

Advanced Simulation Capability for Environmental Management

Fiscal Year 2012 Annual Report



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ASCEM



Message from the Director and Project Managers

Our mission is to protect the nation's water resources for current and future generations. Through the Advanced Simulation Capability for Environmental Management (ASCEM) Initiative and companion Applied Field Research Initiatives, the Office of Soil and Groundwater Remediation is working to deliver transformational science and technology-based solutions to complete the DOE EM cleanup mission. Advanced simulation capabilities are critical for enabling the cleanup mission with cost-effective and sustainable solutions that are protective of human health and the environment. The ASCEM team works collaboratively among a diverse national laboratory team and has many shared successes.

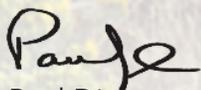


Kurt Gerdes
*Director, Office of Soil and Groundwater Remediation
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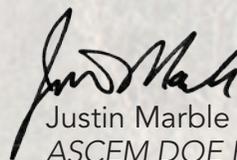
ASCEM was initiated in 2010 by the US Department of Energy (DOE) Office of Environmental Management. ASCEM is a scientific tool and approach for understanding and predicting contaminant fate and transport in natural and engineered systems. ASCEM's modular and open source toolsets will facilitate integrated approaches to modeling and site characterization that enable robust and standardized assessments of performance and risk for EM cleanup and closure activities. Specifically, the ASCEM initiative is aimed at addressing critical EM program needs to better understand and quantify 1) the subsurface flow and contaminant transport behavior in complex geological systems; 2) long-term performance of engineered components including cementitious materials in nuclear waste disposal facilities; and 3) uncertainties and risks associated with DOE EM's environmental cleanup and closure programs. ASCEM will also help transform fundamental science innovation into practical applications deployed by site contractors across the entire DOE complex and is being integrated with the emerging EM endpoints initiative.

The ASCEM project is organized into three technical thrust areas: a user interface (Platform and Integrated Toolset) called Akuna, a computational engine (Multi-Process High Performance Computing [HPC] Simulator) called Amanzi, and deployment with end users (Site Applications). These three areas seamlessly interface to develop the ASCEM toolset and approach.

ASCEM has made significant progress in capability development and a second set of demonstrations was completed in 2012. The demonstrations summarized in this report were performed at the Hanford and Savannah River sites and on a representative waste tank. The project will release an initial research version of the toolsets for evaluation by the EM user community in September, 2013.



Paul Dixon
ASCEM Multi-Lab Program Manager



Justin Marble
ASCEM DOE Program Manager

Responding to the Challenge

In 2009, the National Research Council (NRC) of the National Academies reviewed and validated the U.S. Department of Energy (DOE) Office of Environmental Management (EM) Technology Program in its publication, *Advice on the Department of Energy's Cleanup Technology Roadmap: Gaps and Bridges*. The NRC report outlined prioritization needs for the Groundwater and Soil Remediation Roadmap, and concluded that the complexity and magnitude of the DOE environmental problem justifies long-term investment in environmental remediation science and technology, including predictive capabilities. To address the investment need, DOE EM funded a number of initiatives in 2010. One of the strategic initiatives in the Office of Soil and Groundwater was the development of Advanced Simulation Capability for Environmental Management (ASCEM). ASCEM is a state-of-the-art scientific approach that uses an integration of toolsets for understanding and predicting contaminant fate and transport in natural and engineered systems. The modeling toolset is modular and open source and is divided into three thrust areas: Multi-Process High Performance Computing (HPC), Platform and Integrated Toolsets, and Site Applications (Figure 1). The toolsets facilitate integrated approaches to modeling and site characterization that enable robust and standardized assessments of performance and risk for DOE EM cleanup and closure activities.

During fiscal year 2012, ASCEM made significant progress in capability development. This development occurred in the Platform and Integrated Toolsets as well as with the Multi-Process HPC Simulator. The Platform and Integrated Toolsets capabilities provide a user interface and the tools necessary for an end-to-end simulation analysis including model setup, site data management, model calibration and uncertainty analysis, and model results visualization. The HPC Simulator capabilities increased functionality of process model representations, toolsets for interaction with the Platform, model confidence testing, and verification for quality assurance.

A suite of demonstrations were conducted to guide design and development as well as test and evaluate the ASCEM toolsets. The Phase II Demonstration, completed in September 2012, focused on showcasing integrated ASCEM capabilities. The Hanford Site Deep Vadose Zone (BC Cribs) served as an application site for an end-to-end demonstration of ASCEM at a relatively sparse data site, with emphasis on integration and linkages between the Platform and HPC components. Other demonstrations included attenuation-based remedies at the Savannah River Site F-Area to exercise linked ASCEM components under data-dense and complex geochemical conditions, and detailed simulations of a representative high-level waste tank. End user interactions also continue to be a key consideration for the project to both share information about ASCEM and to solicit input from the user community to guide development.

