ADVANCED SIMULATION CAPABILITY FOR ENVIRONMENTAL MANAGEMENT: INTEGRATED TOOLSETS AND SIMULATOR THAT CAN ENHANCE PUBLIC COMMUNICATION

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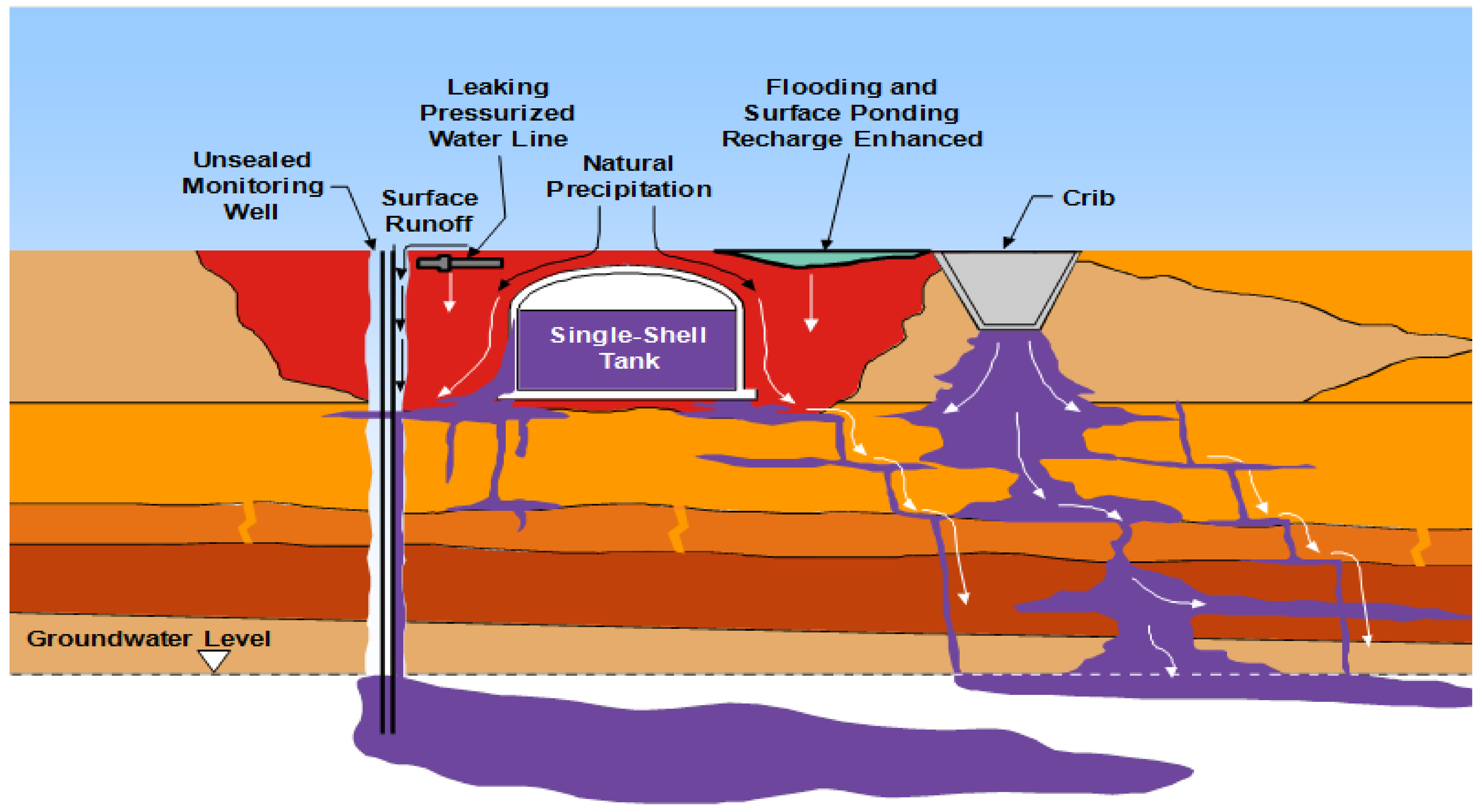
Challenge: Most of the remaining contaminated sites in the EM complex to undergo remediation require additional characterization, most require final remediation decisions, and all of them will require long-term monitoring. The Advanced Simulation Capability for Environmental Management (ASCEM) program is developing an integrated suite of open-source tools that will enable a graded and iterative approach to risk and performance assessments at these waste sites.



