ASCEM

Advanced Simulation Capability for Environmental Management (ASCEM) – Current Status and Hanford Phase II Demonstration Results

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ASCEM

- **Advanced Simulation Capability for Environmental Management**
  - State-of-the-art scientific toolset currently under development for understanding and predicting subsurface contaminant fate and transport across EM complex
- **Organized into three thrust areas**
  - ***HPC*** – open-source, high performance simulator
  - ***Platform*** – tools that facilitate simulation execution
  - ***Applications*** - provide data and feedback to developers

Berkeley Lab

Los Alamos National Laboratory EST. 1943

Pacific Northwest National Laboratory

Oak Ridge National Laboratory

SRNL Savannah River National Laboratory

EM Environmental Management

safety ❖ performance ❖ cleanup ❖ closure

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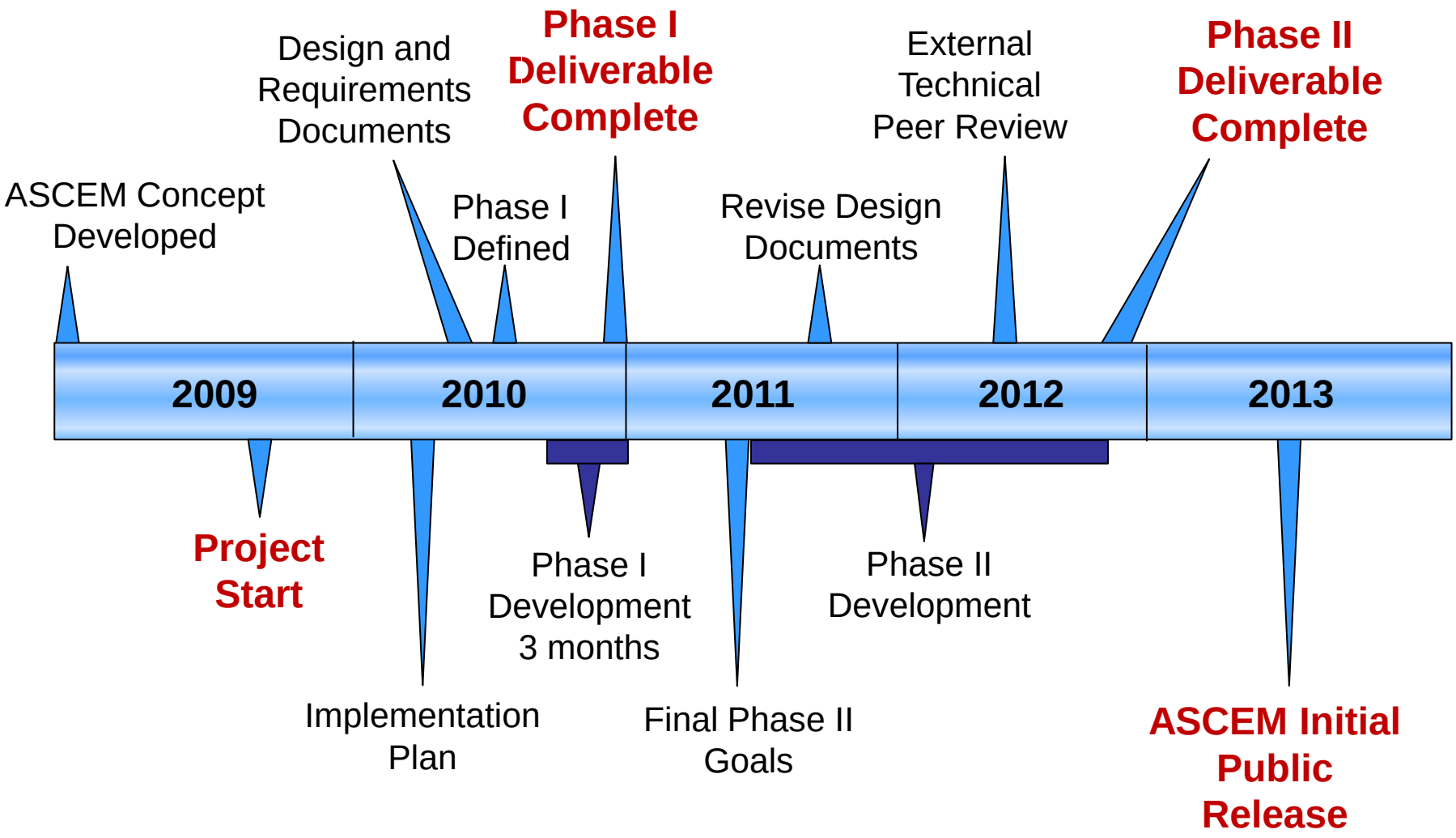
Project Timeline to Date



