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

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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

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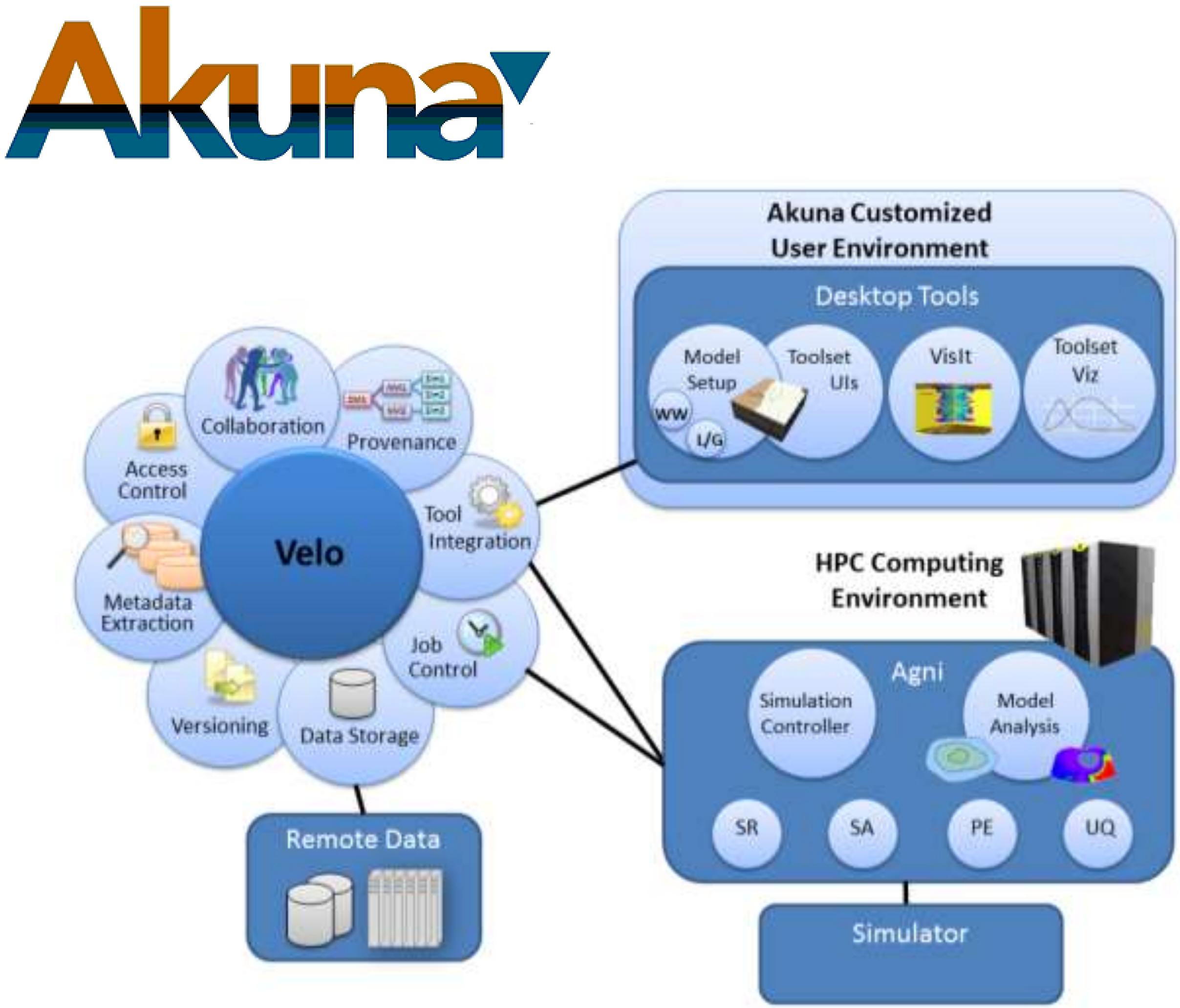
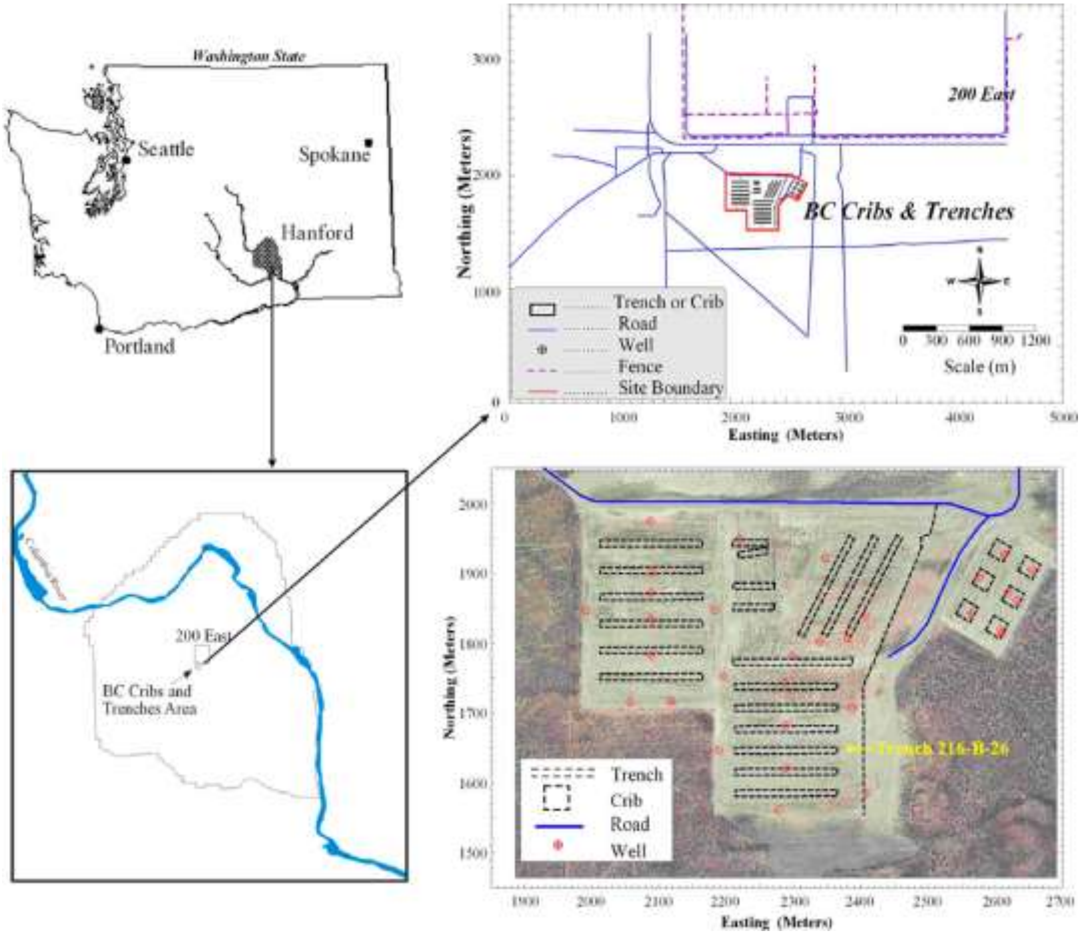
EM Environmental Management safety ❖ performance ❖ cleanup ❖ closure

