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ADVANCED SIMULATION CAPABILITY FOR ENVIRONMENTAL MANAGEMENT – CURRENT STATUS AND PHASE II DEMONSTRATION RESULTS (13161)

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ABSTRACT

The U.S. Department of Energy (USDOE) Office of Environmental Management (EM), Office of Soil and Groundwater, is supporting development of the Advanced Simulation Capability for Environmental Management (ASCEM). ASCEM is a state-of-the-art scientific tool and approach for understanding and predicting contaminant fate and transport in natural and engineered systems. The modular and open source high-performance computing tool facilitates integrated approaches to modeling and site characterization that enable robust and standardized assessments of performance and risk for EM cleanup and closure activities.

The ASCEM project continues to make significant progress in development of computer software capabilities with an emphasis on integration of capabilities in FY12. Capability development is occurring for both the Platform and Integrated Toolsets and High-Performance Computing (HPC) Multiprocess Simulator. The Platform capabilities provide the user interface and tools for end-to-end model development, starting with definition of the conceptual model, management of data for model input, model calibration and uncertainty analysis, and processing of model output, including visualization. The HPC capabilities target increased functionality of process model representations, toolsets for interaction with Platform, and verification and model confidence testing.

The Platform and HPC capabilities are being tested and evaluated for EM applications in a set of demonstrations as part of Site Applications Thrust Area activities. The Phase I demonstration focusing on individual capabilities of the initial toolsets was completed in 2010. The Phase II demonstration completed in 2012 focused on showcasing integrated ASCEM capabilities. For Phase II, the Hanford Site deep vadose zone (BC Cribs) served as an application site for an end-to-end demonstration of capabilities, with emphasis on integration and linkages between the Platform and HPC components. Other demonstrations, addressing attenuation-based remedies at the Savannah River Site F Area and performance assessment for a representative waste tank, illustrate integration of linked ASCEM capabilities and initial integration efforts with tools from the Cementitious Barriers Partnership.

INTRODUCTION

The Advanced Simulation Capability for Environmental Management (ASCEM) program is a multi-National Laboratory effort to develop a state-of-the-art scientific tool and approach for understanding and predicting contaminant fate and transport in natural and engineered systems. ASCEM is being pursued to address a number of challenges related to modeling in the DOE complex, for example:

- Move toward more standardized and consistent analyses using an integrated toolset that is open-source code (i.e., available at no cost to the user community),
- Improve model support for decision-making and demonstrations of regulatory compliance during and at the conclusion of assessment efforts, and
- Provide tools that can present complex information in an understandable manner and provide the capability to explore challenging remediation and disposal problems in greater detail.

ASCEM is being developed to not only have an impact on the decision making at the end of a modeling effort, but it will also provide support for decision-making during the modeling process through tools to prioritize data collection and model refinements expected to have the greatest influence on a decision.

USDOE National Laboratories are actively contributing to the project, including: Los Alamos National Laboratory, Pacific Northwest National Laboratory, Lawrence Berkeley National Laboratory, Savannah River National Laboratory, and Oak Ridge National Laboratory. This broad participation of scientists and engineers enables ASCEM to benefit from experience gained from related activities conducted in a wide variety of different programs. The ASCEM team has recognized the need to integrate more closely with on-going efforts such as the USDOE-EM Applied Field Research Initiatives (AFRIs) and related projects (i.e., Cementitious Barriers Partnership and Landfills Partnership) for an efficient approach to test the tools (Fig. 1) and show relevance for different problem sets across the USDOE complex. ASCEM activities are also leveraging advances in other USDOE programs, including the Offices of Science (Basic Energy Research, Advanced Scientific Computing Research), Nuclear Energy (Advanced Modeling and Simulation, Used Fuel Disposition), and Fossil Energy (National Risk Assessment Partnership).