Mission: The ASCEM initiative supports the reduction of uncertainties and risks associated with DOE EM's cleanup and closure environmental programs by better understanding and quantifying the subsurface flow and contaminant transport behavior and the long-term performance of engineered components in complex geological systems. The ASCEM team is leveraging DOE investments in basic science and applied research including codes developed through the Advanced Scientific Computing Research and Advanced Simulation & Computing programs as well as collaborating with the Offices of Science and Nuclear Energy.

ASCEM Team: The team is composed of scientists and engineers from four National Laboratories.

Los Alamos National Laboratory EST.1943 · Pacific Northwest National Laboratory · Berkeley Lab · Oak Ridge National Laboratory · SRNL Savannah River National Laboratory

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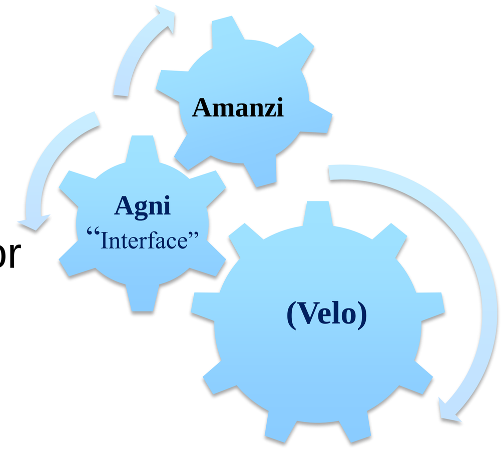
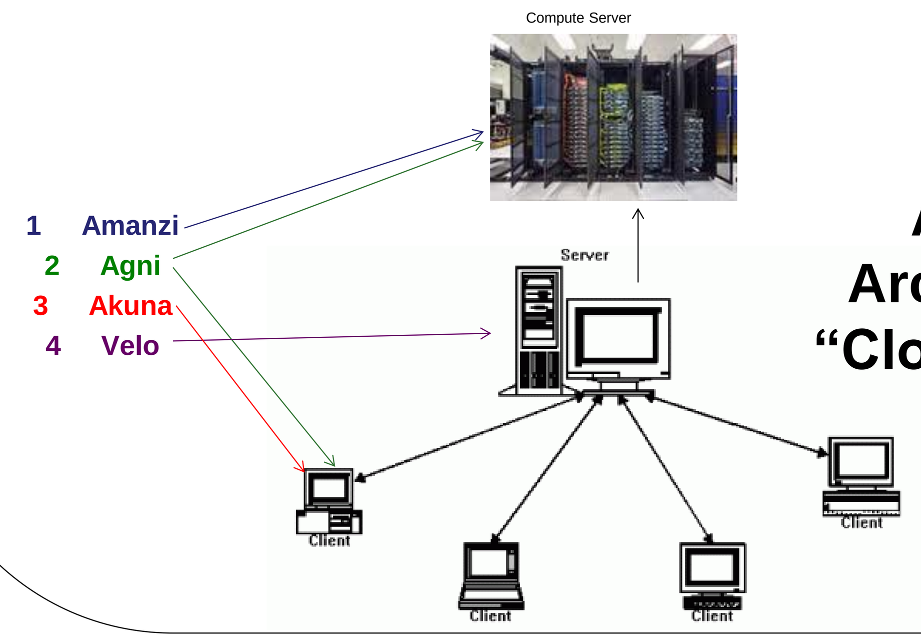
ASCEM Architecture:

ASCEM is managed by a multi-laboratory management team and an NQA-1 compliant QA effort overseeing the ASCEM tool development. The ASCEM program is managed around three

Thrust Areas:

- *Platform and Integrated Toolsets* develops pre- and post-processors that support the modeling workflow. The Toolsets include:
  1. ***Agni*** – the simulation controller
  2. ***Velo*** – the content management system
  3. ***Akuna*** – the modeling workflow UI
- *Multi-Process HPC Simulator* develops **Amanzi,** the flow and reactive transport simulator
- *Site Applications* deploys demonstrations at the sites, and works with potential site users