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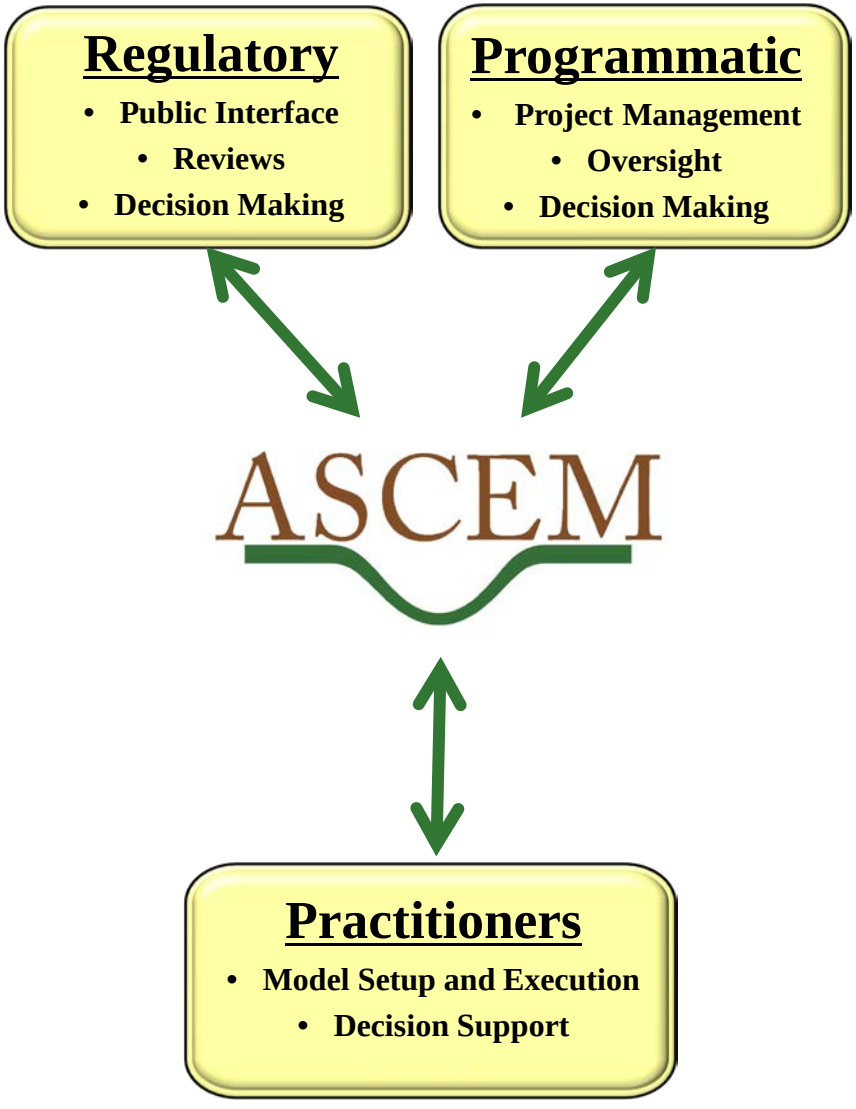
Interactions Shape Development

- **ASCEM team seeks feedback from a broad spectrum of users to guide development efforts**



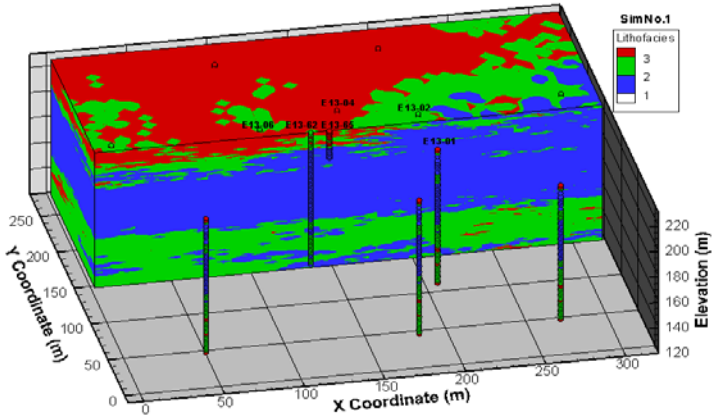
ASCEM Phase II Demonstration

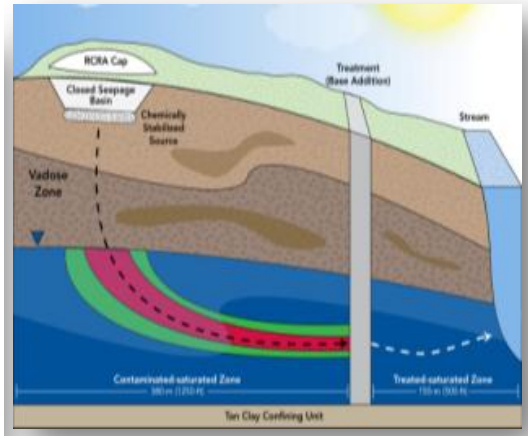
Multiple demonstrations were used to test and evaluate advancement of ASCEM capabilities

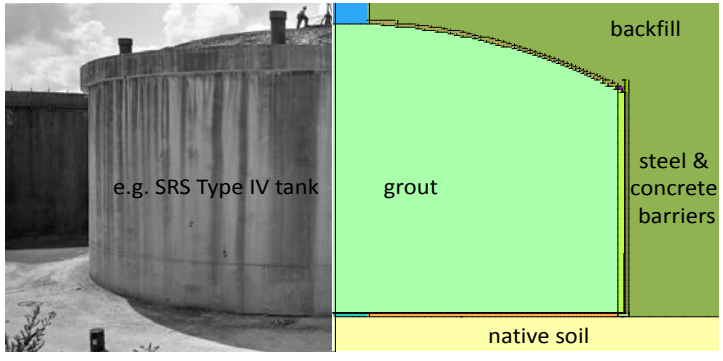
1. End-to-end demonstration of a complete modeling workflow using the Hanford deep vadose zone
   - From data management through simulation and visualization in a sparse data environment

2. Testing of select ASCEM components in a physically and geochemically complex subsurface environment at the SRS F-Area
   - Uncertainty quantification used to identify controls on long-term system behavior over large regions in a data-rich environment

3. Exploring approaches such as Adaptive Mesh Refinement to enhance waste tank PA
   - Unique challenges of engineered systems (e.g., changing properties over time, fine features and large contrasts in material properties)







