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Enhancing Performance Assessments Using the ASCEM Toolset - 15222

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ABSTRACT

The Office of Soil and Groundwater Remediation within the U.S. Department of Energy's Office of Environmental Management (EM) is supporting development of the Advanced Simulation Capability for Environmental Management (ASCEM). ASCEM is an open source and modular computing framework that incorporates new advances and tools for predicting contaminant fate and transport in natural and engineered systems. ASCEM integrates modeling tools into a common workflow that facilitates integrated approaches to modeling and site characterization, and enables robust and standardized assessments of performance and risk for EM cleanup and closure activities.

The ASCEM project includes collaboration with end users engaged in performance assessments and subsurface simulation. Two working groups are engaged in performance assessment activities at the Hanford Site and Savannah River Site (SRS). The Hanford Site working group is focused on evaluating an alternative conceptual model that includes fine-scale heterogeneities. The baseline conceptual model for the performance assessment includes the large-scale stratigraphy at the site. The working group is applying the ASCEM toolset to develop and evaluate alternative conceptual models and evaluate the effect of heterogeneities on long-term transport under rainfall-driven conditions. Because the heterogeneous models require long compute times due to increased model complexity, the simulations are implemented on a high-performance computing platform to reduce simulation times. The ASCEM Akuna workflow enables efficient organization, simulation execution, and processing and visualization of results. Current performance assessments for waste tank closure at the SRS are limited to two-dimensional axi-symmetric representations. The SRS working group is collaborating with the site contractor to address technical review issues by resolving fine-scale tank features and simulating three-dimensional flow with Richards equation for selected closure scenarios using the ASCEM simulator, Amanzi. The Akuna toolset is being applied to support model setup, sensitivity analysis, uncertainty quantification, and visualization.

Both of the ASCEM working groups are addressing issues that cannot readily be evaluated with the existing tools. In these efforts, ASCEM is being used to provide technical underpinnings for ongoing performance assessments.

INTRODUCTION

The Office of Soil and Groundwater Remediation within the U.S. Department of Energy's (DOE's) Office of Environmental Management (EM) is developing 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 (PAs). Two of the current deployments are focused on providing technical support for PAs at the Hanford Site and the Savannah River Site (SRS).

HANFORD SITE PERFORMANCE ASSESSMENT

The DOE Office of River Protection is conducting a PA at the Hanford Site for closure of the single-shell tank (SST) Waste Management Area C (WMA C or the 241-C Tank Farm). WMA C is located in the Central Plateau area near the eastern edge of the 200 East Area of the Hanford Site in southeastern Washington State (Fig. 1). Closure of WMA C requires a long-term PA evaluating the effects of residual tank and ancillary equipment wastes on human health and the environment .

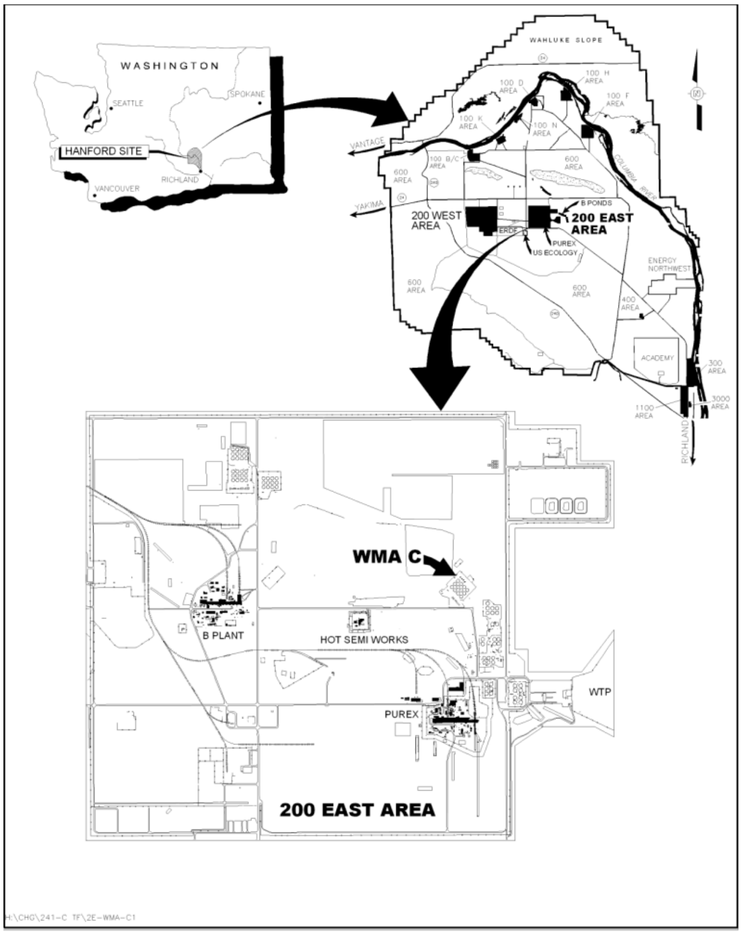


Fig. 1. Location of Waste Management Area C in the 200 East Area at the DOE Hanford Site.

The WMA C PA is assessing the fate and transport of radionuclides and hazardous chemicals for residual wastes left in tanks and ancillary equipment and facilities. Under this closure scenario, the fate and transport calculations will be used to produce estimates of concentrations at downstream locations in the groundwater. From that point, a performance or a risk assessment will apply various human exposure scenarios to estimate potential future risks, including radiological dose and hazardous chemical exposure.