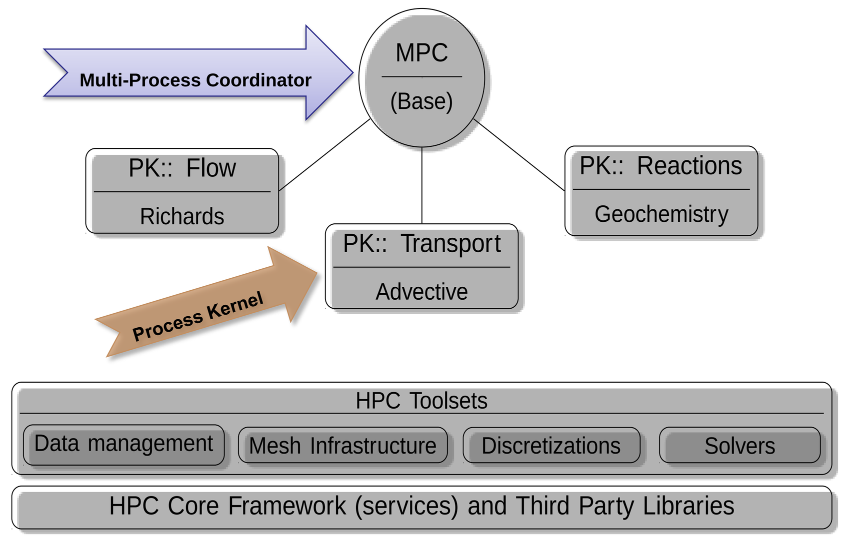
ASCEM Architecture "Cloud Based"

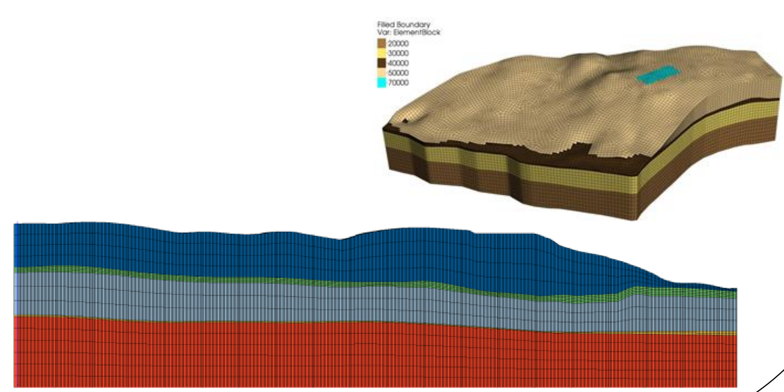
Multi-Process High Performance Computing (HPC) Simulator Thrust

Amanzi uses a hierarchical and modular design that reflects the steps in mapping a conceptual model to a numerical model and producing output for analysis. The ASCEM computational engine is a state-of-the-art extensible, open-source, high performance computing (HPC) modeling system.

Current capabilities:

- Transient unsaturated flow (Richards) and single-phase flow (specific storage/yield)
- Unstructured meshes (polyhedral cells)
- Block-structured AMR
- Volume based sources
- Reactive-Transport (with operator splitting)
- Dispersion (with non-grid aligned flow)
- Alquimia provides a unified API and interface library to simplify the process of using different chemistry engines



