Applications Using the Advanced Simulation Capability for Environmental Management Toolset – 16335

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ABSTRACT

The Office of Soil and Groundwater of the U.S. Department of Energy (DOE) Office of Environmental Management (EM) developed the Advanced Simulation Capability for Environmental Management (ASCEM). The ASCEM toolsets can be used for making informed choices in uncertain and complex environments, where cost-benefits of environmental impacts and human health need to be considered. The deployments and demonstrations show how ASCEM provides a unified framework that facilitates efficient modeling and analyses to address costs and benefits of engineering and remediation decisions:

- Evaluation of engineered remediation and monitoring strategies at the Savannah River Site (SRS) F-Area in collaboration with the Office of Soil and Groundwater Remediation, Attenuation-Based Remedies in the Subsurface Applied Field Research Initiative
- Assessment of performance assessment issues and waste tank closure at SRS
- Evaluation of alternative conceptual models for the deep vadose zone at the Hanford Site, supporting waste tank closure

The ASCEM toolsets enable computationally efficient representations of the complex subsurface systems, including fractured and faulted volcanic and carbonate aquifers, a very deep water table, and multiple contaminant sources. The applications demonstrate that deployment of the ASCEM toolsets provides an opportunity to reduce conservatisms in modeling assessments and allows detailed investigation of alternative conceptual models.

INTRODUCTION

The Office of Soil and Groundwater Remediation within the U.S. Department of Energy (DOE) Office of Environmental Management (EM) developed the Advanced Simulation Capability for Environmental Management (ASCEM). ASCEM provides a workflow [1] consisting of a set of pre- and post-processing tools for translating conceptual models to numerical models. This workflow is based on cloud computing that allows users access to high-performance computing resources. Multiple toolsets are available, including model setup, calibration, sensitivity analysis, and uncertainty quantification; both risk and decision support toolsets are being developed. ASCEM promotes collaborative modeling through file access for multiple users on a shared server.

ASCEM is a modular and open source software infrastructure for understanding and predicting contaminant fate and transport in natural and engineered subsurface systems. The ASCEM toolset facilitates integrated approaches that enable standardized assessments of performance and risk for EM cleanup and closure decisions. The ASCEM project is using a phased deployment approach, starting with site applications that were used to guide software development, and currently with initial deployments to provide technical underpinnings for performance assessments. The deployments include the Savannah River Site (SRS) F-Area, a performance assessment at the SRS H Tank Farm, and evaluation of the deep vadose zone (DVZ) at the Hanford Site.

SAVANNAH RIVER SITE F-AREA

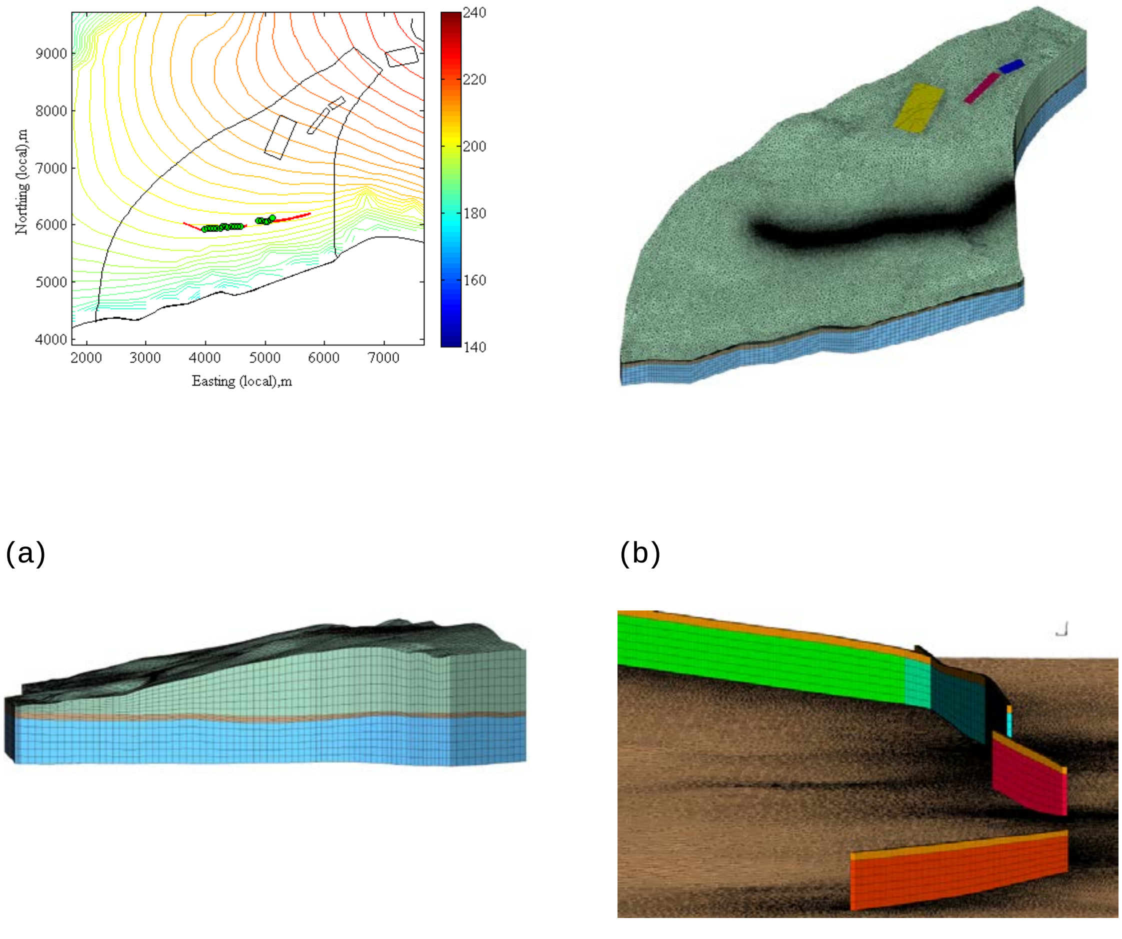
The SRS F-Area working group tested and deployed new capabilities to apply an integrated flow-geochemistry-transport model at the F-Area. The advanced simulation capabilities enabled a systems-based approach that integrates laboratory and field measurements with modeling for long-term management of remediation and monitoring of metals and radionuclides. The model was also applied to explore a new approach for long-term monitoring based on continuous in situ monitoring of geochemical master variables such as pH, electrical conductivity, and water table that control the plume mobility. The ASCEM capabilities 1) provided mechanistic and predictive understanding of contaminant plume mobility and behavior, and 2) were used to evaluate the sensitivity and effectiveness of new monitoring approaches.