The Hanford subcontractor conducting the PA has defined a hybrid modeling approach to perform the needed calculations. In this approach, a physics-based flow and transport simulator (Subsurface Transport Over Multiple Phases (STOMP), [2]) is used to identify transport drivers to the water table. The flow field from STOMP is then abstracted to a system-level model based on GoldSim software [3]. This integrative system-level model is then used to summarize the entire system, from environmental transport to dose or risk, and also provides a framework for sensitivity and uncertainty analyses.

While the modeling that will support the PA considers a wide range of processes contributing to contaminant transport and exposure pathways, regulators and stakeholders have voiced concern over only using major stratigraphy to describe the geologic conceptual model. As shown in the ASCEM Phase II demonstration with BC Cribs [4], heterogeneities may be an important feature influencing subsurface flow and transport. Given that development and execution of heterogeneous conceptual models is outside the Hanford subcontractor’s work scope, the ASCEM project is collaborating with the contractor to apply the toolset and investigate the potential effect of heterogeneities on the long-term fate and transport of tank residuals.

The baseline conceptual model to be used for the WMA C PA is represented by the large-scale stratigraphy at the site. Results of simulations using a heterogeneous conceptual model can be compared to those from the baseline conceptual model used in the PA to evaluate the effect of heterogeneities on long-term transport under rainfall-driven conditions (e.g., in the absence of continued focused water discharges, such as those that have occurred in the past through unplanned releases). To evaluate the impact of heterogeneities, lithofacies distributions are used to develop a facies-based geologic conceptual model. In addition, field-measured water content and soil moisture tension data are being used for parameterization and model calibration. If heterogeneities are determined to have a minimal impact on transport, ASCEM can provide technical defensibility for the baseline conceptual model currently being used in the WMA C PA. If heterogeneities are determined to have a more significant impact, the conceptual and mathematical models can be transferred to the contractor performing the PA.

An additional concern raised by stakeholders engaged in the WMA C PA is the ability of the STOMP simulator to capture sloping surfaces. Because STOMP uses orthogonal grids, sloping surfaces are typically represented in a stair-step fashion, rather than as a continuous surface. Amanzi uses both orthogonal and non-orthogonal grids and is being used to evaluate the impact of gridding. The Amanzi simulation results are also being benchmarked against the STOMP simulator, which will increase confidence in Amanzi simulator and facilitate technology transfer.

WMA C Conceptual Model

WMA C contains twelve 100-series SSTs (535,000-gal capacity) and four 200-series SSTs (55,000-gal capacity; Fig. 2) that are situated approximately 2 m below ground surface. To support the transfer and storage of waste with WMA C, there is a complex system of pipelines, diversion boxes, vaults, and pits. Multiple drywells around each 100-series SST provide leak detection.

Hanford Site geology includes thick sequences of sediments that vary in texture from cobbles and coarse gravels to fine silts and clays. Beneath these sediments are thick basalt flows that form the bottom boundary of the unconfined aquifer. This relatively thin, unconfined aquifer is considered the primary pathway for contaminant transport. Once contaminants reach the water table, contaminants are transported in the aquifer toward the Columbia River.