Examples of End-User Interactions in FY 2012

- Participation in Semi-Annual Business Meetings for the DOE-EM Low-Level Waste Disposal Facility Federal Review Group
- Discussions with the DOE Office of Science, DOE EM, and contractors
- Participation in a workshop for the Paducah Site involving representatives from DOE, EPA Region IV, the Commonwealth of Kentucky, the University of Kentucky and contractors
- Presentation at an IAEA Technical Meeting involving experts involved in modeling activities from more than 25 countries
- Participation in the annual meeting for the Interagency Steering Committee for Multimedia Environmental Modeling
- Briefing on ASCEM for meeting between DOE, South Carolina Department of Health and Environmental Control, EPA Region IV and Savannah River Site contractors

This report highlights advancement in capabilities and demonstrations during fiscal year (FY) 2012 and describes plans for future work, leading to release of a version of ASCEM qualified for regulatory applications in 2015.

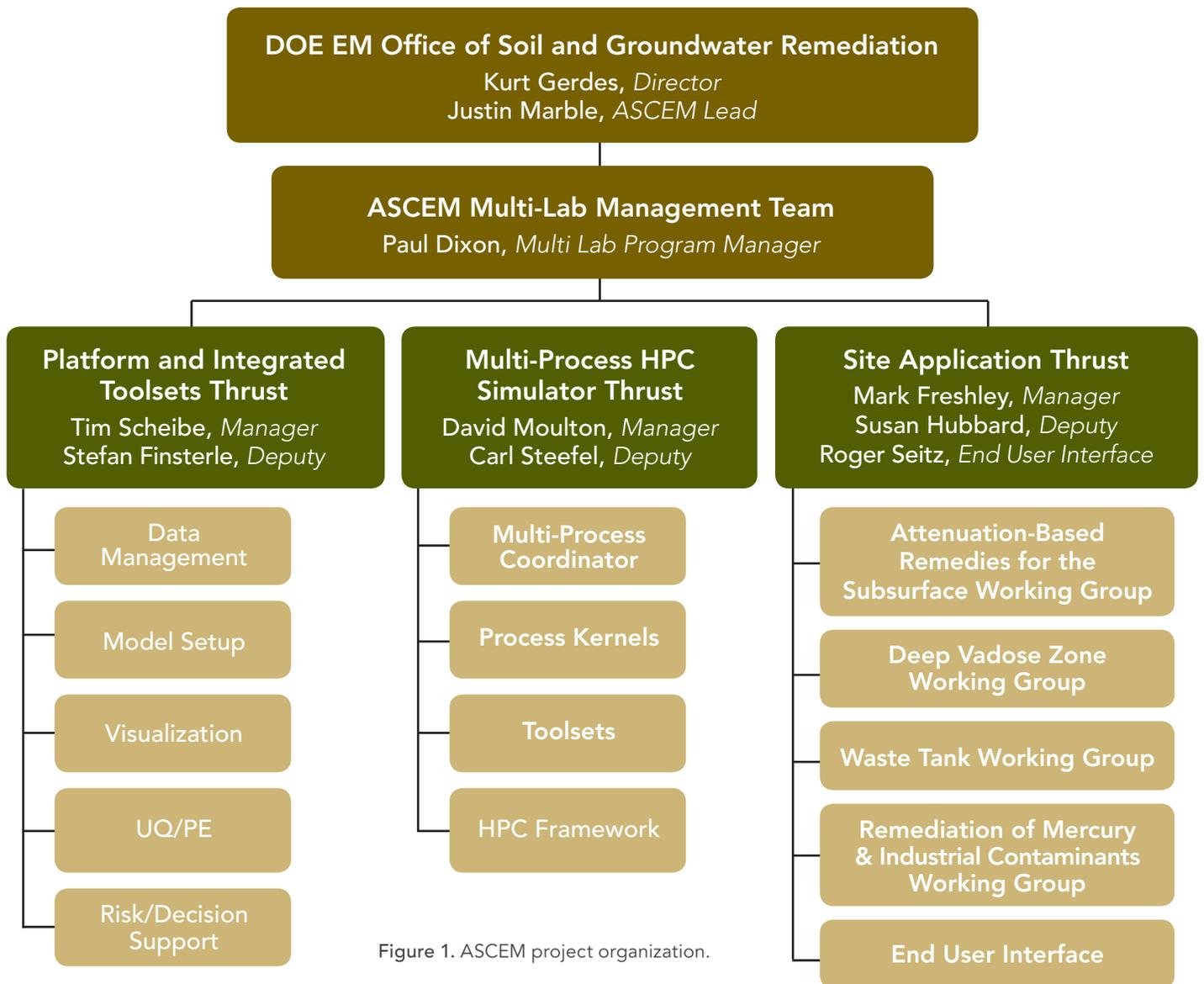


Figure 1. ASCEM project organization.