The F-Area working group applied the ASCEM software to evaluate the effects of past and current engineering systems on flow and the geochemical conditions of the site, and to predict the time frame for transition from active remediation to monitored natural attenuation. A three-dimensional flow and reactive transport model of the F-Area was developed and modified in 2015 to describe the impact of engineered systems and complex geochemical conditions at the site. The Uncertainty Quantification (UQ) toolsets were applied to compute the uncertainty range of predictions for robust decision-making. The model was also used to assess the efficacy of the long-term monitoring strategies through advanced visualization and modeling. The model was used to estimate the plume extent, determine the optimal layout of a monitoring network, and understand the effect of master variables on contaminant mobility.

The three-dimensional hydrological model is based on a previous flow model developed for a larger domain encompassing the overall General Separations Area

(GSA) at SRS [2]. The flow velocity field computed in the GSA flow model was used to define a model domain that follows natural hydrogeologic boundaries (Fig. 1). The hydrostratigraphic units were updated based on recently collected cone penetrometer testing data and surface seismic data [3]. The depth of the Tan Clay, which is known to significantly affect uranium transport, is accurately represented in the new model domain. In addition, the new model includes low-permeability engineered barriers, which were constructed part of the funnel-and-gate system in 2004.

The final mesh used in this study has 1,849,039 cells and 982,998 vertices, representing an order of magnitude greater refinement than the previous model of the GSA [2]. The increased mesh refinement allowed realistic representation of boundary conditions and engineered features in the model.



(a)

(b)

(c)

(d)

Fig. 1. (a) Plan view of the model domain, (b) three-dimensional mesh including three hydrostratigraphic units, the F-Basin site (yellow), and each of the three barriers (red), (c) a cross-section view of the mesh, and (d) a cutaway of the mesh showing the barriers (red, blue, and green) and the Tan Clay interface (brown). In (b) and (c), the top green material region is the upper

aquifer, the middle brown layer is the Tan Clay confining zone, and the bottom blue region is the lower aquifer.

Fig. 2 shows the predicted evolution of the tritium plume. This simulation includes capping of the seepage basin and placement of the low-permeability barriers by changing the barrier material in 2004. The plume initially moves straight down until it hits the water table and then migrates laterally within the upper aquifer. The simulation illustrates the effect of the engineered barrier, and the model predicted that significant tritium was trapped in the vadose zone, showing the long-term effect of capping the basin.