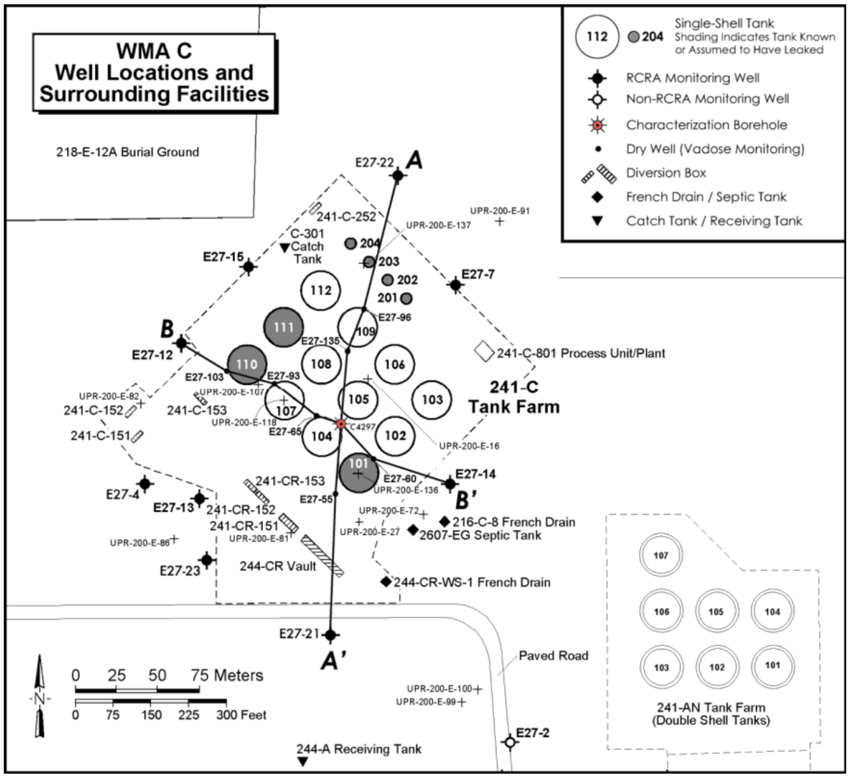
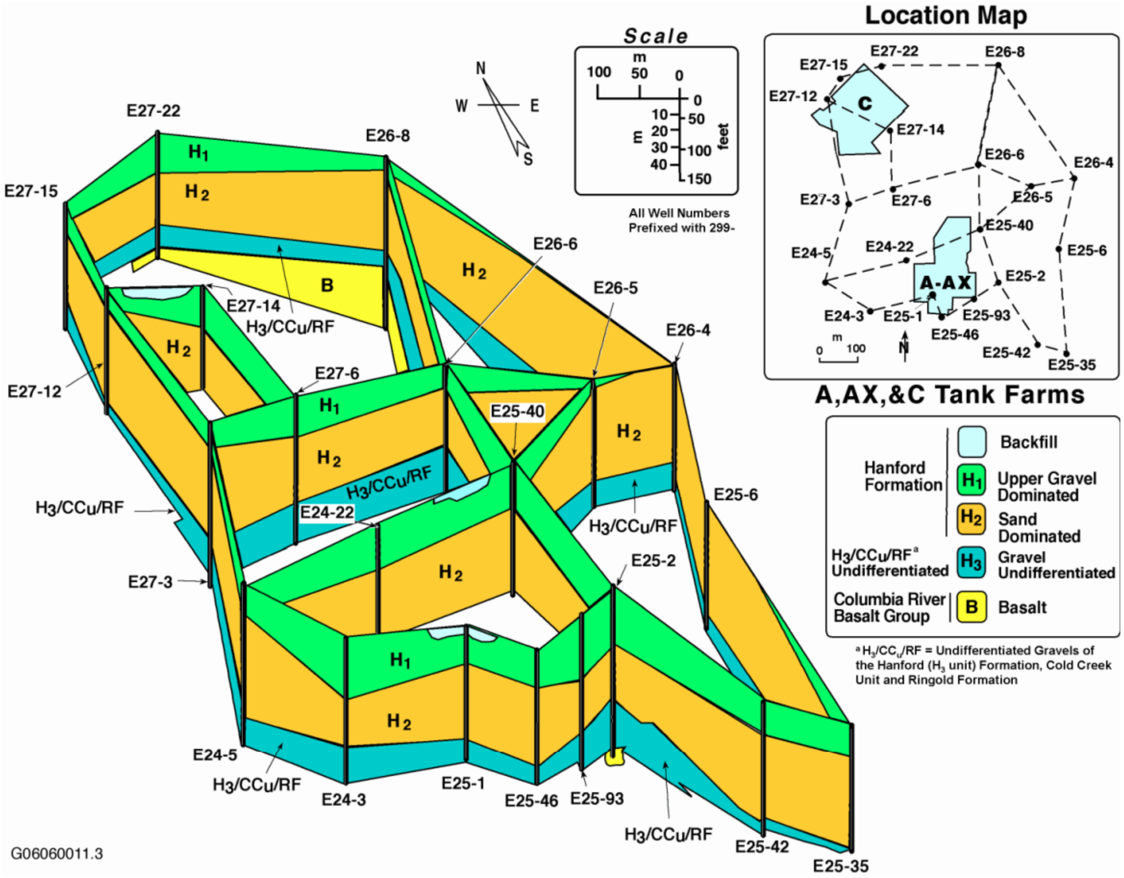


Fig. 2. Waste Management Area C and surrounding facilities.

The sediments are largely composed of the Ringold Formation and Hanford formation units, with the Hanford formation above the Ringold Formation. The Ringold Formation conglomerate is a pebble to cobble gravel with a fine to coarse sand matrix [5]. At the WMA C, however, the Ringold Formation is undifferentiated with the H3 unit of the Hanford formation and the Cold Creek unit (H3/CCU/RF because these units cannot be clearly distinguished at this site. Fig. 3 shows a fence diagram of these units underlying WMAs C and A-AX. As shown in Fig. 3, the Hanford formation comprises most of the vadose zone, and overlies the undifferentiated H3/CCU/RF. The Hanford formation (an informal designation) is up to 64 m thick near the 200 Areas. The formation consists of pebble to boulder gravel, fine- to coarse-grained sand, and silt to clayey silt. These deposits are divided into three facies. The undifferentiated H3 is a gravel unit, above that is the sand-dominated H2 unit, and above the H2 unit is the gravel-dominated H1 unit. Finally, backfill materials consisting of poorly sorted cobbles, pebbles, and coarse to medium sand derived from the H1 subunit of the Hanford formation are distributed around the tanks and tank infrastructure. Overall, the vadose zone is ~75 m thick at WMA C.

Geostatistical Realizations of Lithofacies

The baseline model being used in the WMA C PA represents the stratigraphic framework as homogenous and horizontal stratified units. However, heterogeneities exist within the Hanford formation, which in turn influence vadose zone flow and transport. Hence, approaches that focus on geostatistical simulation of the sequence-stratigraphic relations of lithofacies, as well as continuous property variations conditioned on field-measured water content data, will be used to describe heterogeneity. In this way, the uncertainty in the lithofacies distribution can be quantified.



Reference: PNNL-15955, *Geology Data Package for the Single-Shell Tank Waste Management Areas at the Hanford Site.*

Fig. 3. Fence diagram showing cross-sections through WMA C and A-AX [6].