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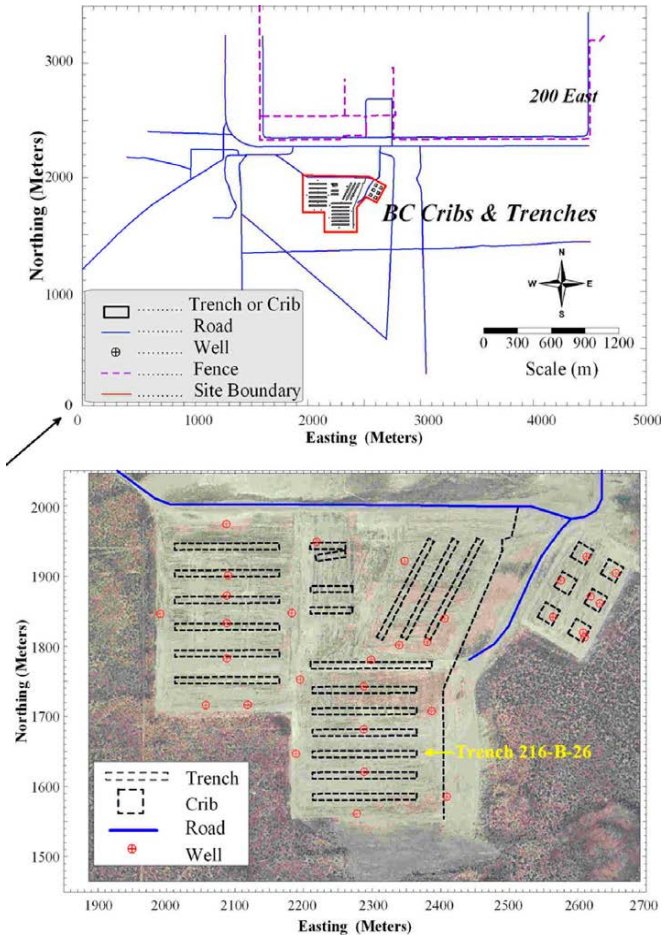
Arid Site Demonstration: Hanford Deep Vadose Zone (DVZ)

- BC Cribs in Hanford Central Plateau
  - Charged with evaluating innovative remediation technologies for recalcitrant Tc-99 in the deep vadose zone

- Phase II Demonstration
  - Scientific goal
    - Establish baseline predictions for Tc-99 in absence of remediation technologies
  - Development goal
    1. Data management
    2. Model setup and execution
    3. Parameter estimation (model calibration)
    4. Visualization
    5. Uncertainty quantification

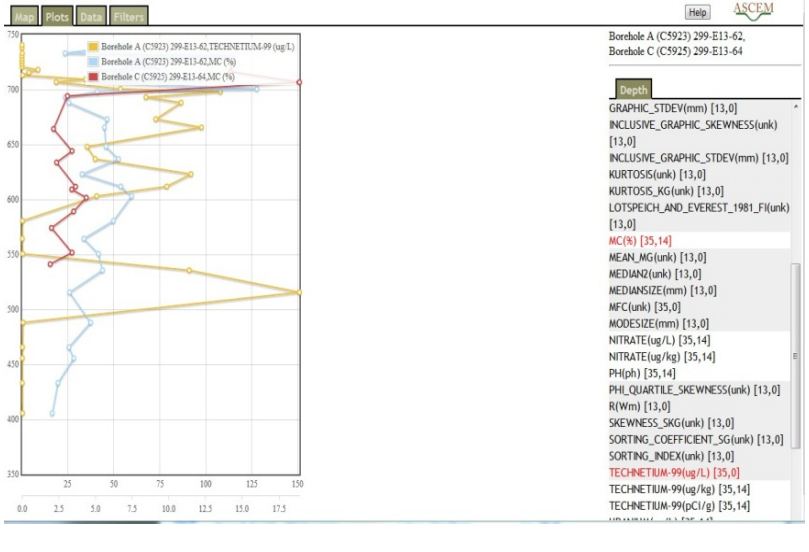


1. Database Management

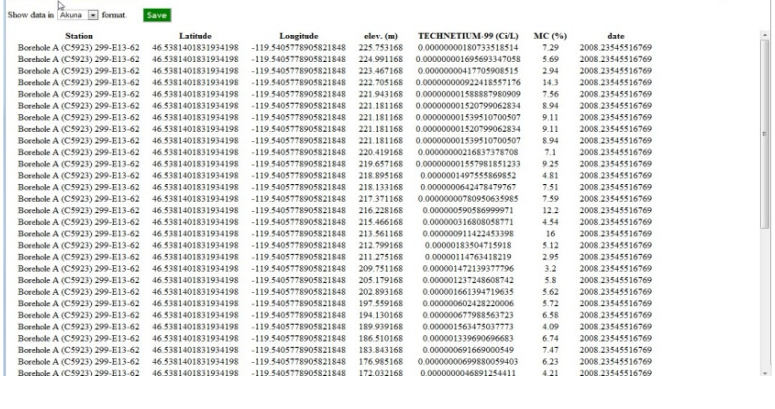
- Click on boreholes
- Plot vertical profiles
- Export data (for input to Akuna)

1)

2)



3)



Station	Latitude	Longitude	elev. (m)	TECHNETIUM-99 (Ci/L)	MC (%)	date
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	225.753168	0.0000000018073318514	7.29	2008.23545516769
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	224.991168	0.0000000016956933470 58	5.69	2008.23545516769
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	223.467168	0.0000000041770590851 5	2.94	2008.23545516769
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	222.705168	0.0000000009224185571 76	14.3	2008.23545516769
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	221.943168	0.0000000015888879809 09	7.56	2008.23545516769
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	221.181168	0.0000000015207990628 34	8.94	2008.23545516769
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	221.181168	0.0000000015395107005 07	9.11	2008.23545516769
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	221.181168	0.0000000015207990628 34	9.11	2008.23545516769
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	221.181168	0.0000000015395107005 07	8.94	2008.23545516769
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	220.419168	0.0000000021683737870 8	7.1	2008.23545516769
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	219.657168	0.0000000015579818512 33	9.25	2008.23545516769
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	218.895168	0.0000001497555869852	4.81	2008.23545516769
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	218.133168	0.0000000642475679767	7.51	2008.23545516769
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	217.371168	0.0000000078095063598 5	7.59	2008.23545516769
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Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	215.466168	0.0000003168080587 71	4.54	2008.23545516769
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	213.561168	0.0000009114224533 98	16	2008.23545516769
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	212.799168	0.0000018350471591 8	5.12	2008.23545516769
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	211.275168	0.0000011476341821 9	2.95	2008.23545516769
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	209.751168	0.0000014721393777 96	3.2	2008.23545516769
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	205.179168	0.0000012372486087 42	5.8	2008.23545516769
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	202.893168	0.0000016613947196 35	5.62	2008.23545516769
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	197.559168	0.0000006024822000 6	5.72	2008.23545516769
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Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	176.985168	0.0000000069988005940 3	6.23	2008.23545516769
Borehole A (C5923) 299-E13-62	46.5381401831934198	-119.5405778905821848	172.032168	0.0000000046891254411	4.21	2008.23545516769