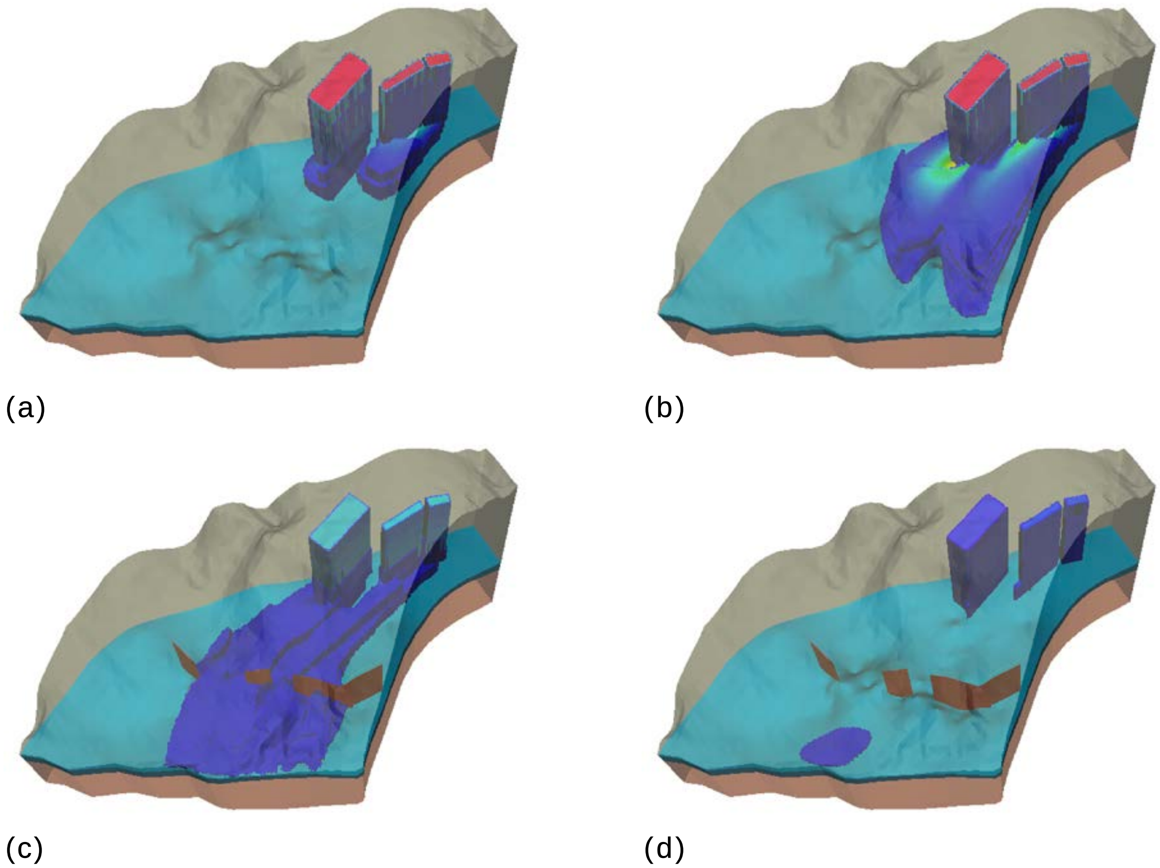


Fig. 2. Simulated tritium plume evolution in the three-dimensional flow and transport model: (a) 1955, (b) 1968, (c) 2005 and (d) 2025. The threshold of 1×10^{-12} mol/L is used to draw the plume boundary, and the brown vertical structures depict the barriers.

The model was used to evaluate the efficacy of different remedial options based on the tritium transfer rate from the site into the creek. Predictions show that capping the basins and installing barriers significantly reduces the flux by up to 30%. Although the model has not been fully calibrated, these results highlight Amanzi's ability to simulate a complex flow process involving seepage, waste discharge, and barriers. This is the first time that Amanzi has been used to simulate large-scale evolution of a three-dimensional plume taking into consideration the effects of variable topography, sharp permeability contrasts, and different remedial options.

While the three-dimensional reactive transport model was under development, correlations between master variables (pH, water table, electrical conductivity) and contaminant concentrations were evaluated using 250 realizations of a two-dimensional model developed by Bea et al. [4]. The correlations between predicted uranium concentrations and pH show they are strongly correlated over time, particularly in the trailing edge of the plume. Additional detail regarding the simulations and results can be found in Wainwright et al. [5].

H TANK FARM PERFORMANCE ASSESSMENT

The H Tank Farm (HTF) focused on an SRS-specific performance assessment. The HTF performance assessment provided an opportunity for testing structured and unstructured capabilities of Amanzi in two- and three-dimensions. The ASCEM toolset was deployed to address a technical concern expressed during a Nuclear Regulatory Commission review of the HTF performance assessment. The specific concern is that the assessment does not adequately assess waste release from the submerged and partially submerged tanks via a preferential pathway [6]. The primary radionuclides of concern with respect to this are strontium-90 (Sr-90) and cesium-137 (Cs-137).

The current HTF performance assessment is based on axi-symmetric flow conditions around the cylindrical waste tanks, and the model uses a two-dimensional radial slice. This representation is adequate for tanks above the water table, where the moisture flow is nominally downward. However, for a fully or partially submerged tank subjected to regional groundwater flow in the aquifer, the flow field is three-dimensional and cannot be accurately represented by the two-dimensional radial flow field. Three-dimensional modeling using a conventional flow and transport simulation code was previously pursued by the SRS performance assessment contractor for a generic scenario. The resulting baseline three-dimensional model was computationally demanding and could not adequately resolve thin geometric features due to meshing constraints. The ASCEM toolset was applied to overcome these difficulties by incorporating more-efficient meshing capabilities, such as adaptive mesh refinement (AMR), flexible unstructured gridding, and using high-performance computing numerical algorithms and hardware. This application resulted in answers to concerns that could not be addressed with baseline computational capabilities.