Using direct push data, lithofacies were identified by multivariate analysis of spectral gamma ray data. This data was used to identify sediment types with different geological and hydrological properties. To date, three lithofacies have been preliminarily identified by clustering Th-232 and K-40 data that are associated with the minor stratigraphic units of the Hanford formation: an H1 and H2-fine association (Lithofacies 1), an H1 and H2-coarse association (Lithofacies 2), and an H2-fine (Lithofacies 3). Only 12 direct-push boreholes were available at WMA C for analysis, and their vertical depth was limited (e.g., above the water table). However, the lithofacies derived from the analysis of the data show good vertical and lateral continuity, as shown in the spatial distribution of lithofacies in Fig. 4.

The next step in this analysis is to develop the indicator variogram models to characterize the spatial continuity of each lithofacies. Conditional indicator simulation techniques will be applied to produce realizations of lithofacies distributed to the upper domain (e.g., Fig. 5). The realizations will then be used as input for flow and transport modeling at WMA C to capture the range of behavior in flow and transport predictions. The resulting three-dimensional geostatistical models of hydraulic conductivity will provide an improved understanding of the heterogeneity of Hanford formation sediments and also will provide geologically plausible constraints on flow and transport modeling of the study area.

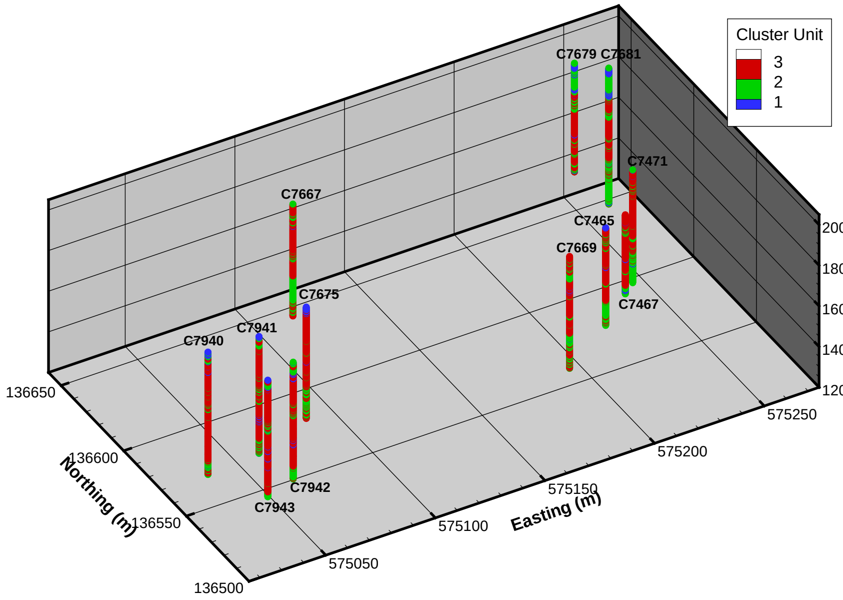


Fig. 4. Spatial distribution of lithofacies.

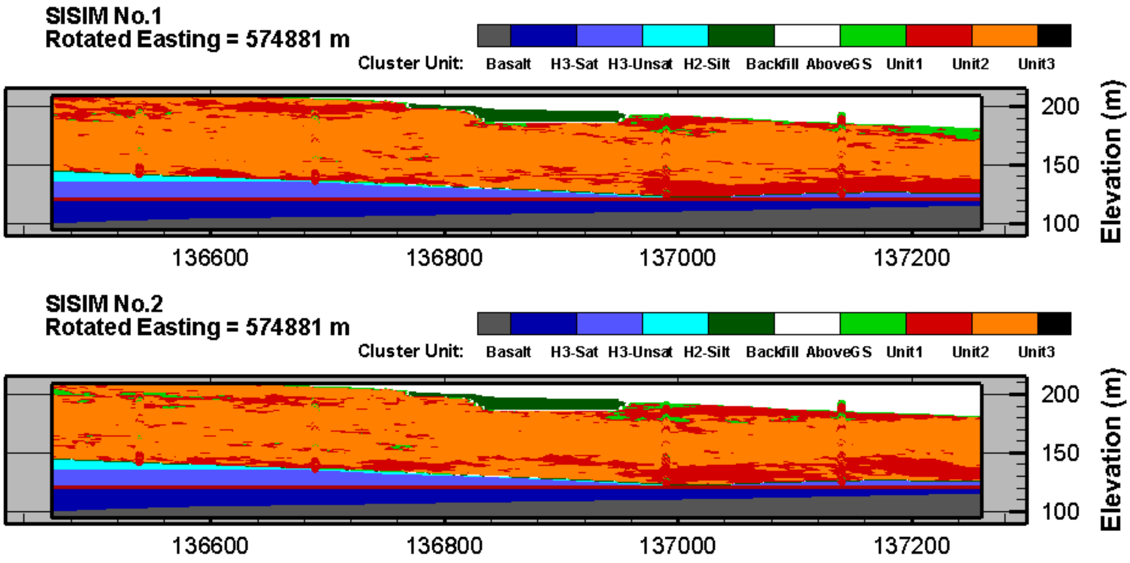
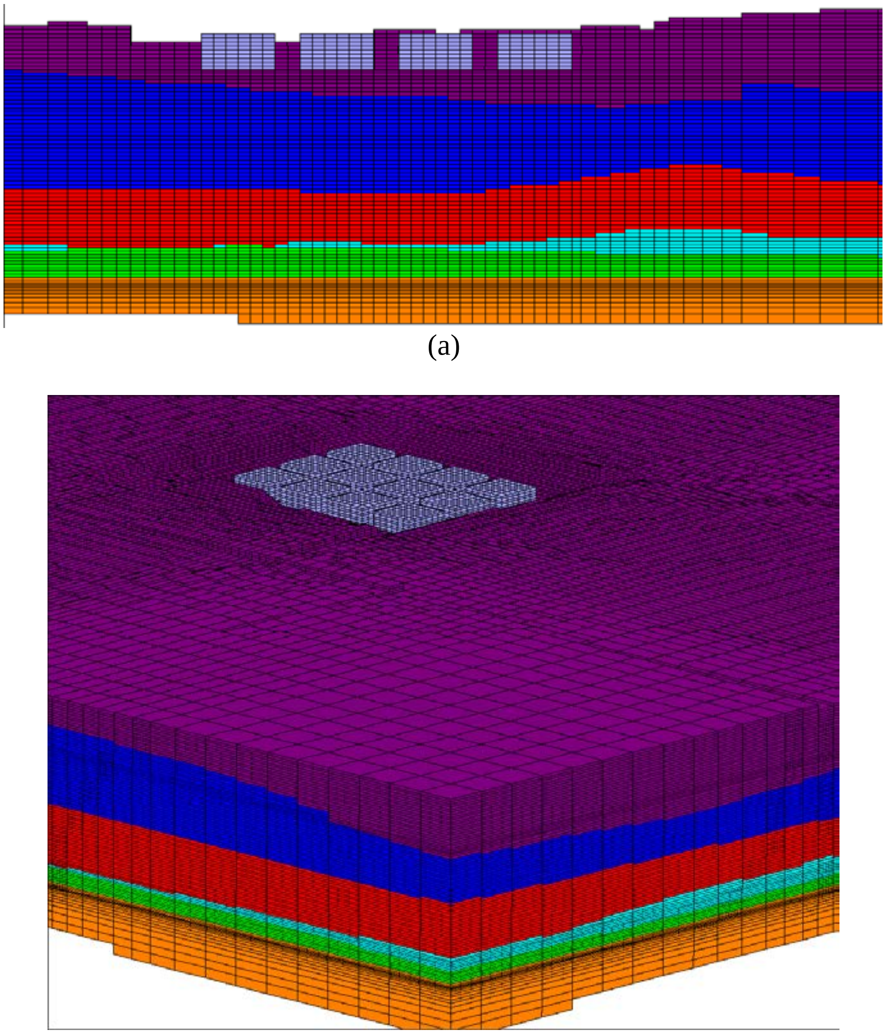