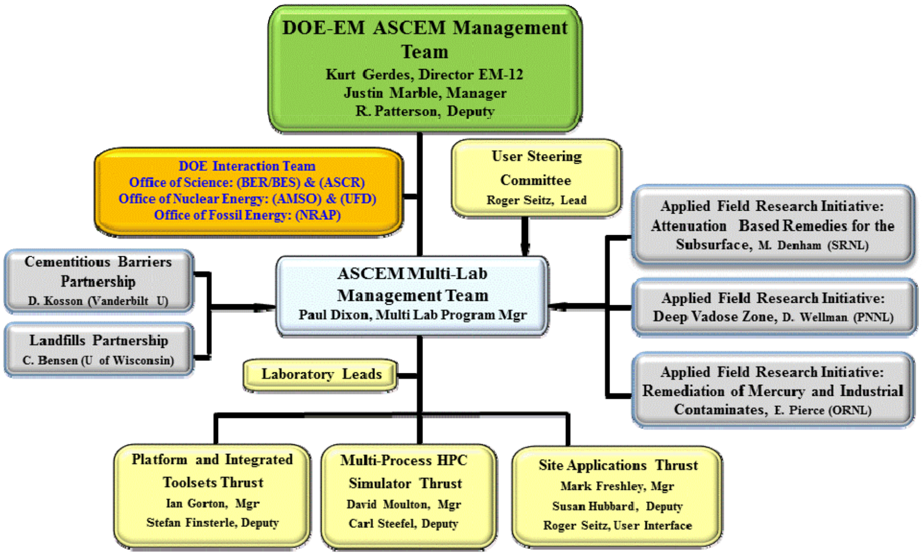


Fig. 1. ASCEM Organization and Leadership.

In addition to leveraging previous and on-going development efforts, the ASCEM team has sought to engage end-users in the development process to ensure that user needs are incorporated into the ASCEM program and its user interface framework. End-user engagement has been a key element of the ASCEM initiative from its inception. Frequent and consistent engagement 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 (PA) and risk assessment practitioners, decision-makers, oversight personnel, and regulators who are engaged in the Department of Energy (DOE) cleanup mission. User engagement is implemented in two areas of the ASCEM project, direct engagement with the management team via a User Steering Committee and broader interactions with the user community as part of the Site Applications Thrust Area [1]. Expanded user involvement working directly with and testing the tools is expected to begin early in 2013 as the first limited user release (Version 1.0) of the ASCEM integrated tools is rolled out.

As part of the development process, ASCEM is implementing site application demonstrations to test and highlight ASCEM components, engage end users in applications, and provide feedback to software developers. The overall approach for ASCEM demonstrations consists of testing components and integrated capabilities at an increasing number of DOE sites and with disparate data sets over time. The Phase II demonstration included examples from the deep vadose zone (DVZ) at Hanford, the F-Area Seepage Basins at the Savannah River Site (SRS), and a representative tank closure performance assessment. The Phase II demonstrations focused on highlighting the integration of different toolsets and capabilities that have been developed to date. This paper is divided into discussions of the structure and capabilities of the toolsets and example (case study) results from the Phase II demonstration, respectively.

ASCEM TOOLSETS

ASCEM is an emerging state-of-the-art scientific approach and software infrastructure for understanding and predicting contaminant fate and transport in natural and engineered subsurface remediation systems. ASCEM is being developed around two core thrust areas: Platform and Integrated Toolsets (called Akuna) and Multi-Process High Performance Computing Simulator (called Amanzi). The general structure and capabilities of Akuna and Amanzi are summarized in this section. The demonstration activities are conducted in the Site Applications Thrust area, which will be addressed in the next section.

Akuna Structure and Capabilities

Development of the Akuna capabilities in the Phase II Demonstration targeted a level of functionality defined by examples and case studies developed by the DVZ, SRS F-Area, and the Waste Tank Performance Assessment Working Groups. These examples defined the primary functionality for the Core Platform, Model Setup and Analysis, Data Management, Parameter Estimation (PE), uncertainty quantification (UQ), and Visualization Toolsets. The overall Platform requirements are defined in a specification of system requirements [3]. A summary of the current Akuna capabilities is included in Appendix B of the Phase II Demonstration Report [2].

The Akuna Toolset is a collection of Java-based desktop graphical user interface (GUI) to support a complete modeling workflow, from model setup to simulation execution and analysis. The toolset is an open-source, platform-independent user environment that is designed to perform basic model setup, Sensitivity Analysis (SA), inverse PE, UQ, launching and monitoring simulations, and visualization of both model setup and simulation results. Features of the model setup tool include visualizing wells and lithologic contacts, generating surfaces or loading surfaces produced by other geologic modeling software (e.g., EarthVision; Petrel), and specifying material properties, initial and boundary conditions, and model output. The model setup tool uses LaGrit for generation of both structured and unstructured model simulation grids. Integration with WorldWind also enables a user to develop a model based on the initial visualization of the site surface topography and geomorphic features.

