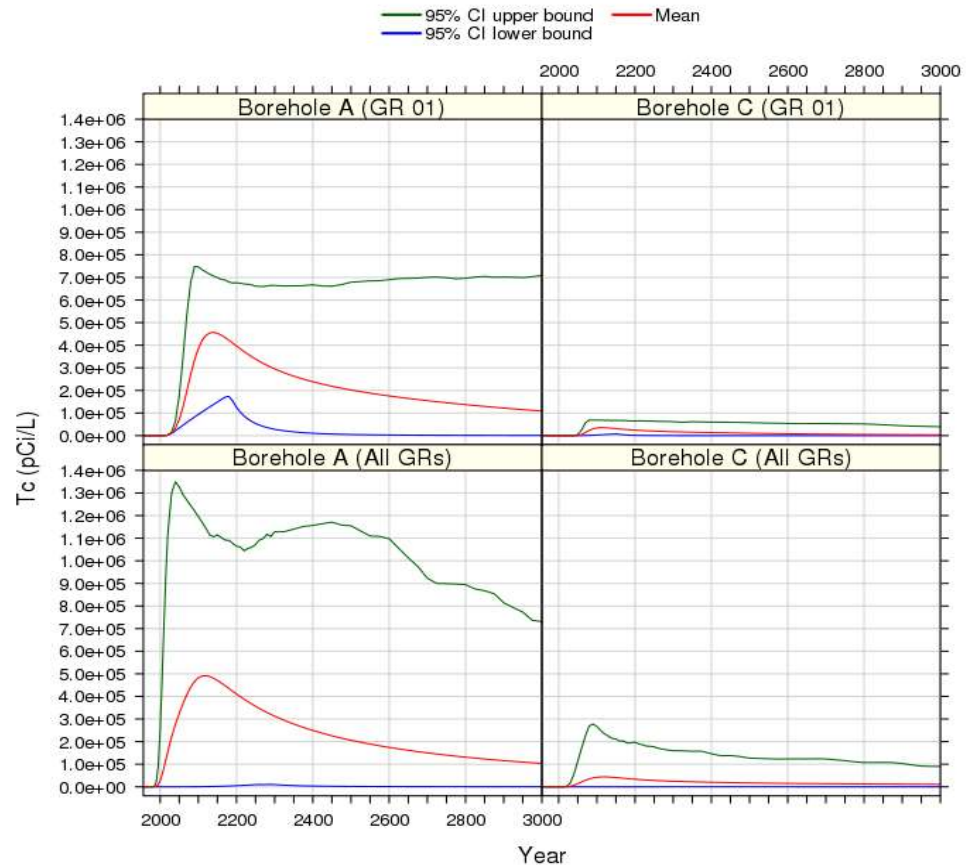


b)



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}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}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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