Fig. 5. Example lithofacies distributions for the upper WMA C domain.

Structured (Orthogonal) Grid

To benchmark the Amanzi simulator against STOMP, an orthogonal (structured) grid was developed with the same discretization used for the PA. A cross-section showing this discretization is shown in Fig. 6a. Note that the contact of the H1 (blue) and H2 (red), for example, is accomplished in a stair-stepped fashion. The oblique view of the grid in Fig. 6b shows the same stair-stepped pattern to capture sloping surfaces, as well as the cubes representing the twelve 100-series tanks at WMA C.


(a)

(b)

Fig. 6. Structured orthogonal grid of WMA C in (a) cross-section and (b) oblique view.

The structured grid serves two purposes. The first is in benchmarking Amanzi results against STOMP. The second is in comparing the differences between a structured and unstructured representation of the major stratigraphy at WMA C. Because the structured grid is coarser than the unstructured grid, it is anticipated that this grid may need some refinements for an adequate comparison.

Results from these simulations will be used to identify the effect of heterogeneities on contaminant transport under a closure scenario. In addition, results will be compared using the structured representation (using the major stratigraphy) to identify any potential numerical impacts from an orthogonal representation of the tanks and the grid.

SRS WASTE TANK PA WORKING GROUP

The SRS Waste Tank PA working group initiated application of the ASCEM toolset to address a technical concern expressed during the ongoing Nuclear Regulatory Commission (NRC) review of the H-Area Tank Farm (HTF) PA. The specific concern is that the PA “does not adequately assess waste release from the submerged and partially submerged tanks via a preferential pathway” [7].