After creating the model, the Akuna Toolset facilitates launching a single forward run to perform a SA, PE, UQ, and visualization of results. Automated job launching and monitoring capabilities allow a user to submit and monitor simulations on high-performance, parallel computers. Visualization of large outputs can be performed without moving the data back to local resources. These capabilities make HPC accessible to the users, who might not be familiar with batch queue systems and usage protocols on supercomputers and other computing platforms.

The Akuna Toolset supports a common workflow for developing and applying a numerical model in support of environmental management. Many workflow elements are repeatedly and iteratively performed as part of the modeling process. Fig. 2 provides a simplified workflow chart. In general, a conceptual understanding of the system to be analyzed is gained from site characterization efforts and monitoring data. This conceptual understanding is then translated into a mathematical model and further implemented in a numerical model. The Akuna's Model Setup Toolset supports the development of a numerical model by describing the model domain with its salient hydrogeochemical features, associated material properties, initial and boundary conditions, forcing terms, as well as information on how space and time are discretized for numerical simulations.

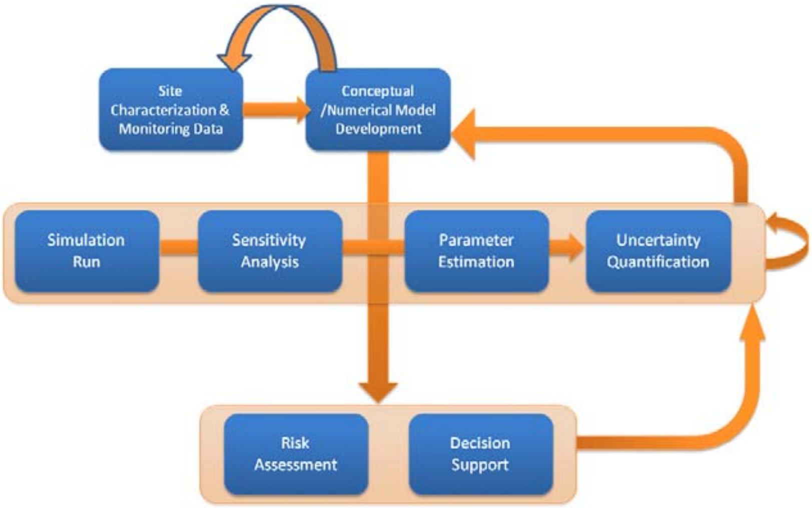


Fig. 2. Schematic of analysis workflow and supporting Akuna Toolsets.

Once an initial numerical model has been developed, the Simulation Run (SR) Toolset is used to launch and monitor a single simulation, the results of which can be analyzed and visualized. In the next step, the Akuna SA Tools are used to to identify parameters that most strongly influence the system behavior, and to examine output variables that are sensitive to model input parameters. These parameters may include material properties, initial and boundary conditions, and generally any aspect of the conceptual model that can be suitably parameterized. The Akuna's PE Toolset can be used to automatically calibrate the model using field measurement results. This step not only provides effective parameter values that can be considered consistent with the data collected at the site, but it also provides estimates of the uncertainty with which the parameters were determined. This information can then be used in the Akuna UQ Toolset to evaluate the uncertainty of model predictions. Akuna's Risk Assessment (RA) Toolset (future capability) will be used for subsequent assessment of environmental and health risks. As a final step, based on the information from these model analyses, the Decision Support (DS) Toolset (future capability) will be used to evaluate and optimize performance measures to help manage DOE's legacy sites.

The toolsets integrated in Akuna are transparent and can be flexibly invoked to accommodate any application's particular workflow. Several major components comprising the Akuna architecture are shown in Fig. 3. The Akuna user interface provides a front end to the simulation workflow. The cross-platform user interface is written in Java and is built on the Velo [4] knowledge management framework. The user interface includes a data browser that provides access to all data, metadata, provenance, and tools associated with the workflow. The VisIt visualization tool has been integrated to support remote visualization of large-scale outputs. A robust open-source content management system is used to manage workflow data and metadata [4]. Shared and private workspaces are supported for collaboration.