User Environment



Application to Hanford BC Cribs

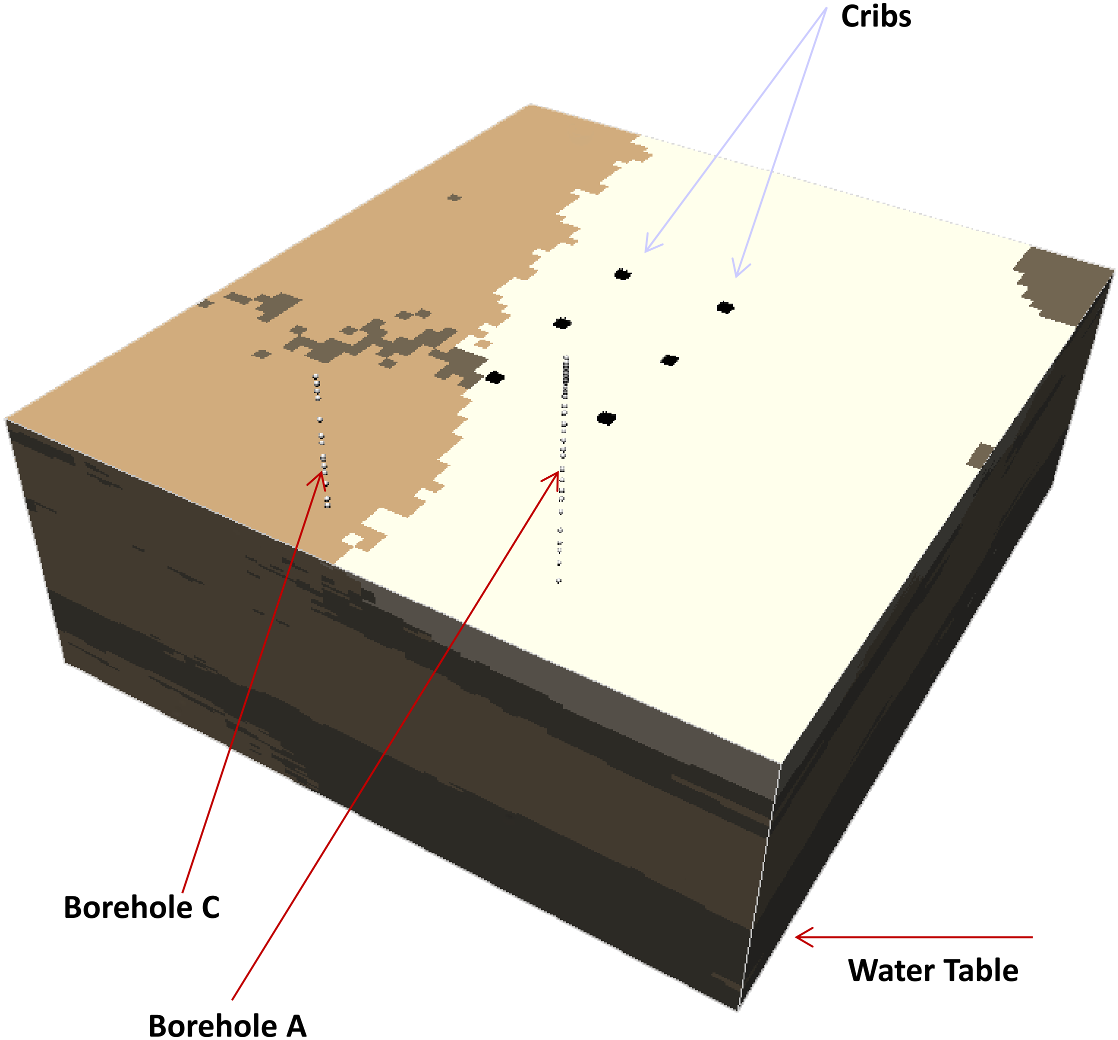
- Former plutonium production site
  - Waste disposed from 1956 to 1958 to 6 cribs
  - Funnel-shaped with sloping sides (~3 x 3 m wide)
- Located a few meters bgs
- Thick vadose zone (~107 m)
- Primary contaminant of concern ^{99}Tc
- Traditional remediation technologies are ineffective
- Evaluate uncertainty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