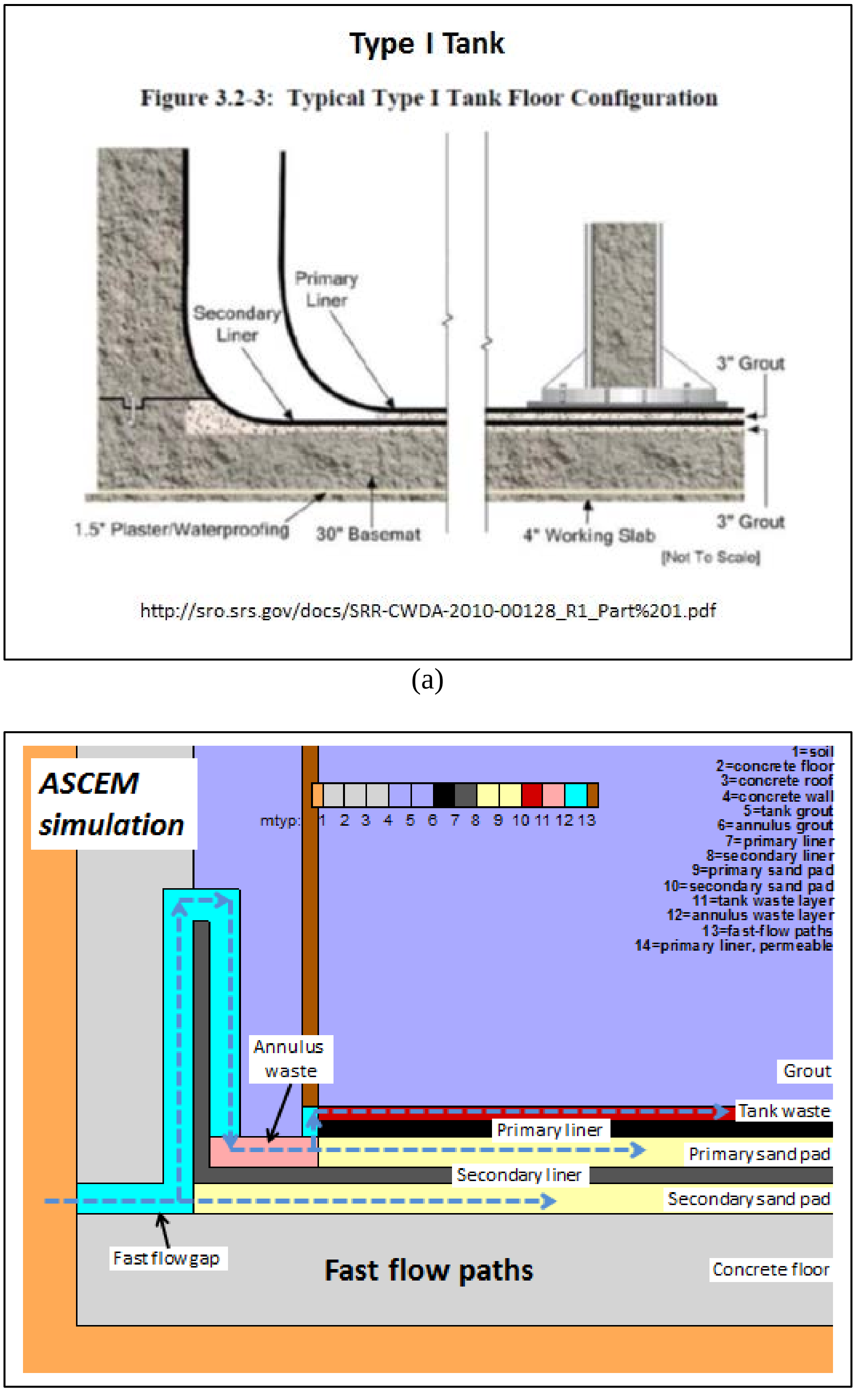
The current HTF PA is based on axi-symmetric flow conditions around the cylindrical waste tanks, and the model uses a two-dimensional radial slice. This representation is adequate for tanks above the water table, where the moisture flow is nominally downward. However, for a fully or partially submerged tank, which is 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. The NRC is concerned about the possibility of (1) early formation of a preferential flow path due to material degradation and/or separation, as examples, grout shrinkage and steel corrosion; (2) the preferential flow path including residual waste layers in the tank annulus and/or sand/grout pads; and (3) significant advective flow through the pathway due to hydraulic gradients in the aquifer/saturated zone. Three-dimensional modeling using a conventional flow and transport simulation code was previously pursued for a generic scenario. However, the three-dimensional model was computationally demanding and unable to adequately resolve thin geometric features due to meshing constraints. The ASCEM toolset is designed to overcome these difficulties by incorporating more efficient meshing capabilities, such as Adaptive Mesh Refinement (AMR) and flexible unstructured gridding, and using high-performance computing numerical algorithms and hardware.

Waste Tank Conceptual Model

Fig. 7 illustrates key features of a submerged SRS Type I waste tank and the simplified conceptual model for implementation in Amanzi. Type II tanks have a similar annulus design. From left to right, an upper 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, a perforation of the primary steel liner due to localized corrosion, the tank waste layer, and similar features on the opposite side of the tank. Preferential flow is also assumed to occur through the pad separating the steel liners from the concrete floor. The fast flow path and liner features are exaggerated in thickness by 10 times in Fig. 7b for clarity, but are represented at true thickness in Amanzi simulations. Material properties and boundary conditions are representative of values published in [8] and values determined from consultation with the SRS Liquid Waste PA contractor.

Amanzi Mesh Development and Application

ASCEM provides two basic meshing capabilities: (1) structured with AMR and (2) unstructured. The structured grid (Fig. 8) is based on multiple grid levels and uses AMR to achieve higher grid resolution where needed, starting from a relatively coarse base-level grid of uniform and orthogonal grid blocks. The unstructured grid (Fig. 9) uses grid cells of variable shape and density in a single grid to achieve local refinement. Both approaches were evaluated in the Waste Tank PA working group application.



(a)

(b)

Fig. 7. Geometry of the (a) physical and (b) conceptual tank features and preferential flow path.