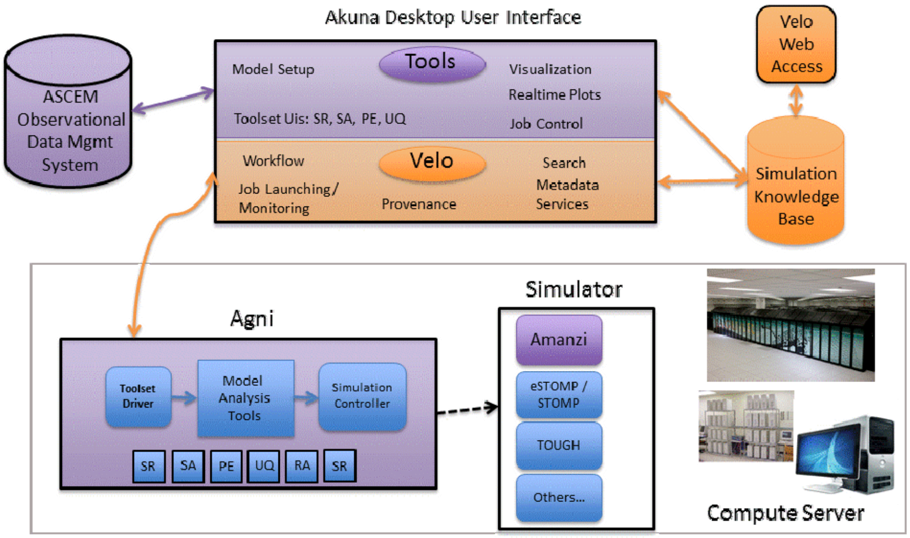


Fig. 3. Akuna architecture.

Agni software—located on the computer server—takes modeling requests from the Akuna client, executes them, and reports information back to the user interface. Agni includes a component for controlling local execution of the simulator as well as the analysis toolsets for SA, UQ, and PE. In the future, tools for risk assessment and decision support will be added. Agni is optimized for use with Amanzi, but support for translation of information to interface with other simulators is also provided.

The ASCEM Observational Data Management System (AODMS) provides data management capabilities to import, organize, retrieve, and search across various types of observational data sets needed for environmental site characterization and numerical modeling (Fig. 4). The AODMS framework provides capabilities to organize, interactively browse on maps, search by filters, select desired data, plot graphs, and save selected data for subsequent use in the modeling process [5].

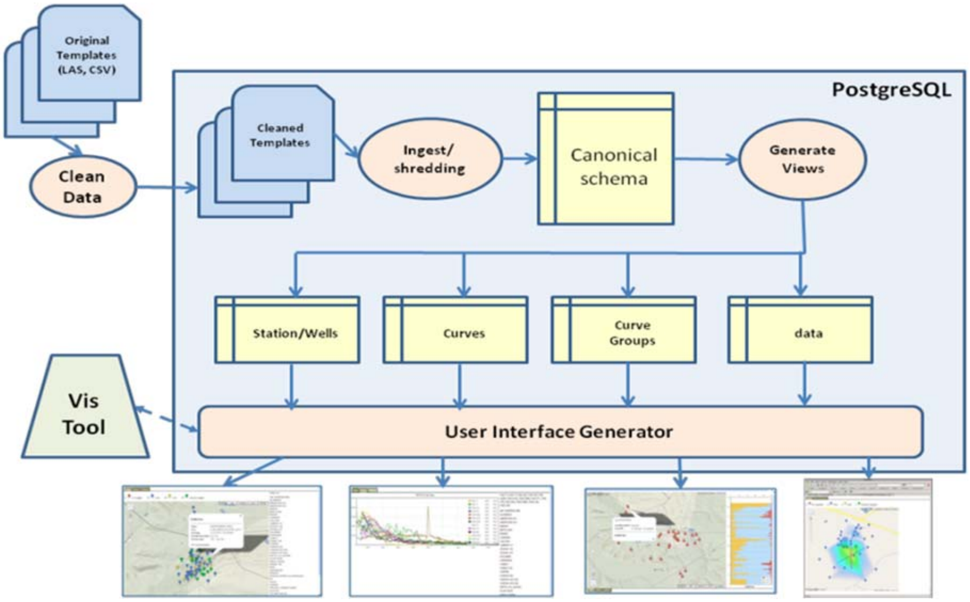


Fig. 4. Schematic diagram of the Observational Data Management System implementation with examples of the user-interface displays in the bottom row.