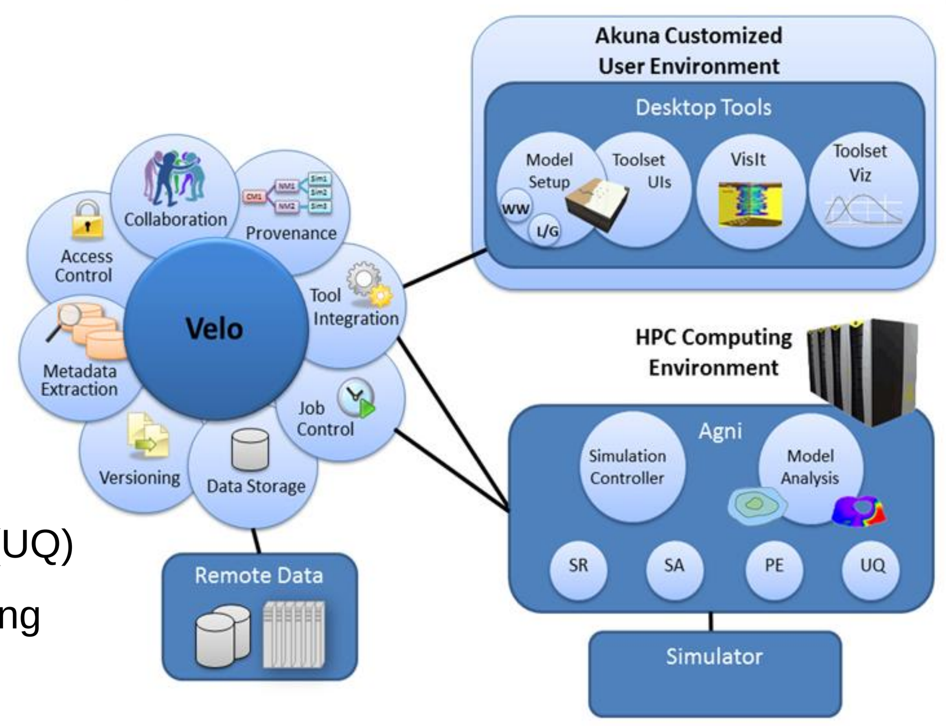


Platform and Integrated Toolsets Thrust

Akuna is an open-source Java-based user environment that supports a complete modeling workflow, from model setup through simulation and analysis.

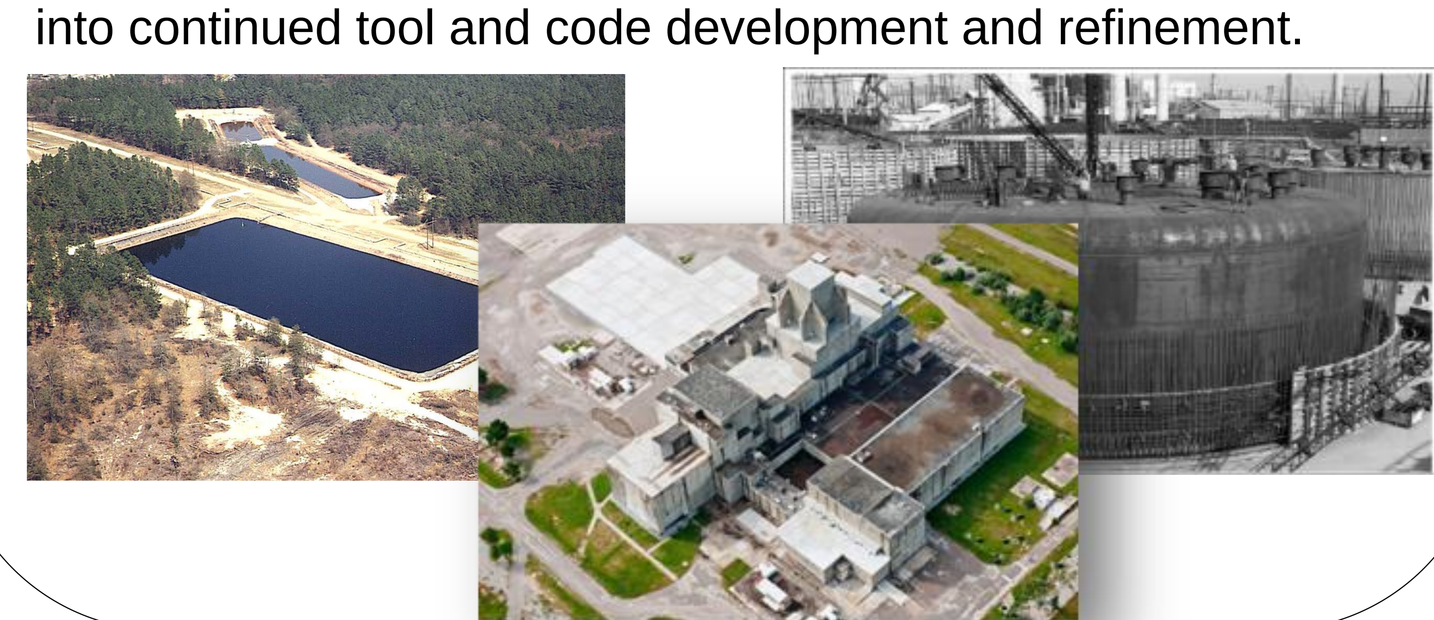
Platform Toolsets:

- Model Setup
- Simulation Toolsets
- Single-Run (SR)
- Sensitivity Analysis (SA)
- Parameter Estimation (PE)
- Uncertainty Quantification (UQ)
- Job launching and monitoring
- Visualization Toolsets
- Supports model execution on diverse computational platforms



Site Applications Thrust:

This Thrust provides expertise and site data for ASCEM capability demonstrations, applications supporting the AFRI test beds, and deployments to specific DOE EM site problems. A key aspect is to provide testing and feedback for developing the HPC and Platform components based on user experience, to disseminate information, and provide training. Along with the ASCEM Regulatory Liaison, this Thrust also establishes contact with end users, solicits their input and conveys this information into continued tool and code development and refinement.