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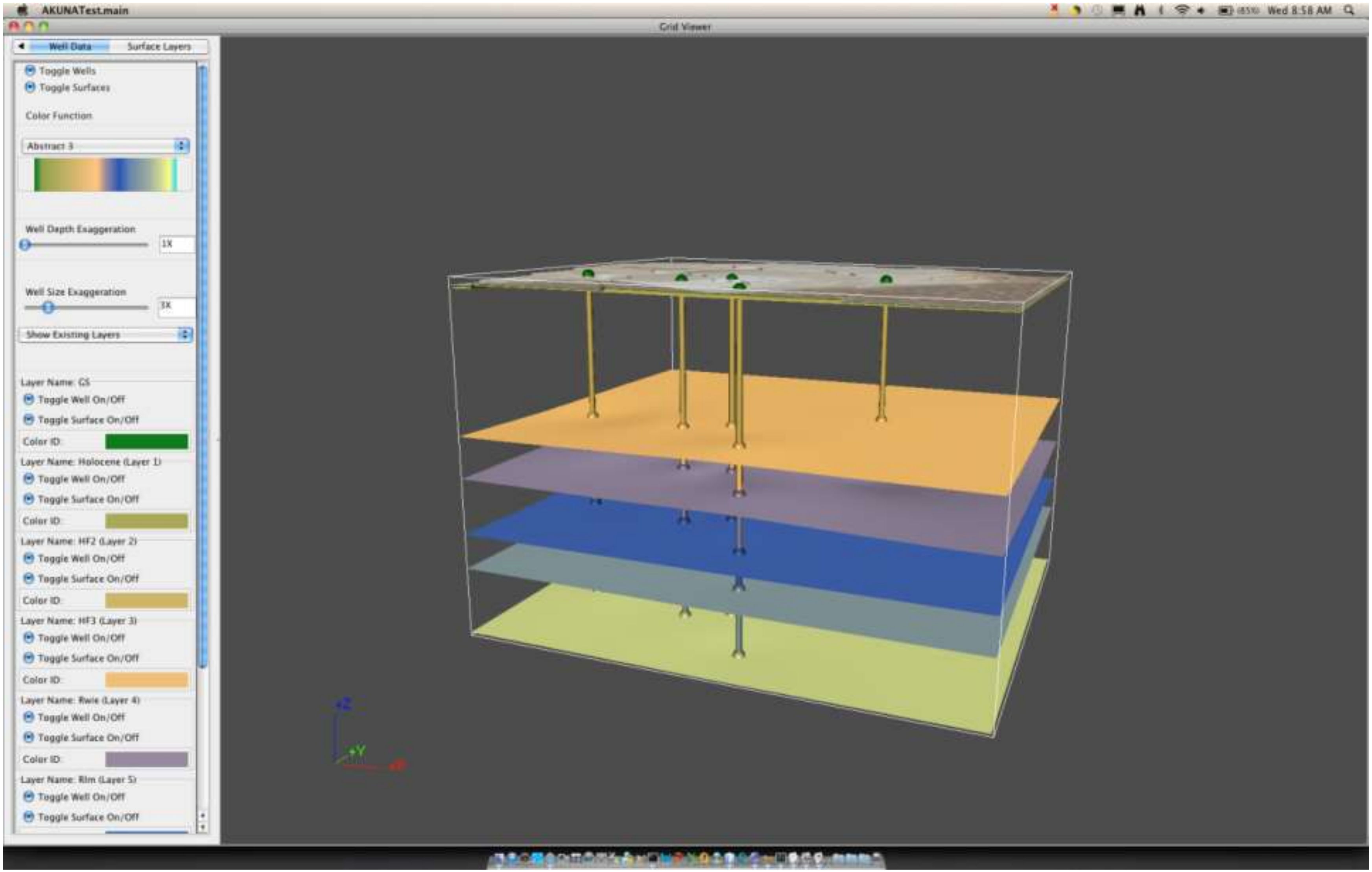
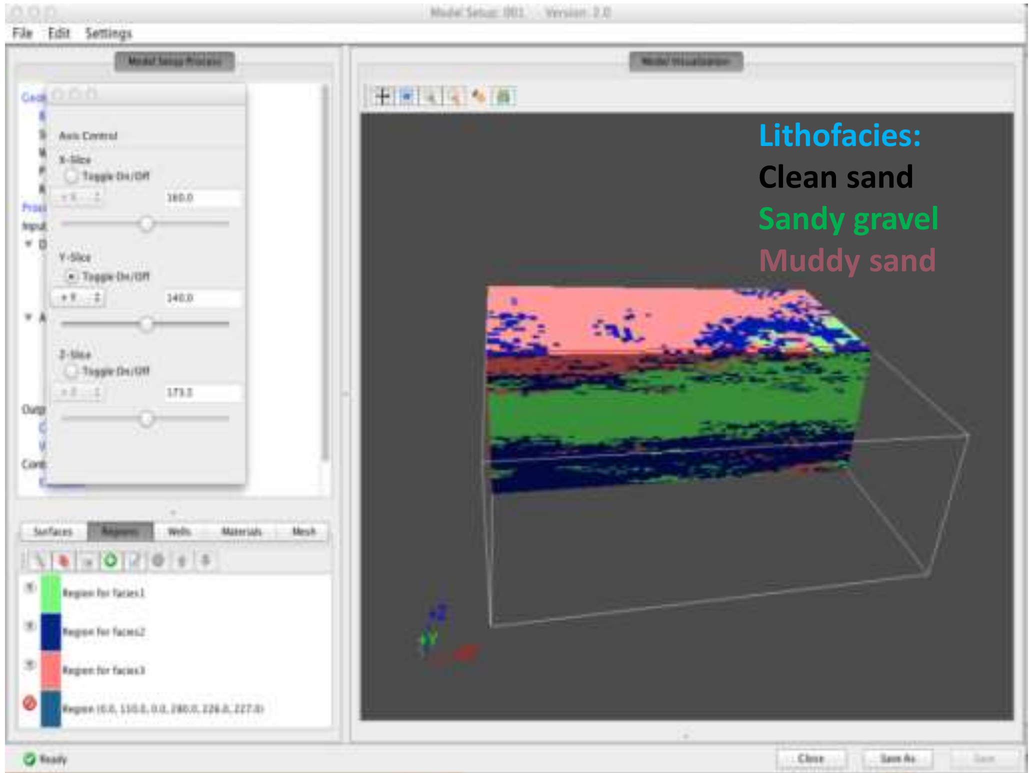
Major Stratigraphy