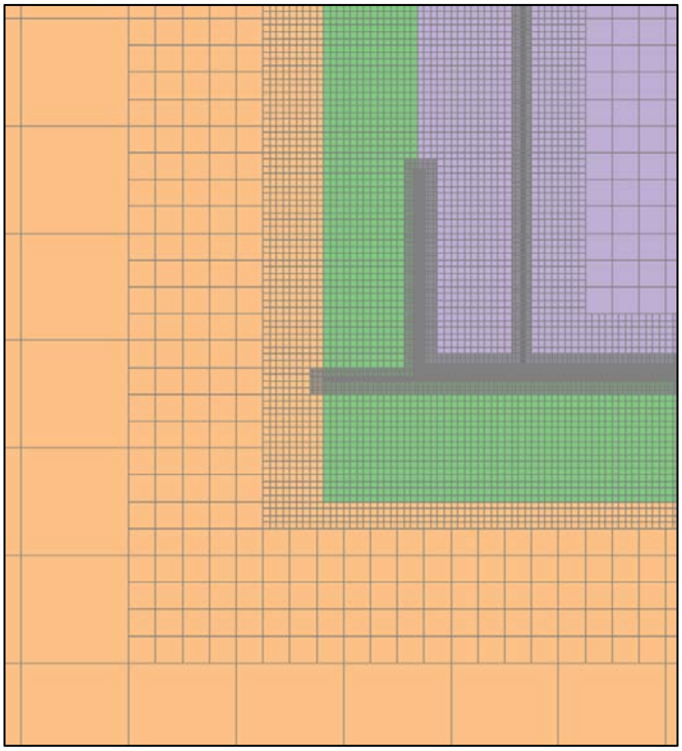


Fig. 8. Structured AMR grid implementation for submerged tank scenario showing four refinement levels at 4x each (profile view).

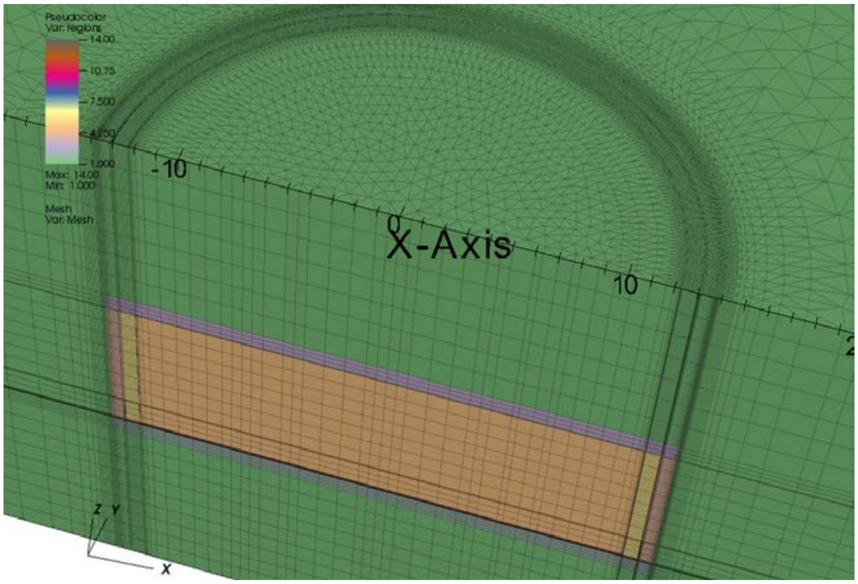
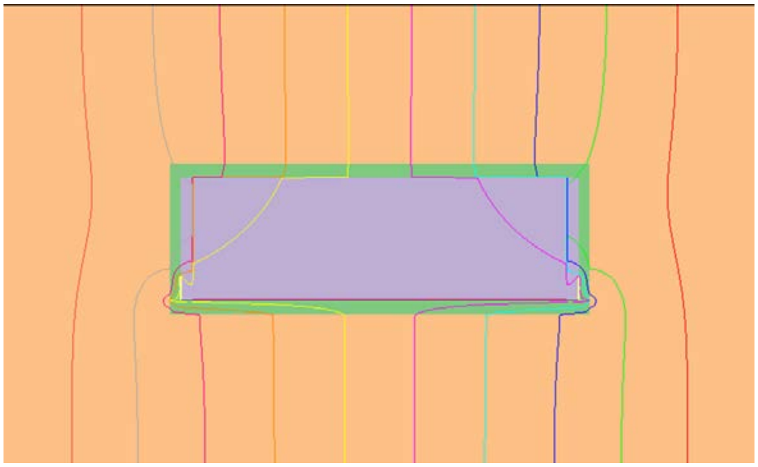


Fig. 9. Unstructured grid implementation for submerged tank scenario (quarter section view).

Flow simulations were performed on prototype two-dimensional models using structured AMR and unstructured grids to assess gridding strategies and to verify model flow predictions against hand-calculations. Fig. 10 illustrates a typical flow simulation using the structured AMR option. A grid resolution study indicated the importance of having fine grid spacing near the fast flow path entrance (Fig. 10b) and exit to resolve the sharp hydraulic head gradients in those regions.

Similar two- and additional three-dimensional flow simulations were conducted for unstructured grids, as well as prototype transport simulations involving Cs-137 and Sr-90, the primary radionuclides of concern in the near-field. Fig. 11 illustrates flow vectors for an example horizontal plane passing through the annulus waste layer component of the fast flow path. The submerged tank simulations also provided a realistic application for developing AMR capabilities and for testing and demonstrating the modeling workflow capabilities of the Akuna user interface.