Fig. 4 illustrates a simplified conceptual model for implementation in Amanzi. A fast flow path is postulated to pass through a concrete construction joint, a shrinkage and/or corrosion gap around the secondary steel liner, a residual waste layer in the annulus, and the sand padding separating the steel liners. The fast-flow path and liner features are exaggerated in thickness by 10 times in Fig. 4b for clarity, but represented at true thickness in Amanzi simulations. Material properties and boundary conditions are representative of values published in [7] and were selected in consultation with the SRS performance assessment contractor.

ASCEM provides two basic meshing capabilities: structured with AMR and unstructured. The structured mesh (Fig. 5) uses AMR to achieve higher grid resolution where needed. The unstructured mesh (Fig. 6) uses grid cells of variable shape and density in a single grid to achieve local refinement. Both approaches were evaluated in the HTF application.

Initial simulations were performed for a two-dimensional slice through the center of the tank using structured AMR and unstructured hex grids. Fig. 7a shows a highly detailed AMR simulation of a non-sorbing and non-decaying tracer after 1000 years, about the time the plume begins discharging to the fast-flow path exiting to backfilled soil.

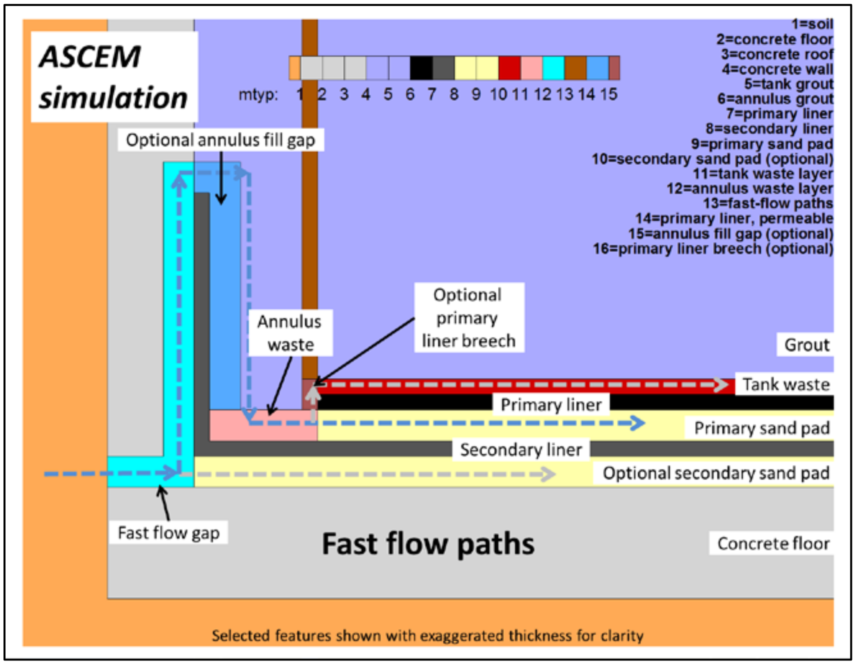


Fig. 4. Geometry of the conceptual tank features and preferential flow path.

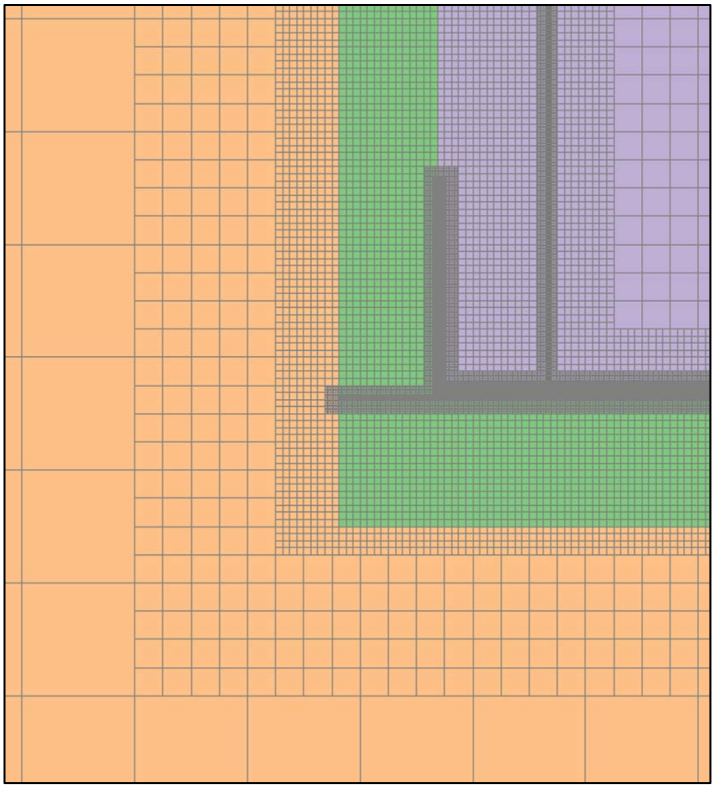


Fig. 5. Structured AMR grid implementation for submerged tank scenario showing four refinement levels at four times each (profile view at time zero).