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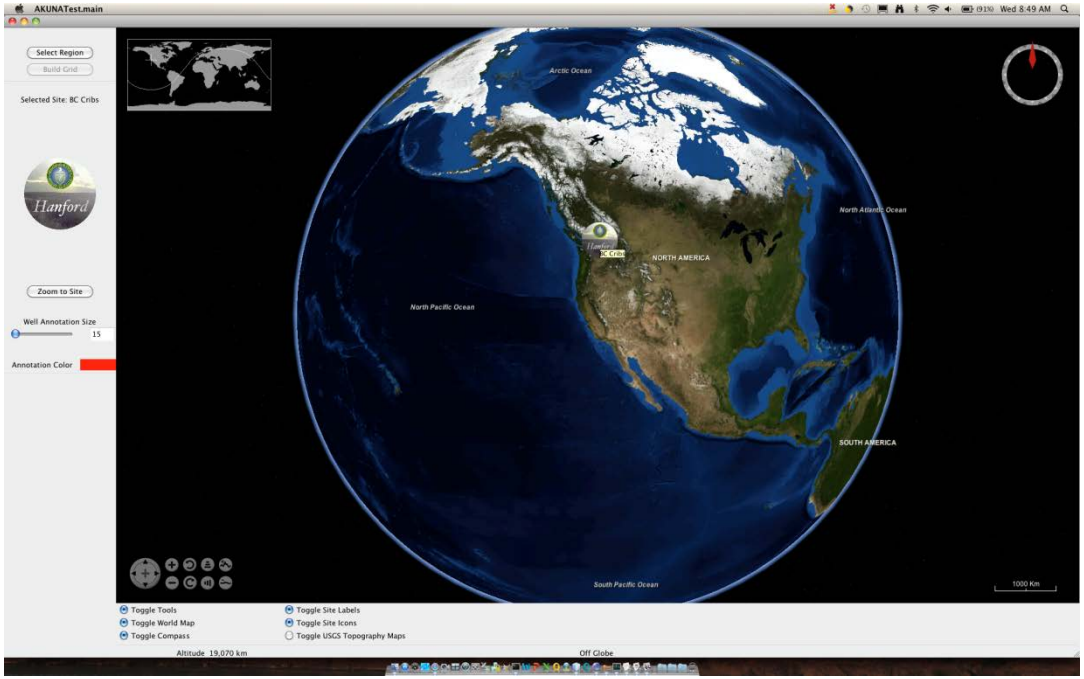
2. Model Setup

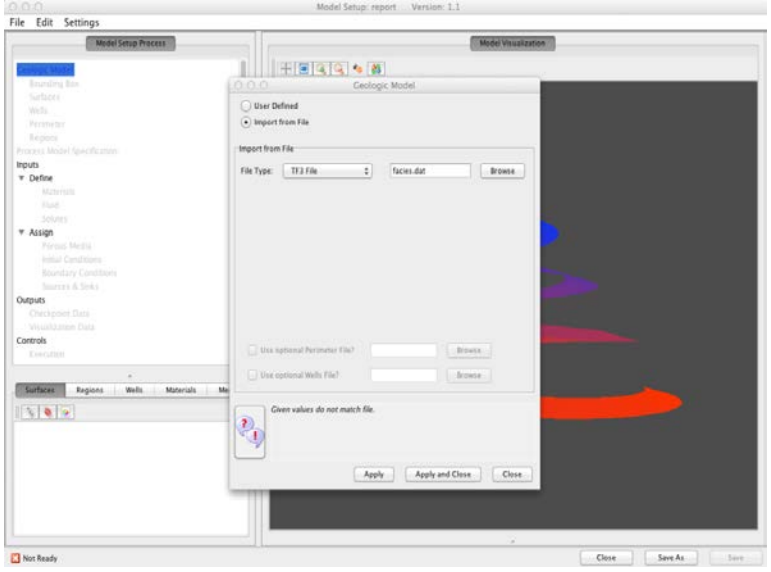


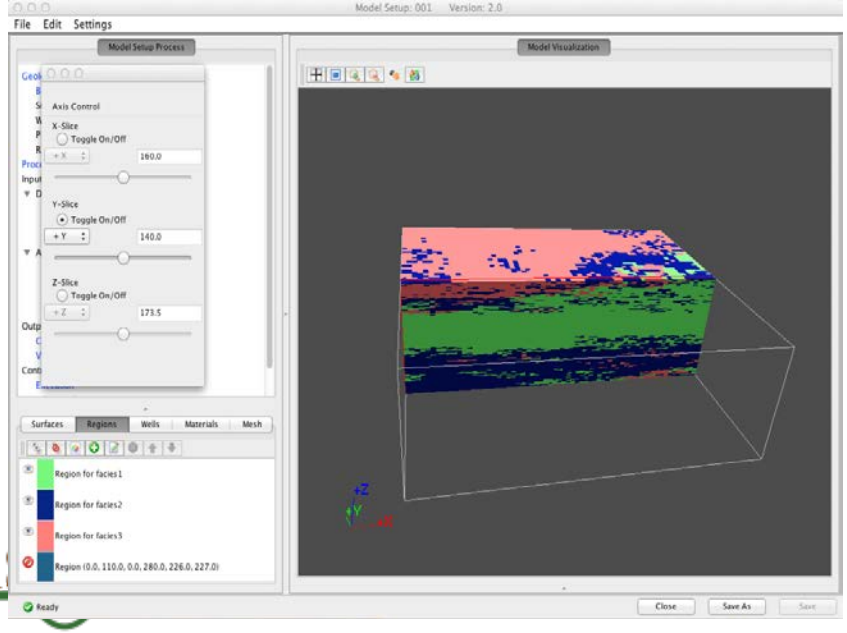
- NASA World Wind
  - Collection of components that interactively display 3D geographic information within Java applications or applets.
    - Open-source
    - Cross platform
- Incorporated into the Akuna Model Setup Tool
  - Used to provide geolocation of site data
  - Select well data for creating model
  - Map simulation results to geospatial locations