Demonstrating Impact

The Platform and HPC Thrusts are focused on development of the ASCEM toolsets, with careful attention to the needs of end users. Frequent and consistent engagement of potential end users is seen as critical to developing user acceptance and eventual deployment and application of the ASCEM toolsets at DOE sites. End users include performance assessment and risk assessment practitioners, decision-makers, oversight personnel, and regulators who are engaged in the DOE cleanup mission. User engagement is implemented through a User Steering Committee and broad interactions with the user community as part of the Site Applications Thrust.

The overall approach for deployment of ASCEM is to demonstrate the capabilities at an increasing number of DOE sites. The demonstrations are implemented through working groups that reside in the Site Application Thrust Area, but rely on close interactions with developers, end users, and collaborators. Collaborations with ASCEM include the DOE EM Soil and Groundwater Remediation Program Applied Field Research Initiatives (AFRIs), the DOE EM Cementitious Barriers Partnership (CBP), and the DOE Office of Science, Biological and Environmental Research Scientific Focus Areas (SFAs).

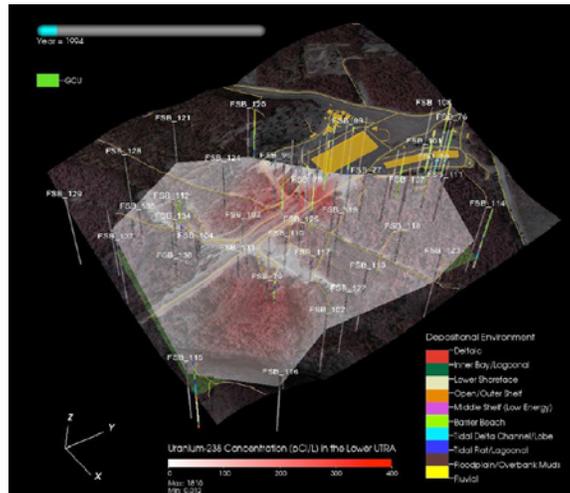


Figure 2. Visualization of the F Area uranium plume and site infrastructure using Vist.

The project performed an early assessment of advances associated with data management, visualization (Figure 2), uncertainty quantification, and HPC in a Phase I demonstration completed during FY 2011. The Phase I demonstration was conducted over a short time period (4 months) and at an early stage of ASCEM development. As a result, the software development teams performed the bulk of implementation and analyses, with minimal involvement of end users.

The purpose of the Phase II demonstration was to highlight integration of ASCEM capabilities and continue advancement of the following specific components: Data Management, Visualization, Uncertainty Quantification, and the multi-process simulator. The demonstration followed a major development phase and relied on the working groups for testing capabilities and providing feedback to developers. The DVZ Working Group focused on a complete end-to-end demonstration of ASCEM capabilities using different conceptual model realizations, with emphasis on integration and linkage between components. The SRS F-Area Working Group focused on demonstrating data management and uncertainty analysis capabilities linked with simulation in a data-rich environment and considering

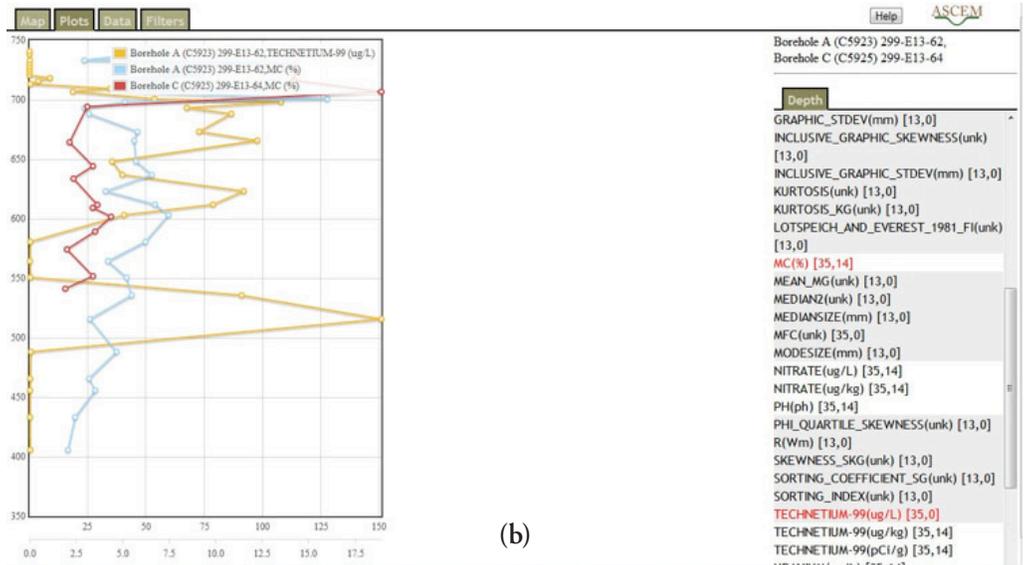
geochemical complexity. The Waste Tank Performance Assessment Working Group exercised HPC using parallel processing to demonstrate adaptive mesh refinement for resolution of fine-scale features in engineered systems.