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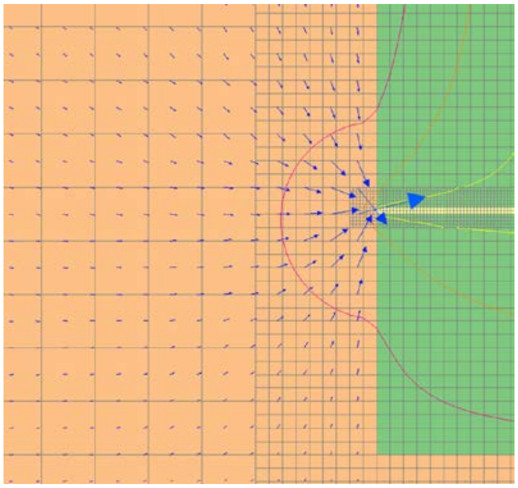

(b)

Fig. 10. Simulated flow using structured AMR for a two-dimensional cross section: (a) hydraulic head profile, (b) velocity field at fast flow path inlet.

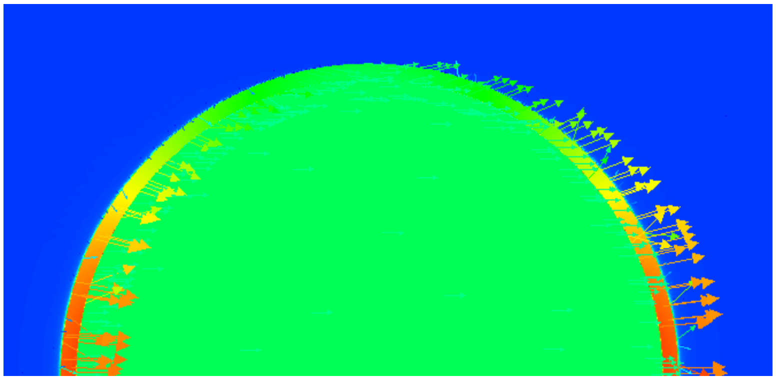

Fig. 11. Simulated velocity field using unstructured prism elements for a three-dimensional half section; plane through annulus waste layer.

CONCLUSIONS

Each of the ASCEM efforts supporting PAs are addressing issues that cannot readily be evaluated with the existing tools. At the Hanford Site for WMA C PA, an alternative conceptual model is being simulated that represents subsurface heterogeneities and determines their impact on long-term transport under rainfall-driven conditions. The heterogeneous conceptual model requires long compute times due to model complexity, so Amanzi is being implemented on a high-performance computing platform to reduce simulation times. Modeling toolsets within the Akuna framework are also being used to demonstrate their utility in data organization, simulation execution, and processing and visualization of results. At SRS, ASCEM is continuing collaboration with the contractor under its PA maintenance program to address NRC technical review issues by expanding the waste tank model to consider patch corrosion and long-term geochemistry changes to reduce conservatism. The Akuna toolset is being applied to support model data management, sensitivity analysis, uncertainty quantification, and visualization. For both EM sites, the ASCEM workflow is providing technical underpinnings for ongoing PAs for cleanup and closure decisions.

REFERENCES

[1] Freedman VL, X Chen, SA Finsterle, MD Freshley, I Gorton, LJ Gosink, E Keating, C Lansing, WAM Moeglein, CJ Murray, GSH Pau, EA Porter, S Purohit, ML Rockhold, KL Schuchardt, C Sivaramakrishnan, VV Vesselinov, and SR Waichler. 2014. “A high-performance workflow system for subsurface simulation.” *Environmental Modelling & Software* 55:176-189. doi:10.1016/j.envsoft.2014.01.030

[2] White MD and M Oostrom. 2006. *STOMP – Subsurface Transport Over Multiple Phases, Version 4: User's Guide*. PNNL-15782, Pacific Northwest National Laboratory, Richland, Washington.

[3] GoldSim Technology Group. 2014. *User’s Guide, GoldSim Probabilistic Simulation Environment*. Version 11.1, Volumes 1 and 2. Goldsim Technology Group, Issaquah, Washington.

[4] Freshley MD, S Hubbard, GP Flach, VL Freedman, DA Agarwal, BJ Andre, YJ Bott, X Chen, JA Davis, B Faybishenko, I Gorton, CJ Murray, D Moulton, JG Meyer, ML Rockhold, A Shoshani, CI Steefel, H Wainwright, and SR Waichler. 2012. *Phase II Demonstration.* PNNL-21900, ASCEM-SITE-2012-01, U.S. Department of Energy Office of Environmental Management, Washington, D.C.

[5] Lindsey KA. 1996. “The Miocene to Pliocene Ringold Formation and Associated Deposits of the Ancestral Columbia River System, South-Central Washington and North-Central Oregon,” *Washington Division of Geology and Earth Resources Open File Report 96-8*, Washington State Department of Natural Resources, Olympia, Washington.

[6] Reidel SP and MA Chamness. 2007. *Geology Data Package for the Single-Shell Tank Waste Management Areas at the Hanford Site*. PNNL-15955, Rev. 1, Pacific Northwest National Laboratory, Richland, Washington.

[7] U.S. Nuclear Regulatory Commission. 2013. *NRC Staff Request for Additional Information on the Draft Basis for Section 3116 Determination and Associated Performance Assessment for the H-Area Tank Farm at the Savannah River Site*. Accessed September 24, 2014 at http://pbadupws.nrc.gov/docs/ML1319/ML13196A133.pdf.

[8] Savannah River Remediation LLC. 2012. *Performance Assessment for the H-Area Tank Farm at the Savannah River Site*. SRR-CWDA-2010-00128, Rev. 1. Accessed September 24, 2014 at http://pbadupws.nrc.gov/docs/ML1304/ML13045A499.pdf.