2. Model Setup

File read on materials

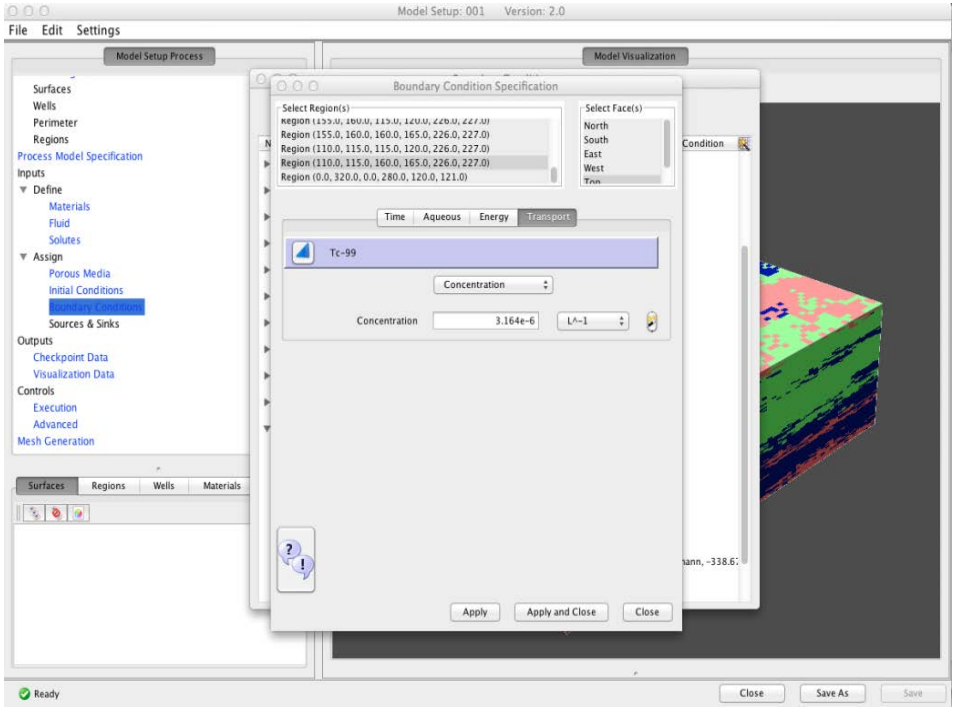
(geostatistical geologic conceptual model; 3 lithofacies; generated 100 realizations of conceptual model)





Lithofacies distribution

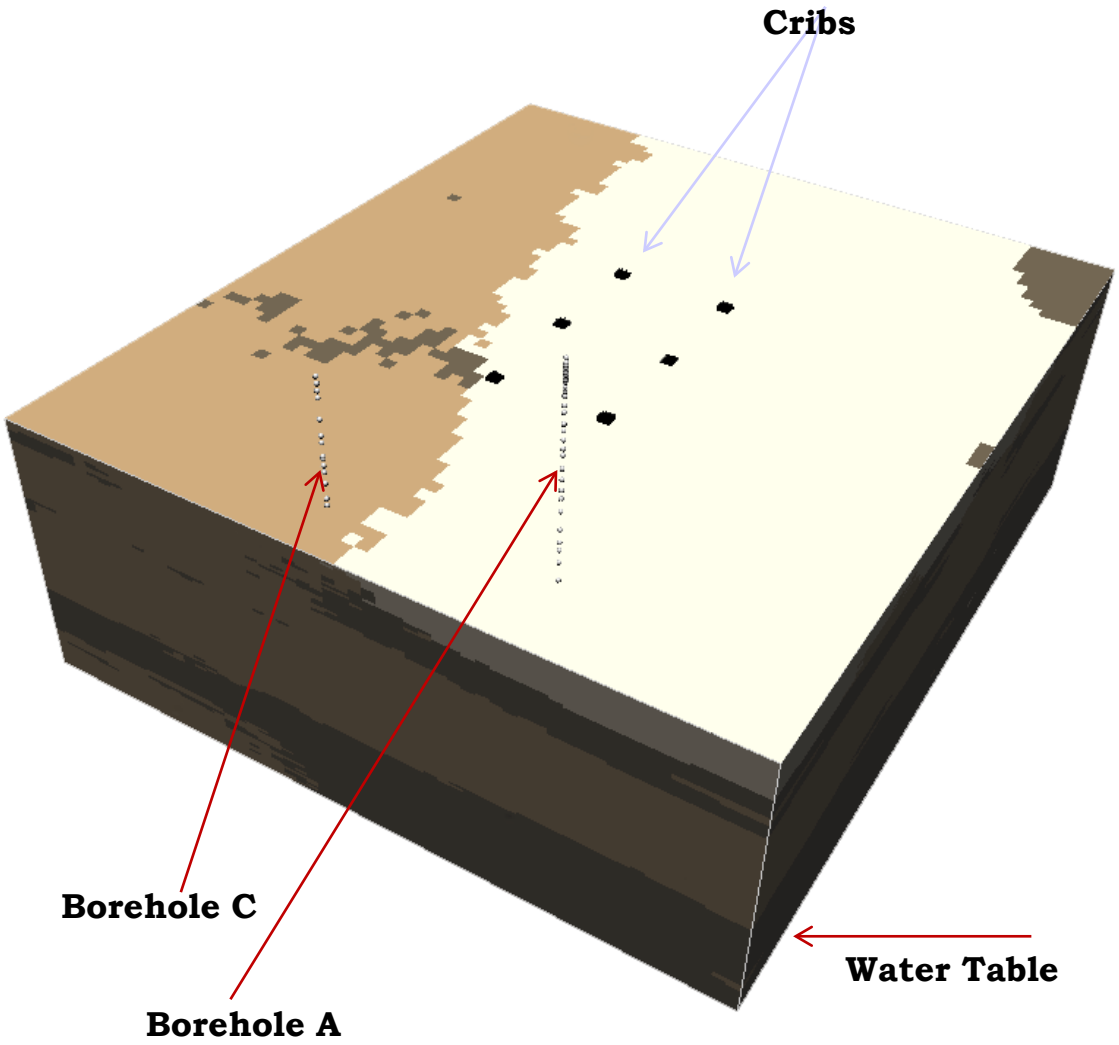
2. Model Setup



Boundary Condition Input

3. Parameter Estimation (PE)

- > 10 million gallons liquid waste released at 6 cribs
  - 1956 – 1958
  - Simulated flow and solute transport (^{99}Tc
- Estimated porosity and permeability
- Examined different realizations of the conceptual model
- Executed PE on 576 cores; 96 cores per run
  - ~24 hrs to complete PE (several iterations)