Phase II demonstration activities 1) advanced many ASCEM-specific components, including Data Management, Model Setup, Parameter Estimation, Uncertainty Quantification, the Multi-Process Simulator, and Visualization; and 2) illustrated how ASCEM toolsets can be used to address DOE EM problems. The end-to-end demonstration showed the advantage of linking Akuna and Amanzi to facilitate model setup, execution, and analysis, including parameter estimation and uncertainty analysis. Amanzi was executed using detailed information on subsurface heterogeneities (a range of parameter distributions) at the plume scale.

Phase II developments for Akuna included new data management methodologies and design of the database infrastructure. The resulting unified database system integrates data from heterogeneous sources having different formats. Data are stored in a uniform format with interfaces that provide automatic generation of views for all relevant data types. This approach makes it easy for users to find data of interest, use filter functions to select subsets, and browse data by visualizing plots, graphs, and plume extents (Figure 3). A graphics viewer, part of the Model Setup tool, was implemented using data from the Hanford Site DVZ. Developments in Akuna's Model Setup Tool allow the user to visualize conceptual models without the need for third-party software (Figure 4). Other Akuna toolsets are used to support a complete modeling workflow, from model setup to simulation execution and analysis through visualization. The demonstrations showed that Akuna tools can be used to manage environmental and simulation data sets, perform model calibration, and conduct uncertainty analyses. Spatial visualization of model results is performed with VisIt, as shown in Figure 5. UQ visualization capabilities allow the user to plot multiple breakthrough curves and analyze a range of responses (Figure 6).

In the Phase II demonstrations, Amanzi was used to simulate unsaturated and saturated flow in heterogeneous systems over large spatial extents and long time frames. For the F Area demonstration, Amanzi simulations were combined with geochemistry and uncertainty analyses to demonstrate use of the toolsets to support future decision making, risk assessment, and site management (Figure 7). At the F Area, uncertainty analysis identified key hydraulic and geochemical parameters that control plume behavior as a function of distance from the contaminant source and over time (Figure 8). For the Hanford Site DVZ, the use of high performance computing allowed a suite of models to adequately capture a range of lithofacies distributions, parameter distributions, and boundary conditions. The Waste Tank Performance Assessment Working Group also highlighted adaptive mesh refinement, where localized regions of enhanced mesh refinement are generated automatically and dynamically to represent combinations of fine-scale features (e.g., material interfaces) and representation of advancing fronts with contrasting properties.

Figure 3. a) BC Cribs and Trenches configuration map view, b) moisture content and technetium-99 concentration profiles in boreholes illustrated using the Data Management Toolset.



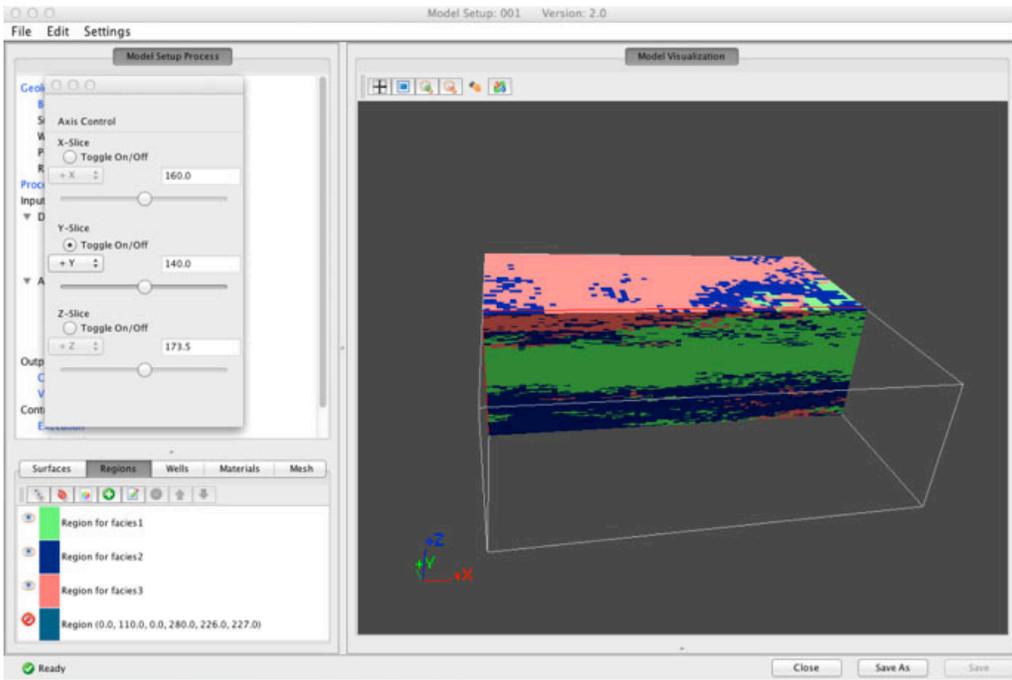


Figure 4. Viewer window in the Model Setup and Analysis Tool showing a heterogeneous conceptual model and a distribution of different facies (sediment types).