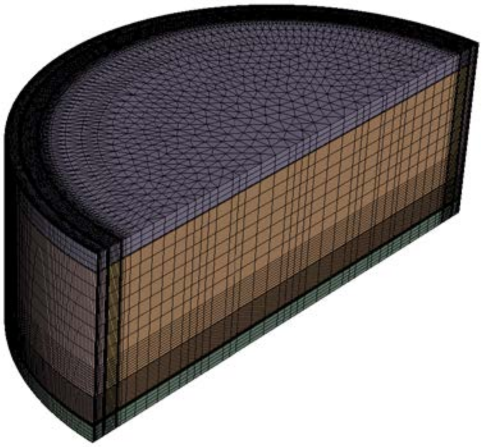


Fig 6. Unstructured grid implementation for submerged tank scenario.

Fig. 7b shows the analogous result for less detailed unstructured grid resolution to increase computational efficiency for a three-dimensional simulation. Greater numerical dispersion from the coarser mesh increases plume spreading and causes earlier initial discharge to the fast-flow path exit. Both effects significantly reduce the peak concentration for a non-conservative assumption for a non-decaying species. However, the opposite is true for a decaying species with a half-life shorter than the advective travel time. In this case, greater plume dispersion allows a portion of the plume to reach the exposure point before the species decays away in transit. Sr-90 and Cs-137 each have a half-life of approximately 30 years, which is short relative to the effective travel time of 1200 years. This nominal travel time is equivalent to about 40 half-lives, which results in decay attenuation for the plume center-of-mass. Thus, dispersion has significant impact on concentrations in the plume leading edge, and a coarser grid will generate conservative predictions for Sr-90 and Cs-137.

Both the structured AMR and unstructured hex grid simulations predict significant dilution of the species concentrations slowly exiting the wall-floor and mixing with a relatively high aquifer velocity field in the surrounding backfill soil. Tracer concentrations immediately outside the fast-flow path are ~25 to 50 times lower than those inside the wall-floor joint. Decay over the nominal travel time of 1200 years and dilution in the aquifer result in insignificant Sr-90 and Cs-137 concentrations in backfill soil.

Rigorous representation of the full three-dimensional tank geometry demonstrates that the two-dimensional analog is substantially conservative (Fig. 8). Unlike the two-dimensional simulations, the wall-floor joint and wall-liner gap form a continuous flow pathway between the up-gradient and down-gradient sides of the tank (Fig. 8, top image), which reduces the hydraulic gradient across the waste zones. As a result, the three-dimensional simulation indicates orders of magnitude lower concentrations outside the tank compared to two-dimensional simulations.

The results demonstrate that deployment of the ASCEM toolset provides an opportunity to reduce conservatisms in performance assessment of closed HTF waste tanks under certain conditions through three-dimensional, high-resolution flow and transport simulation.