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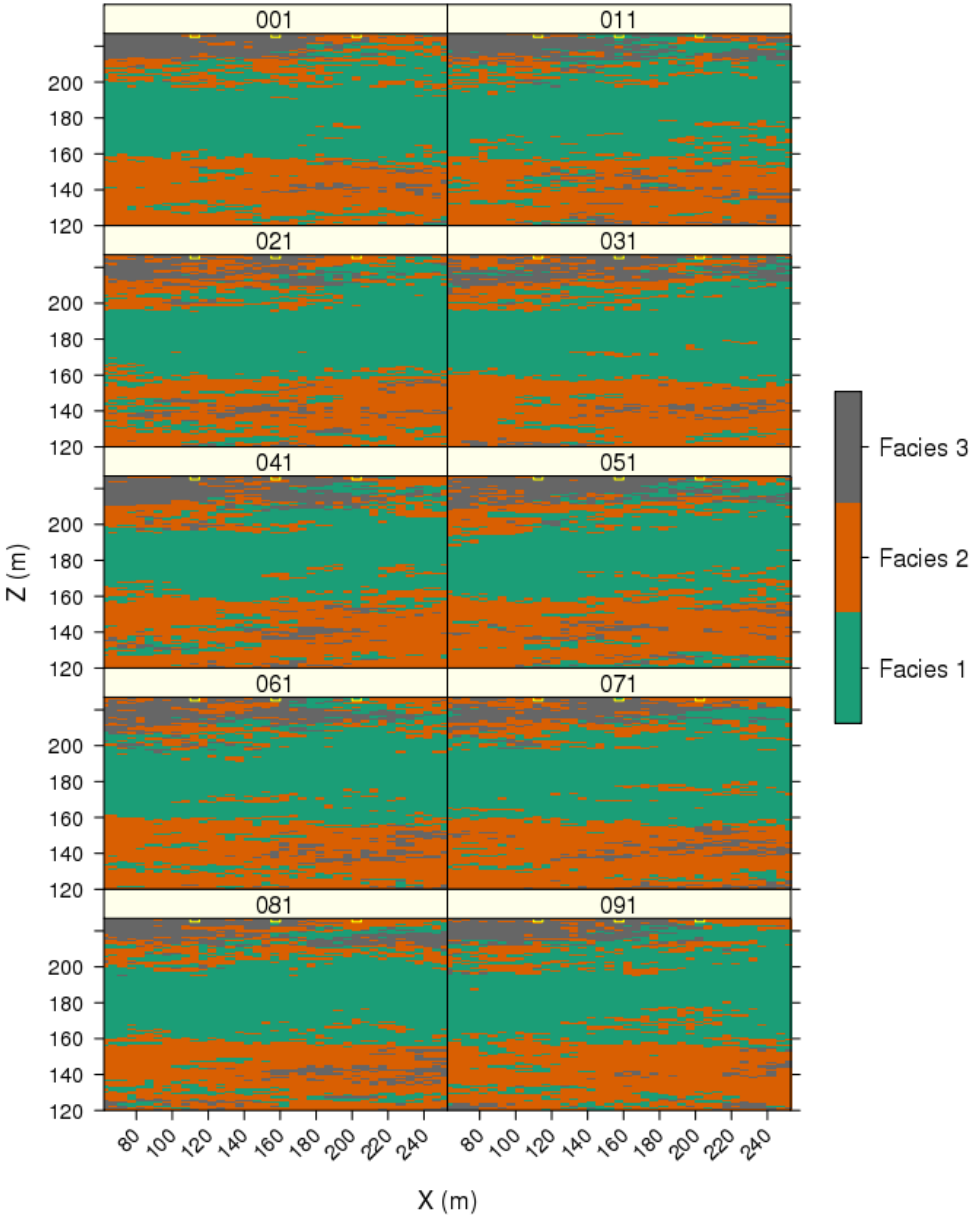