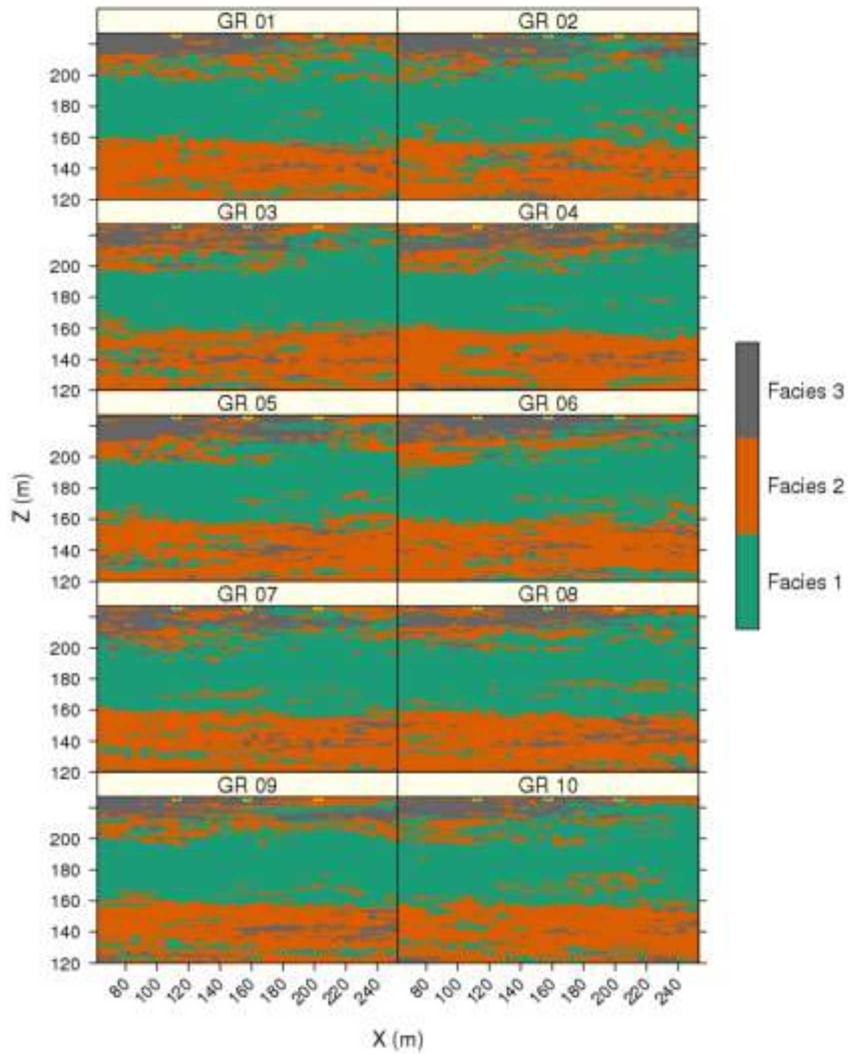
Incorporation of Heterogeneity

- 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 hetereogeneities captured