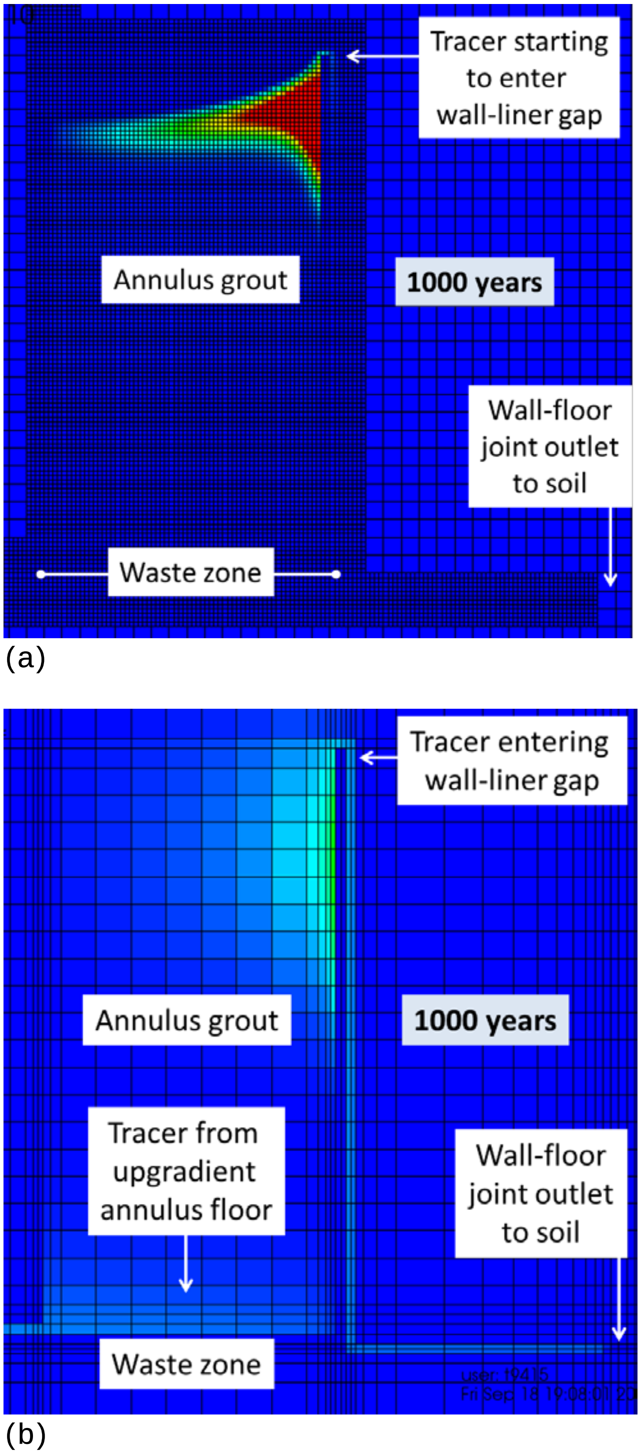


Fig. 7. Simulated two-dimensional tracer transport for (a) structured AMR and (b) unstructured hex grids.

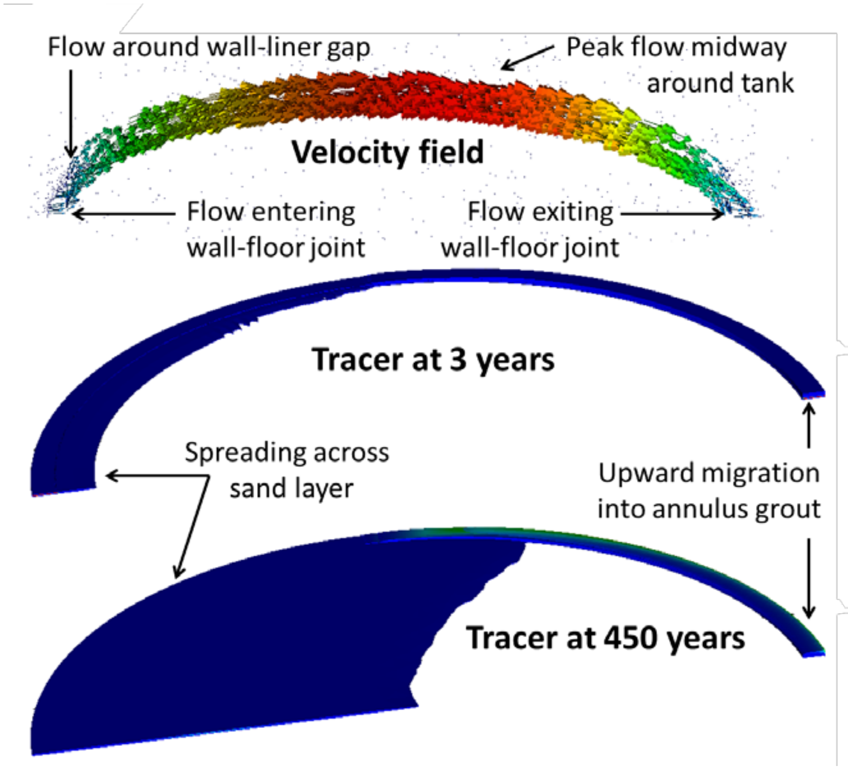


Fig. 8. Simulated velocity field and tracer transport for three-dimensional tank geometry.

DVZ WORKING GROUP

The DVZ working group focused on a demonstration of ASCEM to evaluate alternative conceptual models associated with a performance assessment of the single-shell tank (SST) Waste Management Area C (WMA C or the 241-C Tank Farm) at the Hanford Site. The performance assessment is being conducted by the DOE Office of River Protection for closure of WMA C.

The WMA C performance assessment will assess the fate and transport of radionuclides and hazardous chemicals for residual wastes left in tanks and ancillary equipment and facilities. Under this closure scenario, fate and transport calculations will be used to estimate concentrations at downstream locations in the groundwater. While the performance assessment considers a wide range of processes contributing to contaminant transport and exposure pathways, concerns have been voiced over only using major stratigraphy to describe the geologic conceptual model. As shown in the ASCEM Phase II demonstration at BC Cribs [8], heterogeneities may be an important feature impacting subsurface flow and transport. The Hanford DVZ working group used the ASCEM toolset to investigate the possible impact of heterogeneities on the long-term fate and transport of tank residuals.

The DVZ demonstration of ASCEM used a geostatistical approach that focused on representing sediment types to describe heterogeneity within each stratigraphic unit. The sediment types were identified by multivariate analysis of spectral gamma ray data from direct-push boreholes and were represented with different geological and hydrological properties. Several realizations of the conceptual model were used as input for flow and transport models using Amanzi to examine the potential range of behavior in flow and transport.

An unstructured mesh was used to represent discontinuous material types and properties as well as engineered features (e.g., tanks) within WMA C. Preliminary results showing hypothetical technetium-99 (Tc-99) plumes for three conceptual model realizations at one snapshot in time (year 3520) are shown in Fig. 9. Fig. 10 shows breakthrough curves of flux-average Tc-99 concentrations at a 100-m down-gradient plane for the same three realizations. The results shown in these figures indicate that the facies-based representation of subsurface heterogeneity at WMA C yields similar transport behavior, attributable to the subtle differences in the distributions of the three facies, and the similarities in their parameters.