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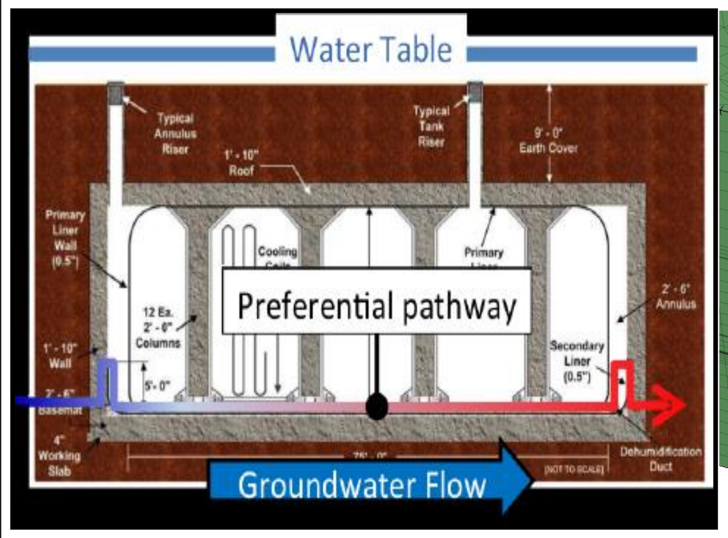
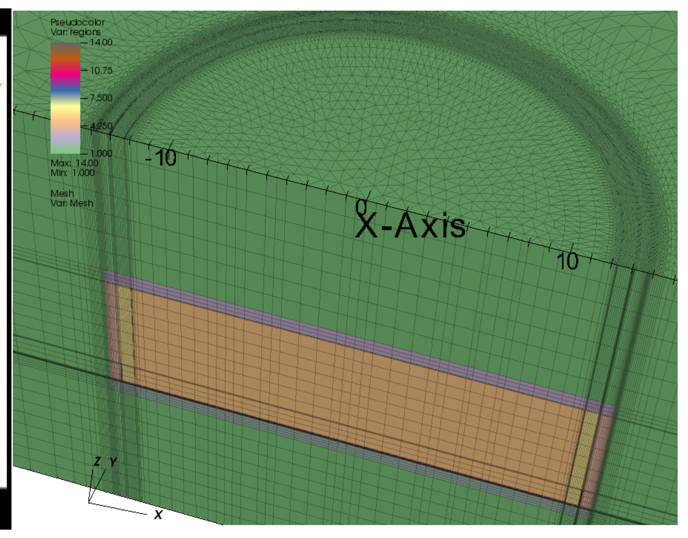
Savannah River Site (SRS) Waste Tank Closure

Several waste tanks in the SRS H Tank Farm are fully or partially submerged below the water table. The NRC issued a Technical Evaluation Report identifying concerns that the H Tank Farm PA does not adequately assess waste release from the submerged and partially submerged tanks via preferential pathways and that a low-permeability cover will not isolate these tanks from subsurface flow. Rigorous simulation of the flow field around a submerged tank and through a preferential pathway requires 3D modeling with a variable resolution mesh.

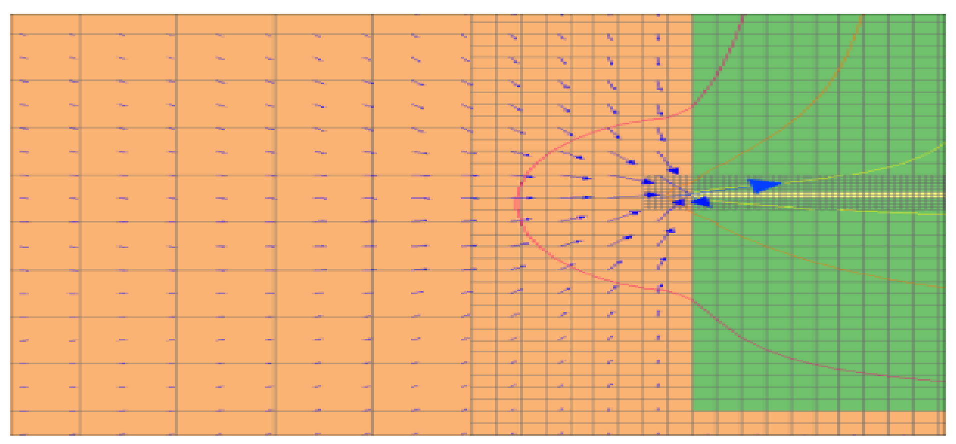
The Amanzi HPC simulator meets these modeling requirements