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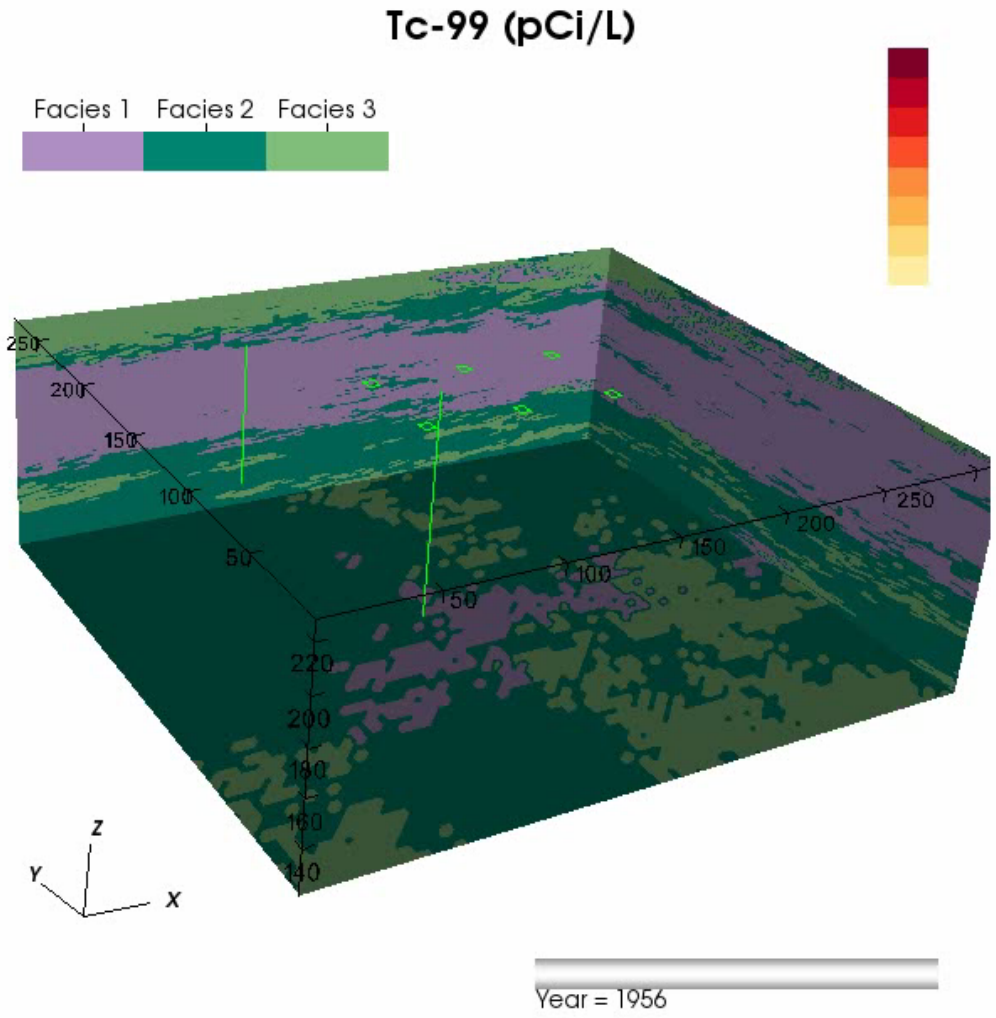
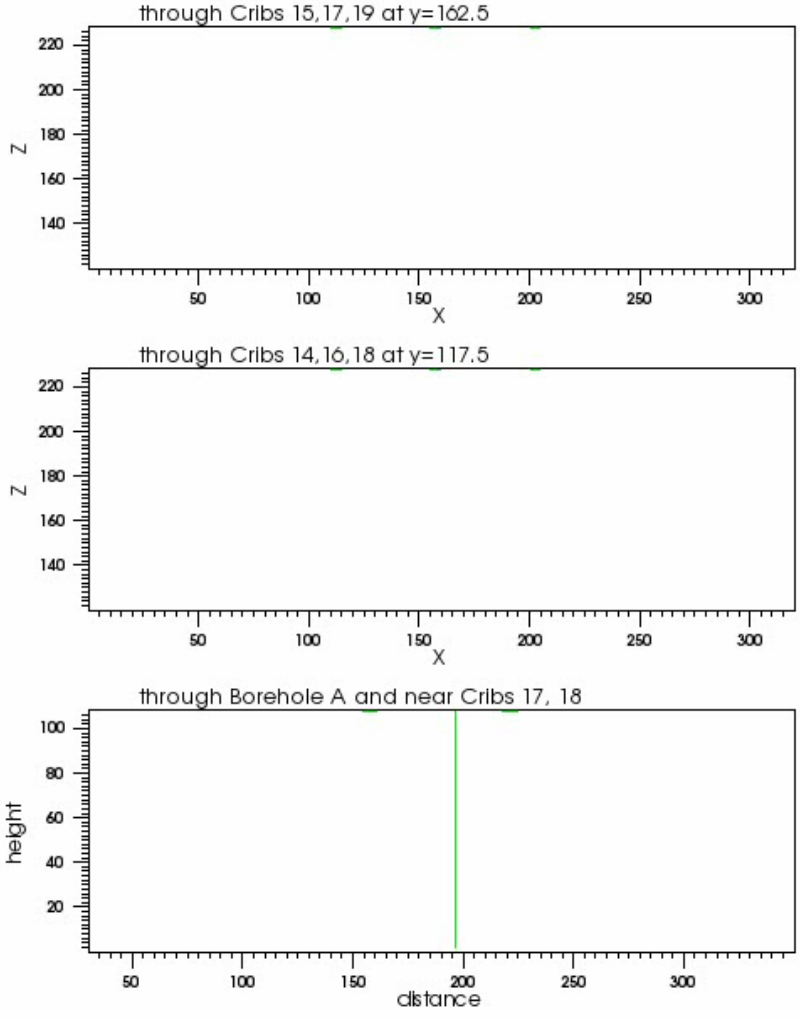
4. Simulation Results - Visualization





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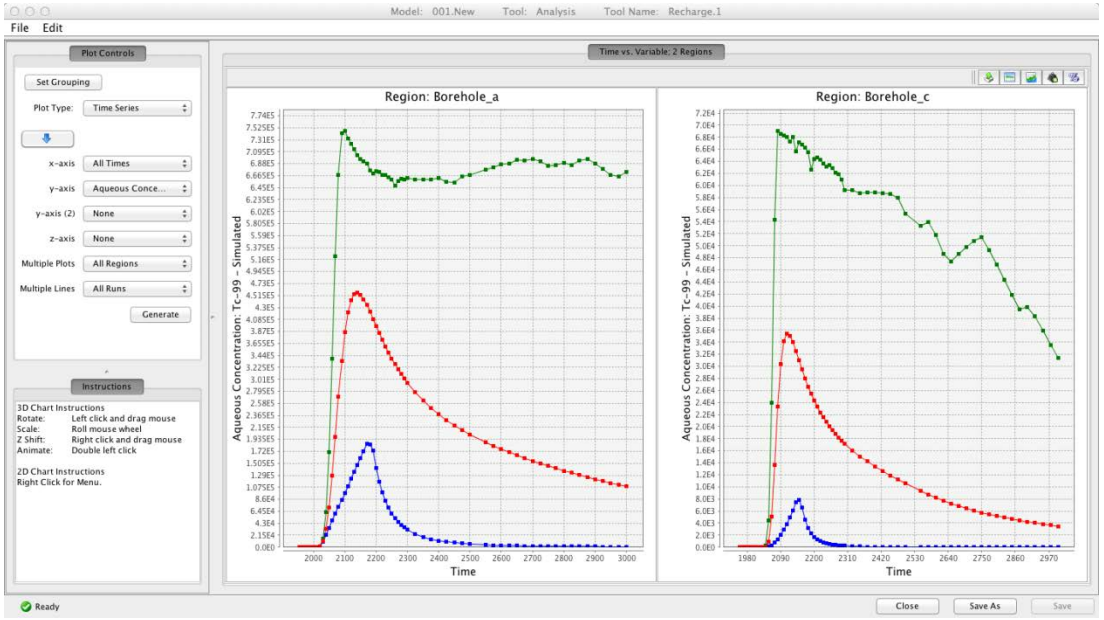
5. Uncertainty Quantification (UQ)