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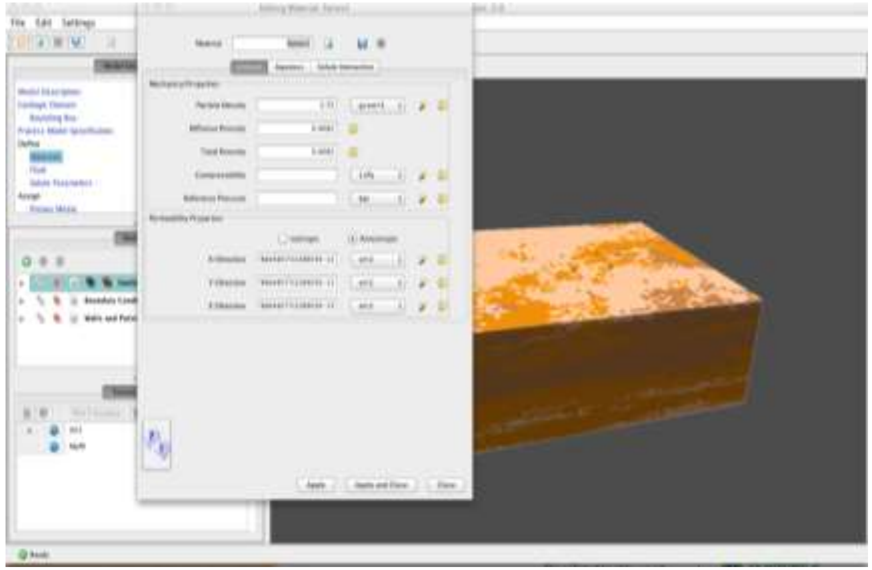
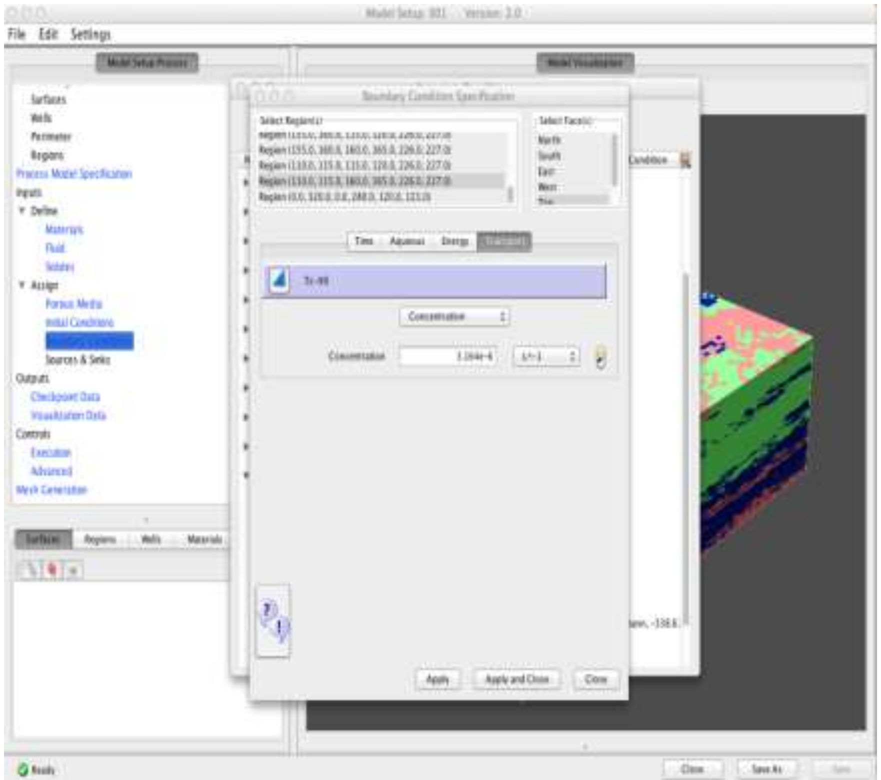
Property Assignments and Boundary Conditions