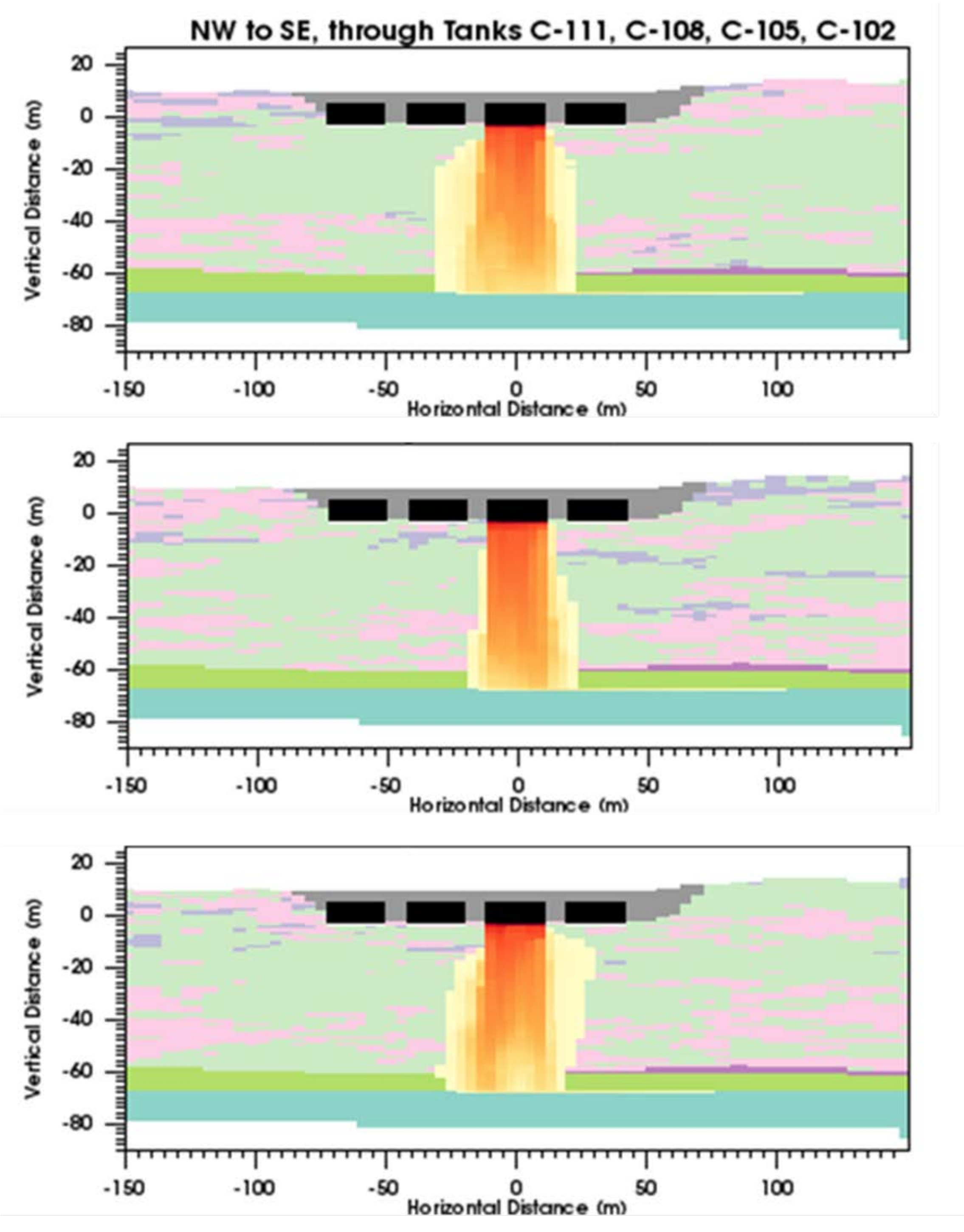


Fig. 9. Snapshots of a hypothetical Tc-99 plume from residual tank wastes at year 3520 for three conceptual model realizations of the subsurface for WMA C.