Akuna UQ Visualization

- Varied rainfall rate for 100 simulations for 2012 – 3000
  - Rates represent management actions
- Metrics
  - Travel times to water table
  - Peak concentration and arrival time
  - Time at which a threshold concentration is exceeded
  - Time period of exceedance



Mean and 95% confidence intervals for the Tc-99 breakthrough curves beneath Boreholes A and C

Future Development

- Akuna:
  1. Enhance UQ, PE, SA capabilities
  2. Tight integration of visualization and analysis
  3. Usability enhancements based on user feedback
  4. Initial Decision Support Toolset
  5. Incorporation of Risk Evaluation toolset

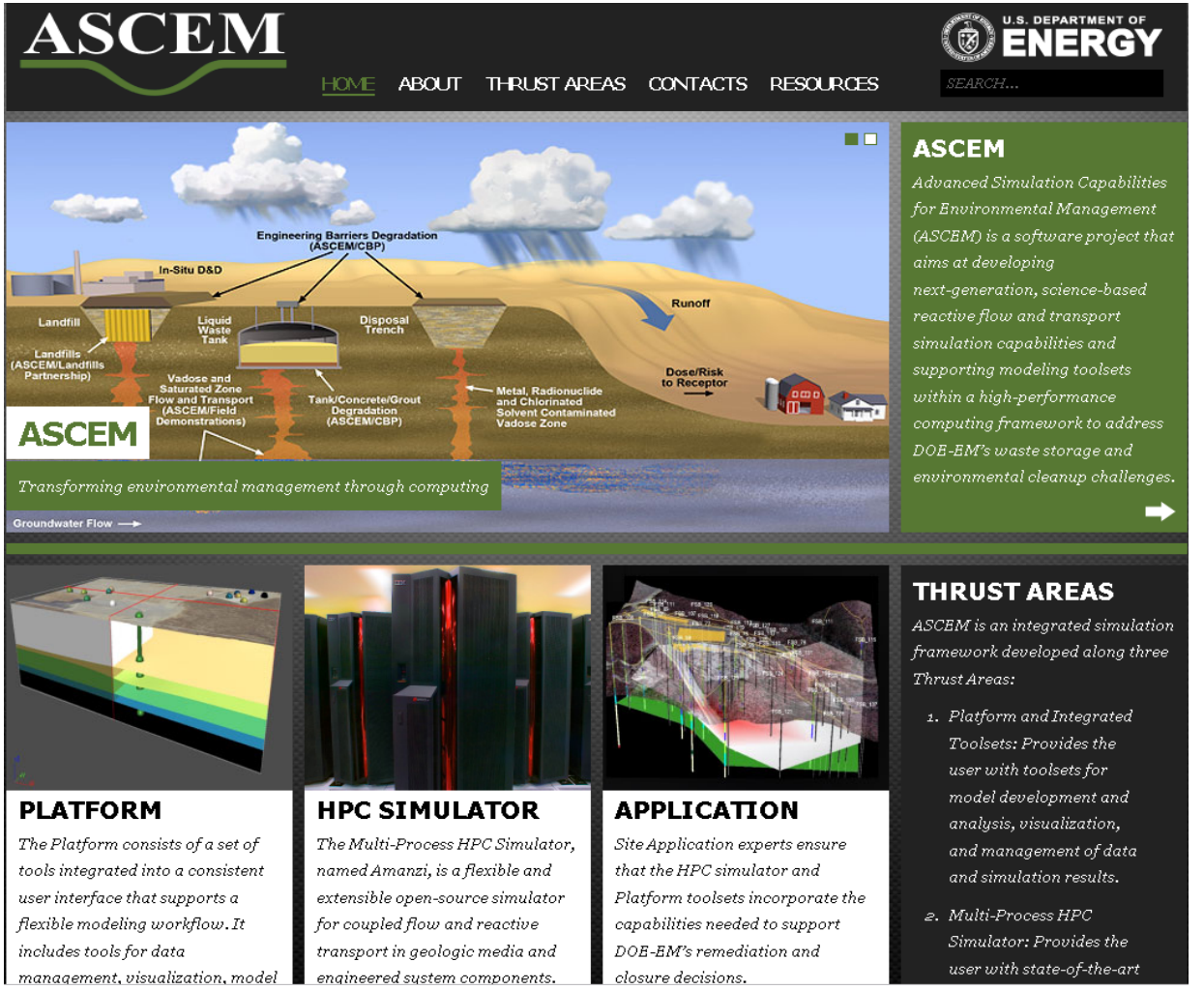
- Amanzi:
  1. Enhance performance on emerging architectures
  2. Flexible and extensible interface for geochemistry
  3. Multi-phase flow with thermal processes for modeling desiccation

- BC Cribs:
  1. Phase II Demo established baseline conditions for Tc-99 transport
  2. Subsequent demos will examine impact of remedial technologies (e.g., soil desiccation)

- Enhance outreach and application to sites demonstrating the potential impact of minimizing abstractions and flexible “what if” analysis.

- NQA-1 qualification of ASCEM codes for regulatory release

Questions



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