Hydraulic Property Input

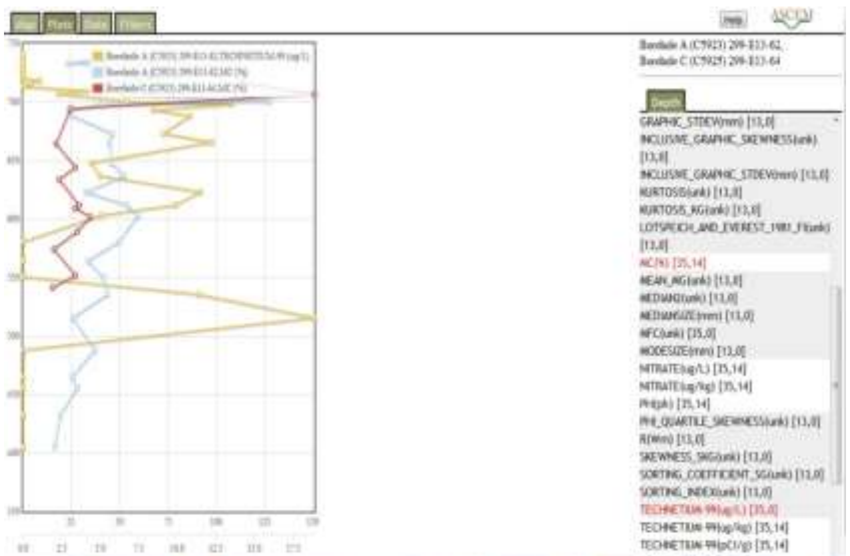


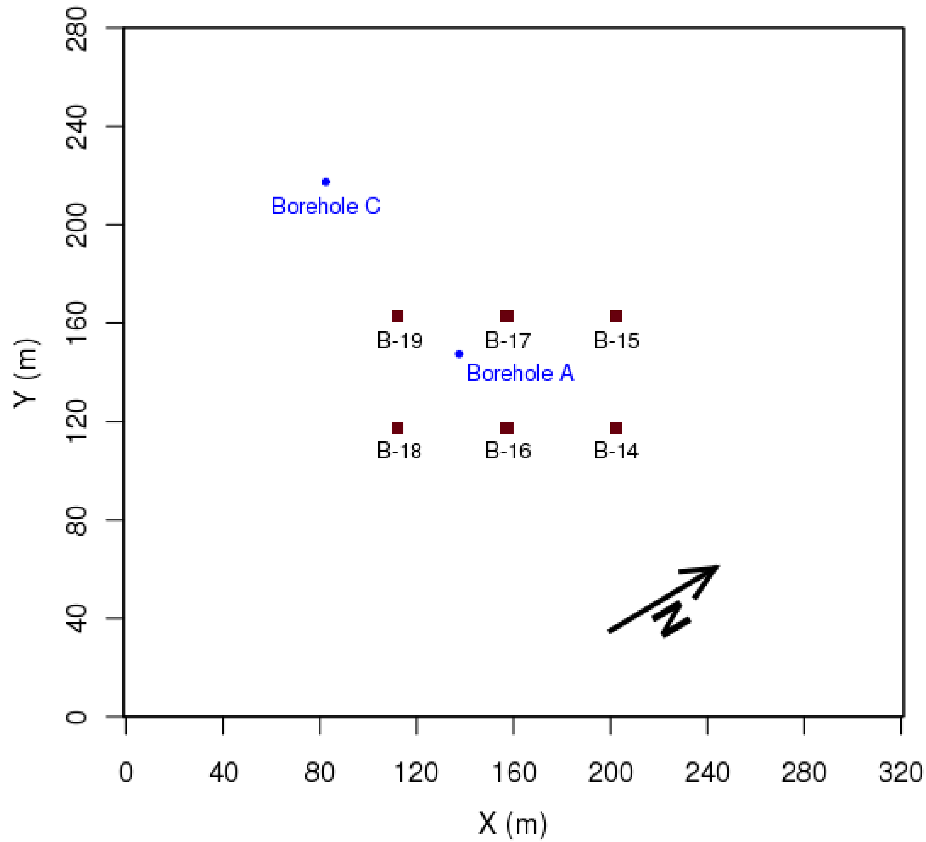


Boundary Condition Input

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