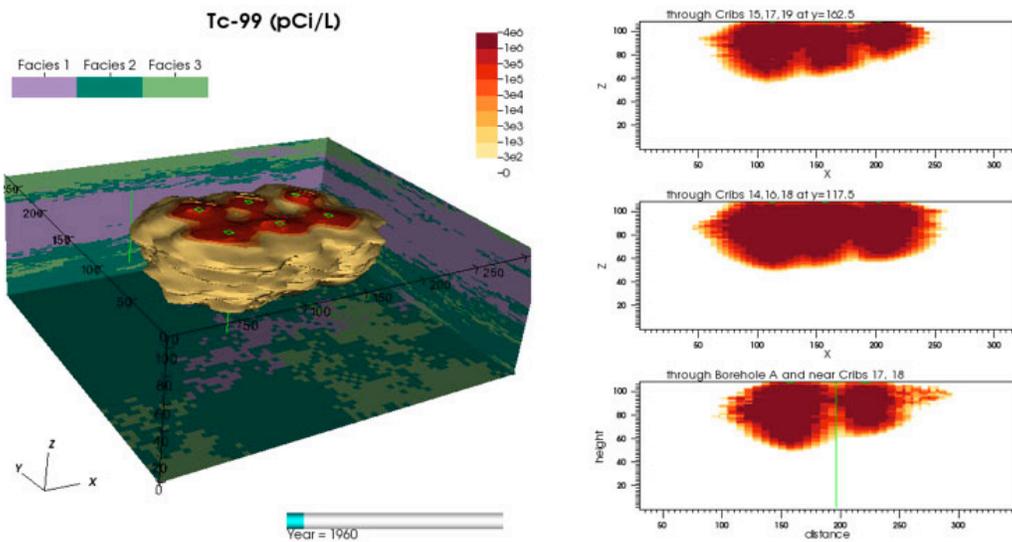


Figure 5. Predicted distribution of technetium-99 released from the cribs in 1960 using VisIt to visualize Amanzi simulation results.



Figure 6. Screen shot from the Uncertainty Quantification Toolset showing mean and 95% confidence intervals for the contaminant breakthrough curve at a monitoring well.

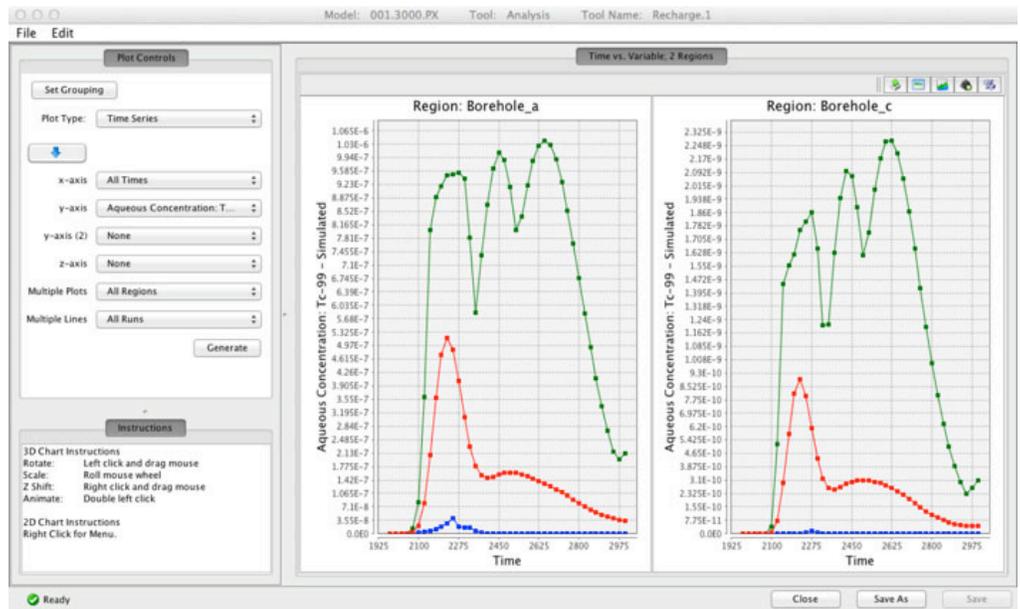
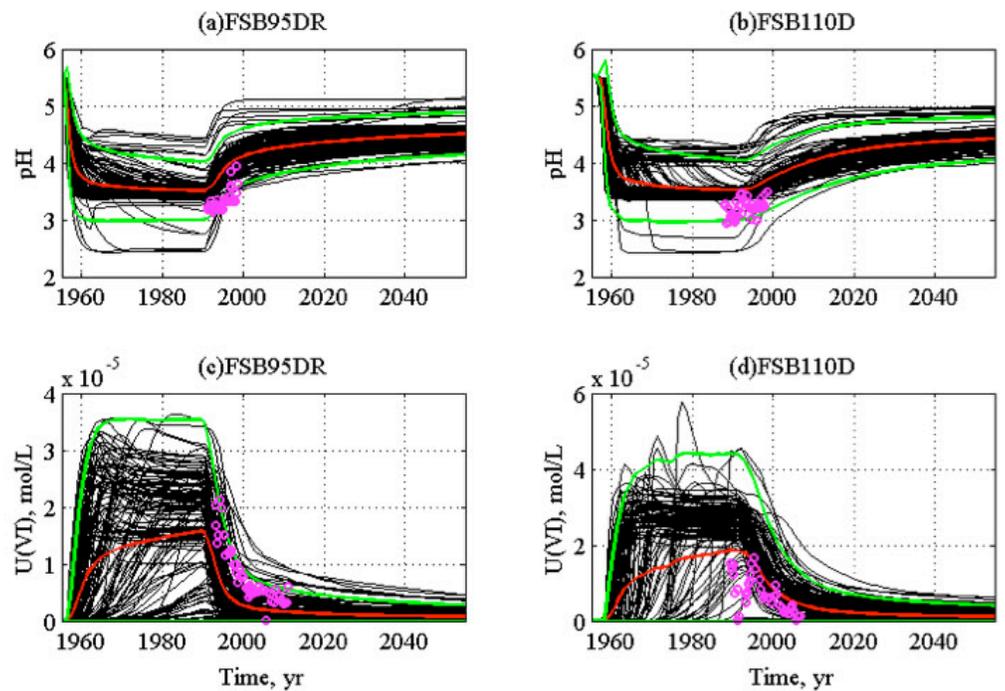