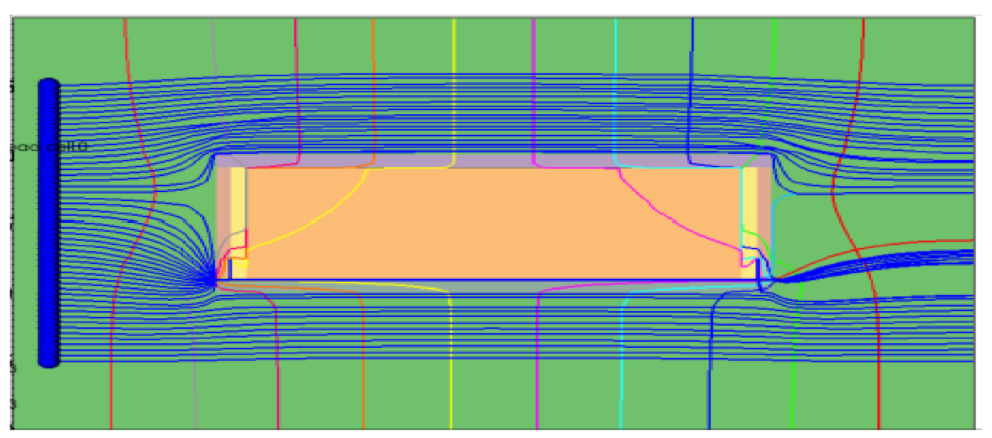
The conceptual model for a central cross-section with preferential flow paths is shown (left), along with the three-dimensional unstructured mesh with preferential flow paths (right). Structured AMR and unstructured capabilities of Amanzi are being demonstrated.





The numerical model for the two-dimensional structured mesh with calculated flow vectors for a preferential flow path on the central cross-section (top figure below) and calculated path lines (bottom figure) with preferential flow paths were generated using four levels of mesh refinement.



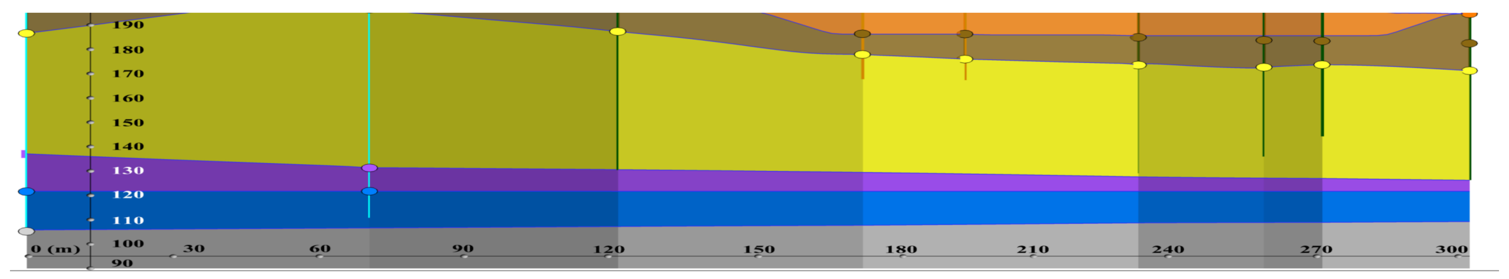


Site Application Examples:

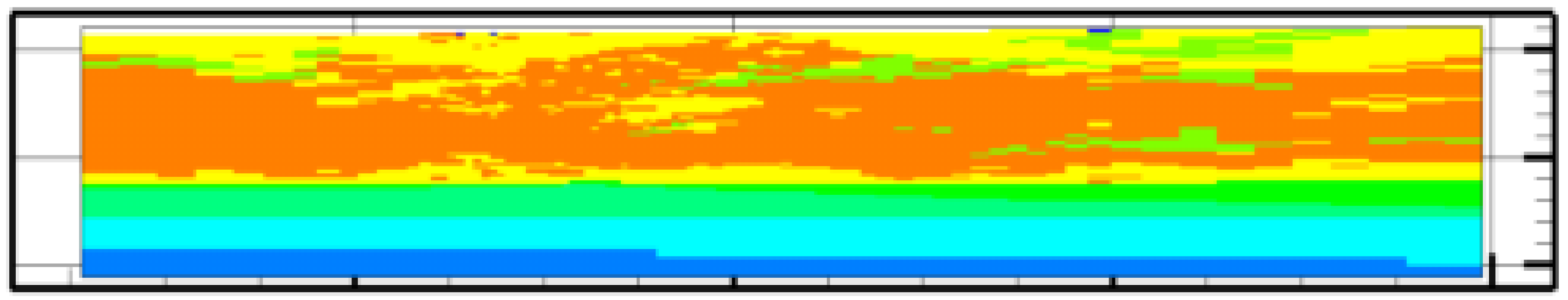
Hypothetical Calculations for Residual Waste Release in Vadose Environments:

Comparison of Geological Heterogeneities

Geological conceptual model based on major stratigraphy



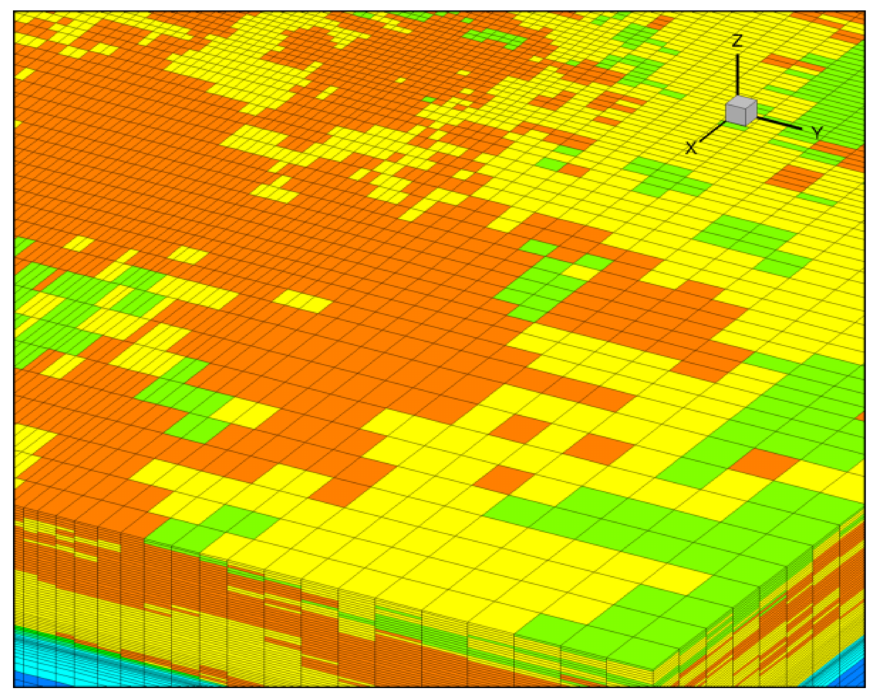
Geologic conceptual model incorporating heterogeneities (based on KUT data using sequential indicator simulation)



Hydraulic property estimates differed between the models because there is not a 1:1 correspondence between major stratigraphy and lithofacies

Simulation Setup:

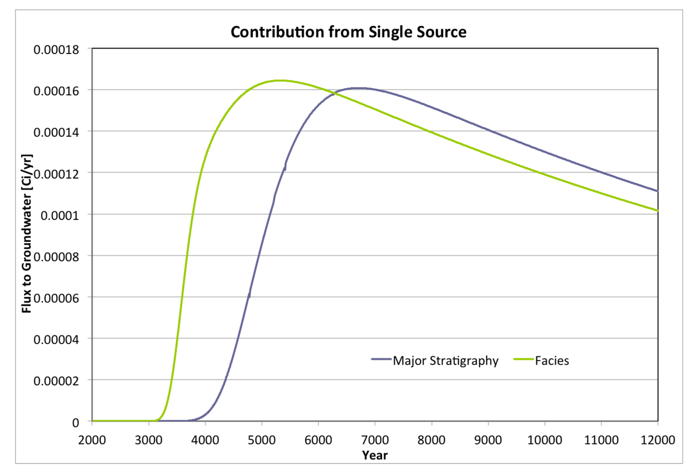
1. Diffusive release of conservative solute
2. Recharge boundary condition at surface
3. Water table at bottom of domain



Preliminary Results

Compared mass flux to water table for major stratigraphy and facies-based model for both