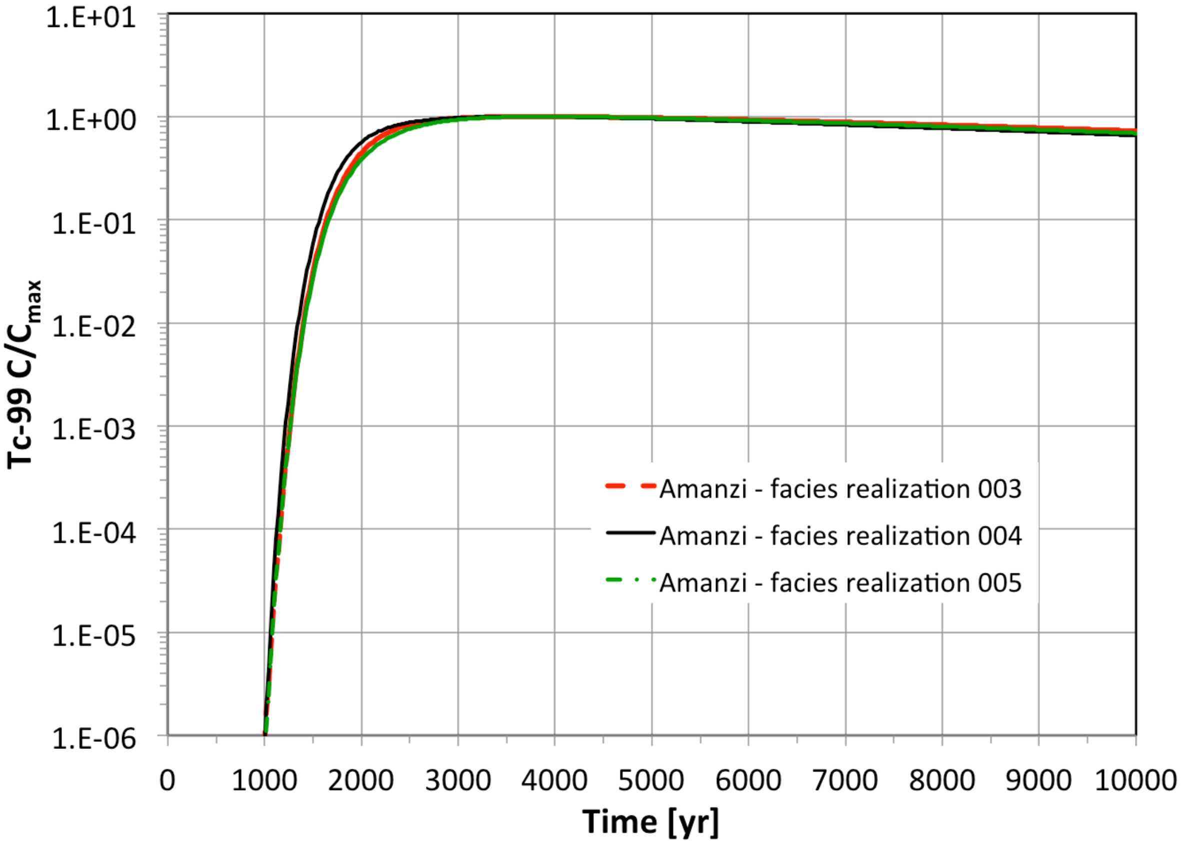


Fig. 10. Preliminary flux-average concentration results at a 100-m down-gradient plane.

CONCLUSIONS

The demonstrations and deployments are intended to highlight ASCEM capabilities for evaluation of remediation strategies and performance assessments over baseline capabilities. Development of ASCEM has matured to the point where it was deployed to address specific issues facing the SRS and Hanford Site.

Modeling is a tool that can be used for making informed choices in uncertain and complex environments, where cost-benefits of environmental impacts and human health need to be considered. The Akuna software integrated with Amanzi provides a unified framework that extends simulation capabilities, facilitates efficient modeling and analyses, and can address costs and benefits of decisions made at waste sites. This efficiency, and ease of access to analysis methods, maximizes available information to address and mitigate sources of uncertainty in subsurface analyses.

The analysis of the SRS F- Area included detailed simulations using a three-dimensional unstructured mesh that accounted for fine-scale discretization to represent the engineered barriers, seepage basin, and injection/extraction wells. Increased mesh refinement allowed realistic representation of boundary conditions and engineered features in the model. Simulation of the system included changes over time for capping the seepage basin and placement of the low-permeability barriers in 2004, a significant improvement in modeling dynamic changes of engineered systems. Access to high-performance computing resources enabled a more refined mesh and model complexity to be simulated. A two-dimensional model was used to correlate between master variables (pH, water table elevation, and electrical conductivity) and contaminant concentrations. These results confirm the effectiveness and robustness of a new approach for long-term monitoring using master variables, although they need to be compared with the three-dimensional reactive transport model.

For the waste tank performance assessment, two- and three-dimensional flow and transport simulations were completed to assess waste release from submerged and partially submerged tanks via a preferential pathway. Results from two- and three-dimensional modeling revealed the critical need for three-dimensional modeling to correctly represent the influence of fast-flow path features on advective flow through residual waste zones. The results demonstrate that deployment of the ASCEM toolset provides an opportunity to reduce conservatisms in performance assessment of closed HTF waste tanks under certain conditions through three-dimensional, high-resolution flow and transport simulation.

The Hanford DVZ application was used to investigate the possible impact of heterogeneities on the long-term fate and transport of tank residuals at WMA C. The demonstration included significant effort to test new capabilities of Amanzi to handle engineered features and improve robustness of the simulator. The demonstration showed that ASCEM can be used to evaluate alternative conceptual models and uncertainty without the need for simplifying assumptions to meet computational requirements.

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