Figure 7. Breakthrough curves and their uncertainty ranges generated from Monte Carlo analyses for pH (a and b) and uranium concentrations (c and d) at different locations. The black lines are the predicted breakthrough curves, red lines are the mean predicted curves, green lines are the mean ± 2 standard deviations (the lower bound is set to zero, when it is negative in c and d), and the magenta points are observations.



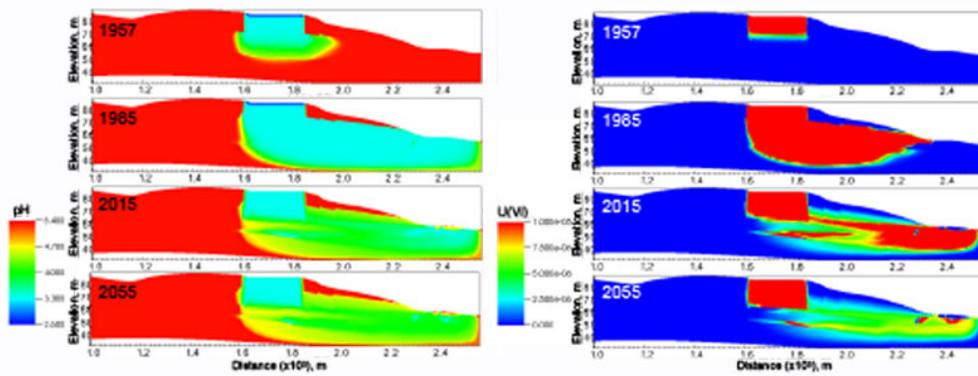


Figure 8. Results of two-dimensional Amanzi simulations of the pH (left column) and uranium concentration (right column) evolution over time at the SRS F-Area using an unstructured grid aligned with a three-layer geologic model.

User Steering Committee

The ASCEM project maintains interactions with a User Steering Committee (USC) to advise the management team and DOE-EM regarding programmatic and regulatory considerations related to the implementation of performance and risk assessments. The USC represents interests from the management and technical perspective at contractor, regulatory and DOE organizations that will be involved in application and review of analyses conducted with the tools. USC Meetings are scheduled to coincide with significant accomplishments and development milestones on the project. Two meetings were held during 2012. The first meeting focused on a demonstration of the initial capabilities developed in the Platform Thrust Area and included updates on the status and plans for the project, plans for the Phase II demonstration, and a discussion of initial results. The second meeting included discussion of progress on capability development and the status of the Deep Vadose Zone Working Group demonstration.

Looking Forward

During FY 2013, the project is focused on completing a release of the ASCEM toolset with example problems and tutorials. The ASCEM toolset will be made available for downloading and the end user community will be engaged directly. Additional end user interactions will also continue to occur through the USC, formed to provide feedback to the project.

In FY 2014, the Platform and Integrated Toolset will continue capability enhancements to provide support for model development and analysis tasks. The Data Management structure will continue to be enhanced and integrated with Visualization tools. A key focus will be on creation of interfaces to enable the data management system to be easily queried and data extracted to provide integration with other Platform Toolsets. The Model Setup and Analysis Toolset will be enhanced with new capabilities to support conceptual/numerical model generation, different mesh types, and geochemistry models. Improvements to usability, robustness, and performance will also be made. Akuna will be enhanced for improved workflows, model management, and new algorithms available in the toolsets. Attention will be given to performance and usability of the environment. New capabilities

will be added to the Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis toolset. Commonalities in the toolsets will be exploited to improve performance. An initial version of the Decision Support Toolset will be designed and implemented. The interface between Akuna and Amanzi, known as Agni, will be enhanced to improve robustness and performance.