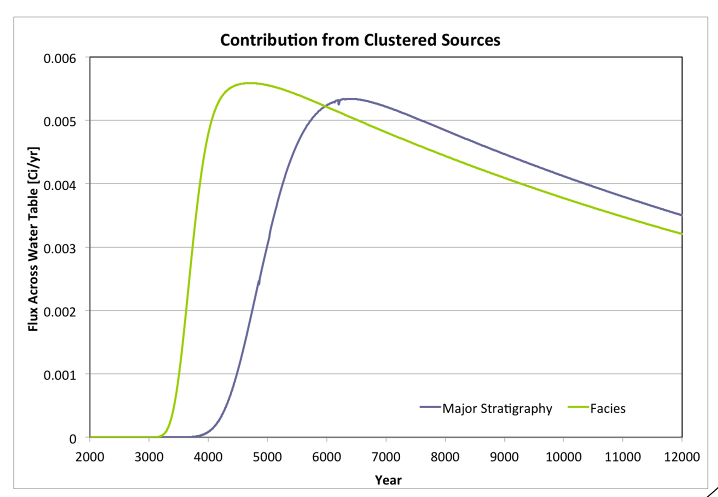
- ❖ Individual residual source
- ❖ Group of clustered residual sources



Principal impact between different conceptual models

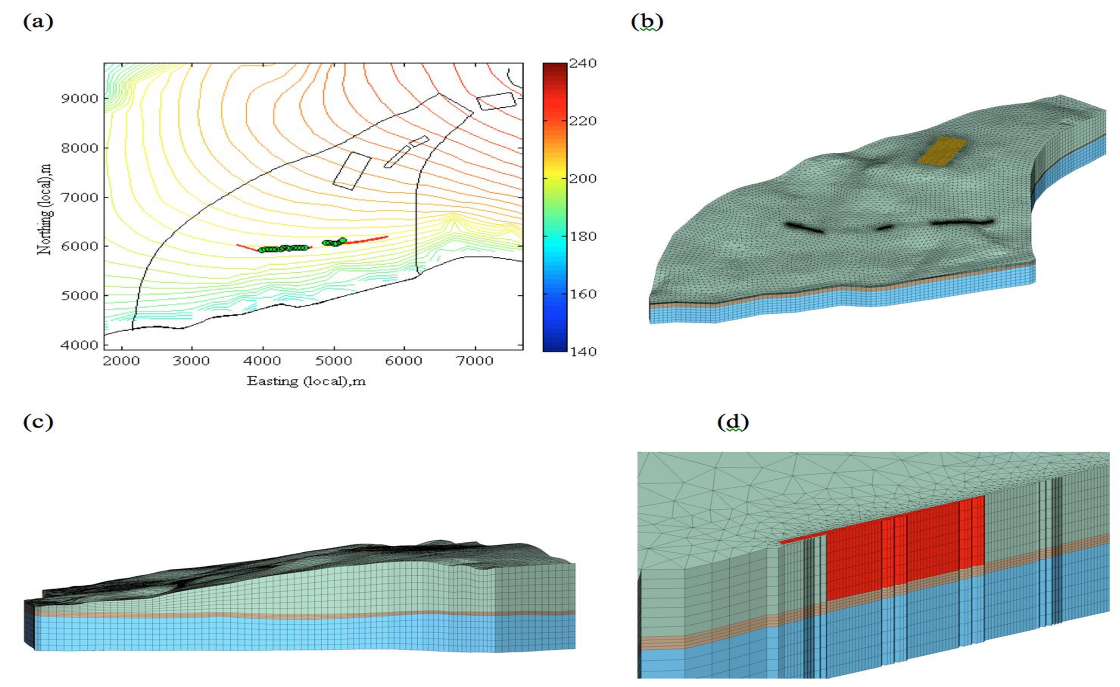
- ❖ Peak concentration delayed by nearly 3000 yrs
- ❖ Peak concentration decreased ~10%

Impacts most likely due to differences in hydraulic property assignment



Savannah River Site (SRS) F-Area Seepage Basins

The SRS F-Area seepage basins (below, upper left) were constructed as unlined impoundments for low-level waste solutions from the F-Area Separations facility. The basins were closed in 1989, capped in 1991, with recent remediation focused on using a base injection to neutralize the acidic groundwater, and retard the contaminant plume.



The modeling domain is shown on the left along with flow barriers. The unstructured prismatic mesh is shown on the right with the refinement around the barriers clearly visible.

Plume Modeling results

The plume lies directly below the basins in 1955 (upper left). By 1968 the plume is beginning to migrate towards the four-mile branch. By 2005 (lower left), some of the plume is hitting the barriers and being forced through the gates for base injection, and by 2055 (lower right) the plume is shrinking.