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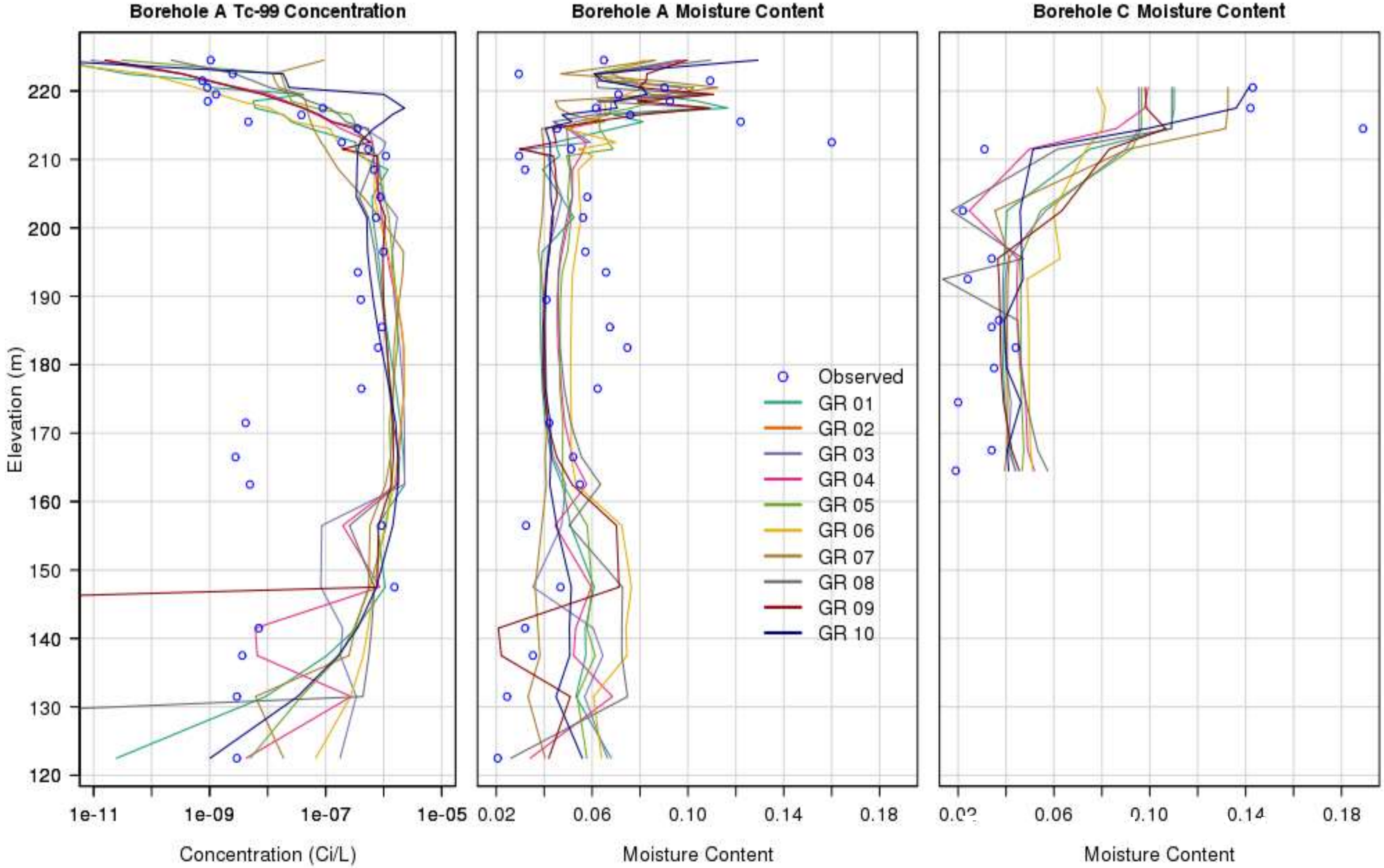
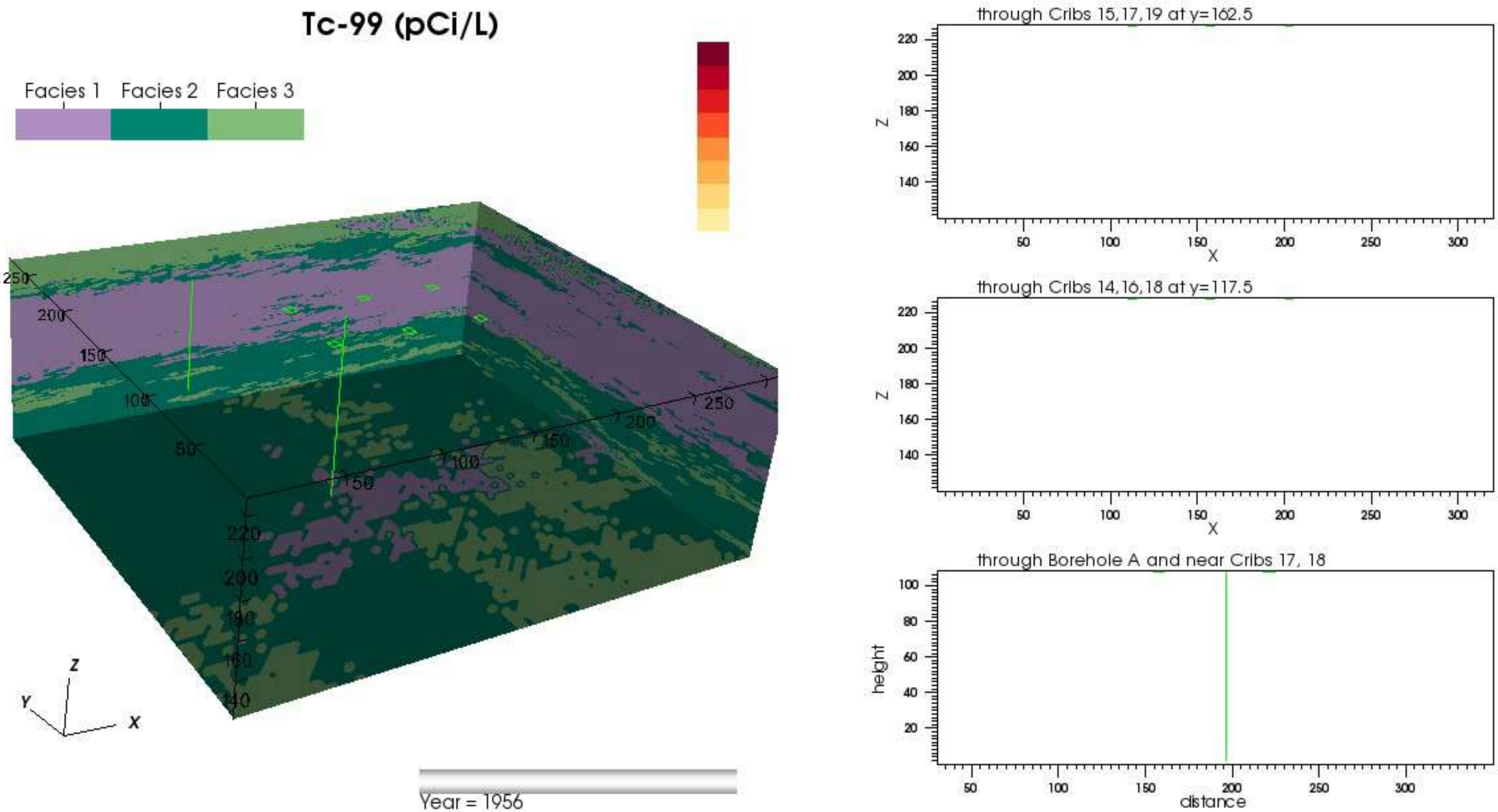
Parameter Estimation