Enhancements to Amanzi, the HPC Simulator, will continue to focus on improving performance and robustness. Additional features will be added to Amanzi, such as the representation of source terms to model the base injection wells at the F-Area and new representations of geochemical heterogeneity. Improvements to the robustness of discretizations and the efficiency of the nonlinear solvers will also be made. The input specification used by Akuna to drive Amanzi will continue to evolve, adding support for new features, and making existing features easier to specify. A new geochemistry interface, dubbed Alquimia, will be added to facilitate the use of other geochemistry libraries as Process Kernels (PKs) in Amanzi. This is a cost-effective way to significantly enhance the geochemistry available in Amanzi, while better addressing the flexibility that the community needs. In addition to enhancing the portable build system, the automated testing and reporting framework will be completed to improve the reliability of all components.

The Site Applications Thrust Working Groups will continue applying ASCEM to DOE EM-relevant problems. Working group activities that include interactions with end users will be a specific focus of the Site Applications Thrust in an effort to integrate ASCEM into the DOE EM community and gaining broader feedback on capabilities of the toolsets and performance. The SRS F-Area Working Group will engage the user community at SRS to focus demonstration activities on engineered treatments conducted at the site. The demonstration will evaluate the possibility of replacing active groundwater remediation with natural and enhanced attenuation strategies for final end-state decisions. The DVZ Working Group will focus on expanding the demonstration to include other processes and providing test cases and expertise to support model development and testing. The Waste Tank Performance Assessment Working Group will complete work on advancements in the areas of Adaptive Mesh Refinement (AMR) implementation on structured grids, radioactive decay and progeny ingrowth, consideration of changing material properties as a function of time, and collaboration with CBP on a joint demonstration. Other opportunities for applying ASCEM to relevant problems at DOE EM sites will be sought to engage end users and begin transferring the toolsets to the user community. An Oak Ridge Mercury Working Group will begin an active demonstration including implementation of a surface–water component.

The ASCEM capabilities developed by DOE-EM will help provide efficient and cost-effective transition to site closure end states. Through the working groups and end-user engagement, ASCEM will sequentially test and demonstrate capabilities that will enable it to be used to guide site decision making to develop long-term paths to completing the DOE cleanup mission.

Appendix: Publications and Presentations for the Advanced Simulation Capability for Environmental Management Project

Peer Reviewed Publications

Bea SA, H Wainwright, N Spycher, B Faybishenko, S Hubbard, and ME Denham. 2012. "Identifying key controls on acidic-U(VI) plume behavior at the Savannah River Site, using reactive transport modeling." *Journal of Contaminant Hydrology* (in press).

Faybishenko B. 2011. "Fuzzy-Probabilistic Calculations of Evapotranspiration." Chapter 5 in *Evapotranspiration – Remote Sensing and Modeling*, InTech Publisher, pp. 81-96. ISBN 978 953-307-808-3.

Meyer J, W Bethel, J Horsman, SS Hubbard, H Krishnan, EH Keating, L Monroe, R Strelitz, P Moore, G Taylor, B Torkian, TC Johnson, and I Gorton. 2012. "Visual Data Analysis as an Integral Part of Environmental Management." *IEEE Transactions on Visualization and Computer Graphics* 18(12):2088-2094.

Tokunaga TK, J Wan, and ME Denham. 2012. "Estimates of vadose zone drainage from a capped seepage basin, F Area, Savannah River site." *Vadose Zone Journal* 11(3), DOI: 10.2136/vzj2011.0131.

Williamson M, J Meza, D Moulton, I Gorton, M Freshley, P Dixon, R Seitz, C Steefel, S Finsterle, S Hubbard, M Zhu, K Gerdes, R Patterson, and YT Collazo. 2011. "Advanced Simulation Capability for Environmental Management (ASCEM): An Overview of Initial Results." *Technology and Innovation* 13(2):175-199, 1949-8241. DOI: 10.3727/1949822411Z13085939956625.

Abstracts

Agarwal D, A Wiedmer, B Faybishenko, J Hunt, G Kushner, A Romosan, A Shoshani, and T Whiteside. 2012. "A Methodology for Management of Heterogeneous Site Characterization and Modeling Data." *XIX International Conference on Computational Methods in Water Resources* (CMWR 2012, June 2012).

Faybishenko B and G Flach. 2012. "Uncertainty Quantification of Evapotranspiration and Infiltration from Modeling and Historic Time Series at the Savannah River F-Area." *Fall 2012 American Geophysical Union Meeting*, San Francisco, California, December 2012.

Freedman, VL. 2012. "Uncertainty Assessment at BC Cribs at Hanford Using the ASCEM Toolset." Abstract submitted to AGU 2012 Fall Meeting, San Francisco, California.