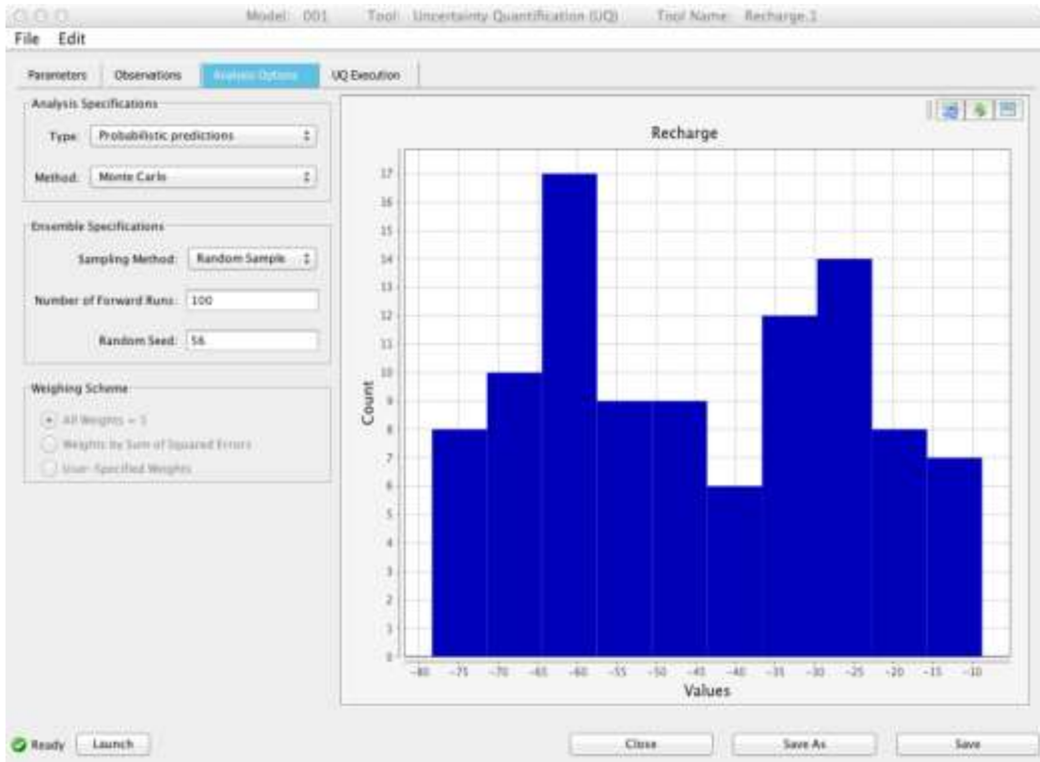


Simulation 1956 – 2008



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

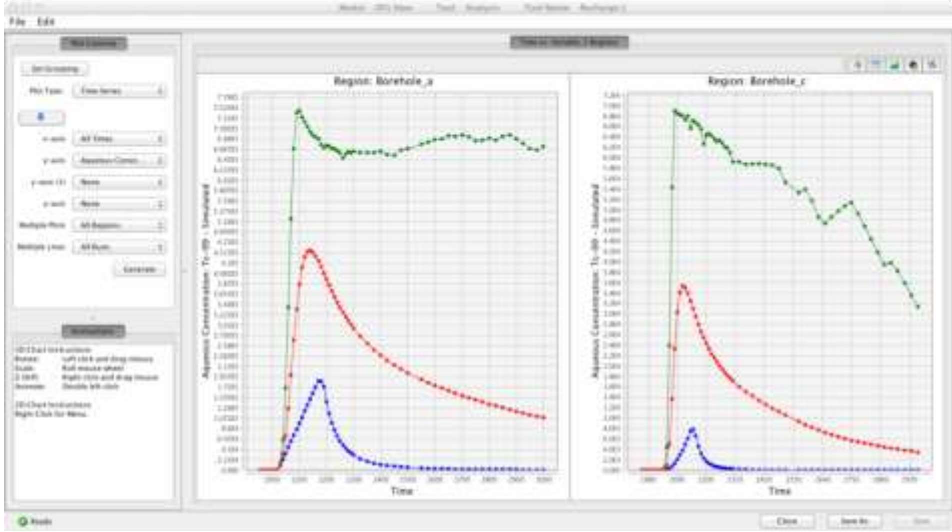


Screenshot from UQ Toolset: Histogram of Recharge Rates

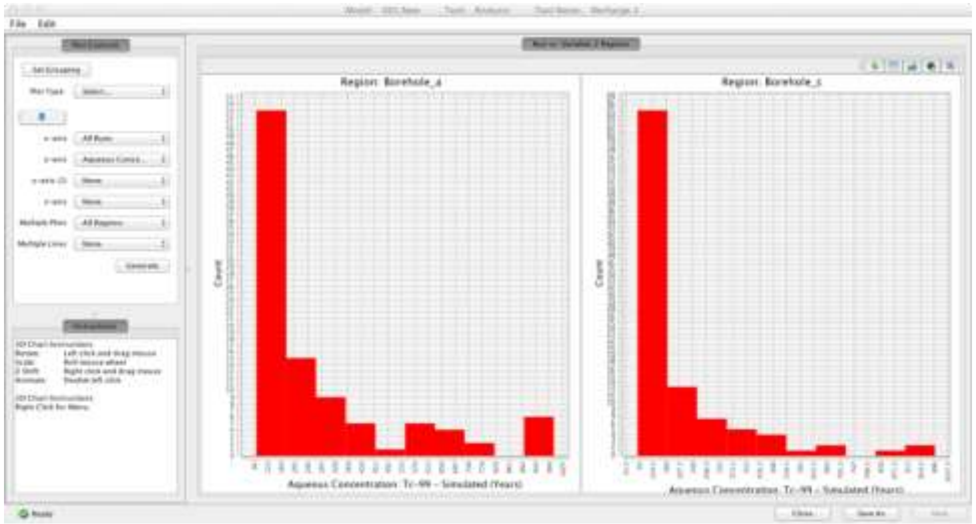
Uncertainty Quantification

- 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)

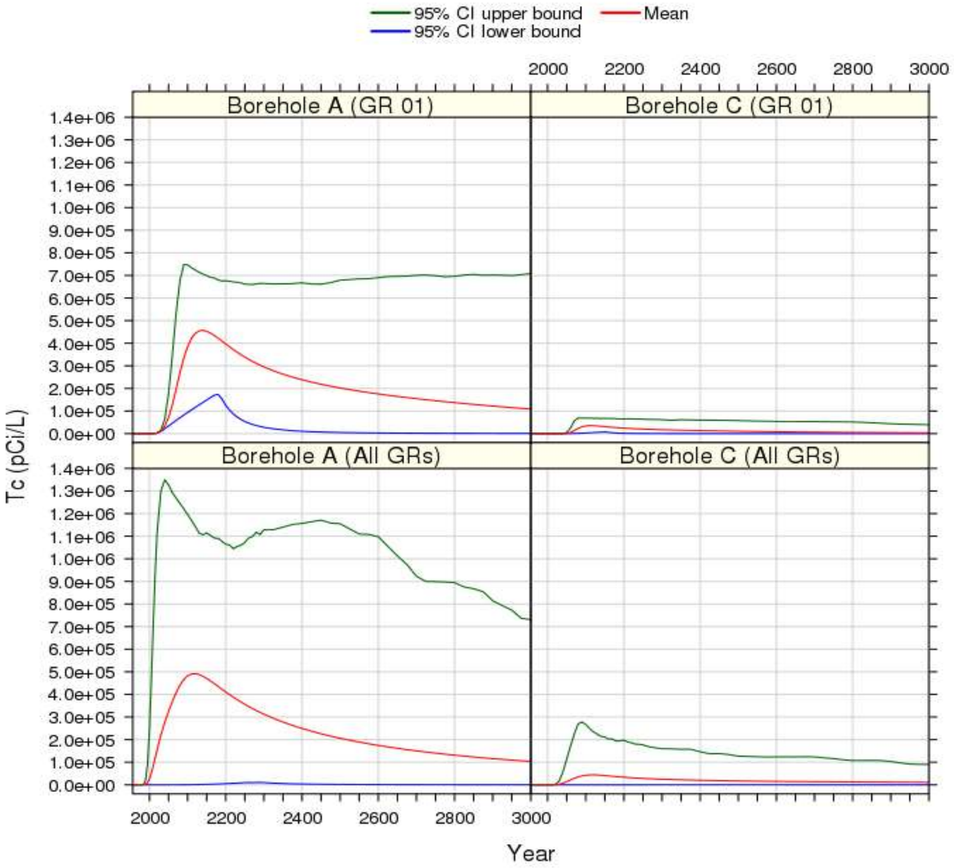


b)



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!

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