Freshley MD, JD Moulton, I Gorton, SS Hubbard, VL Freedman, G Flach, CI Steefel, SA Finsterle, and P Dixon. 2012. "Advanced Simulation Capability for Environmental Management (ASCEM): Development and Demonstrations." *Subsurface Biogeochemical Research Annual Meeting*, April 30 - May 2, 2012, Wardman Park Hotel, Washington, D.C.

Meyer J, EW Bethel, J Horsman, S Hubbard, H Krishnan, A Romosan, E Keating, L Monroe, R Strelitz, P Moore, G Taylor, B Torkian, TC Johnson, and I Gorton. 2012. "Visual Data Analysis as an Integral Part of Environmental Management." *IEEE Visualization 2012*, Seattle, Washington, October 14–20, 2012.

Moulton JD. 2012. "Amanzi: A Parallel Open-Source Flow and Reactive-Transport Simulator for Environmental Applications." *Computational Methods in Water Resources, XIX International Conference Methods in Water Resources* (CMWR 2012), University of Illinois at Urbana-Champaign, June 17–22, 2012.

Moulton JD, CI Steefel, I Gorton, V Freedman, and P Dixon. 2012. "Amanzi: A Parallel Open-Source Flow and Reactive-Transport Simulator for Environmental Applications." *InterPore*, May 14–16, 2012, Purdue University, West Lafayette, Indiana.

Schuchardt KL, DA Agarwal, SA Finsterle, CW Gable, I Gorton, LJ Gosink, EH Keating, CS Lansing, J Meyer, WAM Moeglein, GSH Pau, EA Porter, S Purohit, ML Rockhold, A Shoshani, and C Sivaramakrishnan. 2012. "Akuna - Integrated Toolsets Supporting Advanced Subsurface Flow and Transport Simulations for Environmental Management." *XIX International Conference on Computational Methods in Water Resources (CMWR 2012)*, University of Illinois at Urbana-Champaign, June 17–22, 2012.

Wiedmer A, JR Hunt, B Faybishenko, D Agarwal, GP Flach, T Whiteside, P Bennet, L Bagwell, A Romosan, and SS Hubbard. 2011. "Mass Balances and Uncertainty in Radionuclide Transport at the SRS F-Area Seepage Basins Groundwater Plume." *American Geophysical Union*, Fall Meeting, December 5–9, 2011, San Francisco, California.

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Freshley M, V Freedman, S Hubbard, I Gorton, D Moulton, and P Dixon. 2012. "Advanced Simulation Capability for Environmental Management: Development and Demonstrations." *Waste Management Symposium*, February 26–March 1, 2012, Phoenix, Arizona.

Gorton I, C Sivaramakrishnan, G Black, S White, S Purohit, M Madison, and K Schuchardt. 2011. "Velo: Riding the Knowledge Management Wave for Simulation and Modeling." In *Proceedings of the 4th International Workshop on Software Engineering for Computational Science and Engineering (SECSE 2011)*, pp. 32–40. Association for Computing Machinery, New York.

Meza JC, JD Moulton, I Gorton, SS Hubbard, M Freshley, and P Dixon. 2011. "Advanced Simulation Capability for Environmental Management." *SciDAC*, July 10–14, 2011, Denver, Colorado.

Meza JC, SS Hubbard, MD Freshley, I Gorton, JD Moulton, and ME Denham. 2011. "Advanced Simulation Capability for Environmental Management (ASCEM): Early Site Demonstration." *Waste Management Symposium*, February 27–March 3, 2011, Phoenix, Arizona.

Seitz R, M Freshley, P Williamson, K Dixon, Y Gerdes, and Y Collazo. 2011. "Identification and Implementation of End-User Needs During Development of a State-of-the-Art Modeling Toolset." *Proceedings of the 14th International Conference on Environmental Remediation and Radioactive Waste Management*, ICEM2011, September 25–29, 2011, Reims, France.

Seitz RR, MD Freshley, P Dixon, SS Hubbard, V Freedman, B Faybishenko, G Flach, I Gorton, S Finsterle, JD Moulton, CI Steefel, and J Marble. 2013. "Advanced Simulation Capability for Environmental Management – Current Status and Phase II Demonstration Results." *Waste Management Symposium*, February 24–28, 2013, Phoenix, Arizona.

Zhu M, J Meza, D Moulton, I Gorton, M Freshley, P Dixon, R Seitz, J Wengle, R Patterson, and R Nelson. 2010. "A New Initiative for Developing Advanced Simulation Capabilities for Environmental Management (ASCEM)." *Proceedings Waste Management Conference*, March 7–11, Phoenix, Arizona.

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DOE – U.S. Department of Energy. 2010. *Advanced Simulation Capability for Environmental Management (ASCEM): Independent Peer Review and Assessment Team Report*. Office of Environmental Management, U.S. Department of Energy, Washington, D.C.

Freshley M, S Hubbard, V Freedman, and G Flach. 2012. *Phase II Demonstration Plan*. ASCEM-SITE-11-02, U.S. Department of Energy, Washington, D.C.

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