As part of the Phase II Demonstration, new visualization templates for VisIt were developed to automate the process of generating visualizations of structured and unstructured meshes, of model setup and PE results, and for generating two-dimensional and three-dimensional animations from large-scale HPC simulations for selected analytes. The templates, written in Python, enable a user to generate complex visualizations with a single-button click in the Akuna GUI. The templates automatically scale and label axes, select intuitive color schemes and camera angles, and generate animations of time-varying data sets. These data can be viewed in an interactive mode, which allows the user to modify the initial visualization provided by the template to adjust variables, color schemes and camera angles. The visualization can also be created in the background; for instance, to generate an animation using many simulation output time steps. In this case, when the execution of the parallel rendering code is complete, the resulting images and video animations are returned to the Akuna user interface and displayed as a thumbnail image.

Amanzi Structure and Capabilities

The Multi-Process HPC Simulator, named Amanzi, provides a flexible and extensible simulation capability for ASCEM. Amanzi supports a wide range of process complexity in flow and reactive transport models, and supports the graded and iterative approach to performance and risk assessment required by EM. Amanzi is designed, developed, and has been tested on a range of computer architectures, from laptops to supercomputers, to access advanced computational power as needed.

To ensure Amanzi’s design and capabilities support the range of conceptual models developed using Akuna, high-level requirements, including the underlying mathematical formulations of the models, was developed [6]. After prototyping key high-level concepts for the Phase I Demonstration [7], an initial design document was developed for Amanzi [8]. During Phase II, significant advances were made toward accomplishing this design and establishing key Amanzi capabilities. Some of these advances, which are discussed in more detail in this section, include transient saturated/unsaturated flow; the van Genuchten and Brooks-Corey water retention models; a flexible high-level model representation and input specification; a wide variety of geochemical processes including surface complexation, aqueous speciation, and several sorption models; parallel input/output for visualization and restarts; and a hierarchical verification and validation testing framework. Amanzi has performed parallel 3-D single runs on over 1000 processors using the Hopper Cray XE6 at the National Energy Research Scientific Computing Center (NERSC) and is readily driven by Akuna/Agni for UQ and PE studies.

The Multi-Process HPC Simulator takes as input a conceptual model, which describes a set of coupled processes such as flow and reactive transport. The conceptual model is expressed mathematically by a system of differential and algebraic equations that represent the relevant conservation laws, constitutive laws, equations of state, and reactions. Various parameters required for the model are specified, along with initial and boundary conditions. To represent this system of equations on a computer, a mesh (grid) is provided with the model. A mesh may be thought of as a collection of discrete cells or grid blocks that fill the domain of interest. For a given mesh, a relationship between variables (e.g., pressure), parameters (e.g., permeability), and mesh geometry is developed. This process is referred to as discretization, and gives rise to a system of equations that represent the model.

The hierarchical and modular design of the Multi-Process HPC Simulator reflects the steps in translating a conceptual model to a numerical model to produce simulation output. At the highest level, the Multi-Process Coordinator (MPC) and the Process Kernels represent the conceptual model (Fig. 5). The Process Kernels are high-level objects that represent processes such as flow, transport and reactions. The MPC manages the coupling of the Process Kernels that comprise the conceptual model, as well as the data.

At the next level of design, the HPC Toolsets include Mesh Infrastructure, Discretization, Reactions, and Solvers. The Mesh Infrastructure Toolset provides interfaces and supporting routines to leverage existing mesh representation libraries. The Discretization Toolset provides procedures that generate the discrete system of equations from a given continuum model on a mesh. The Reaction Toolset implements geochemical reactions such as aqueous speciation and sorption. At the lowest level, the HPC Core infrastructure provides low-level services such as data structures to operate on parallel computers, input and output, and error handling.

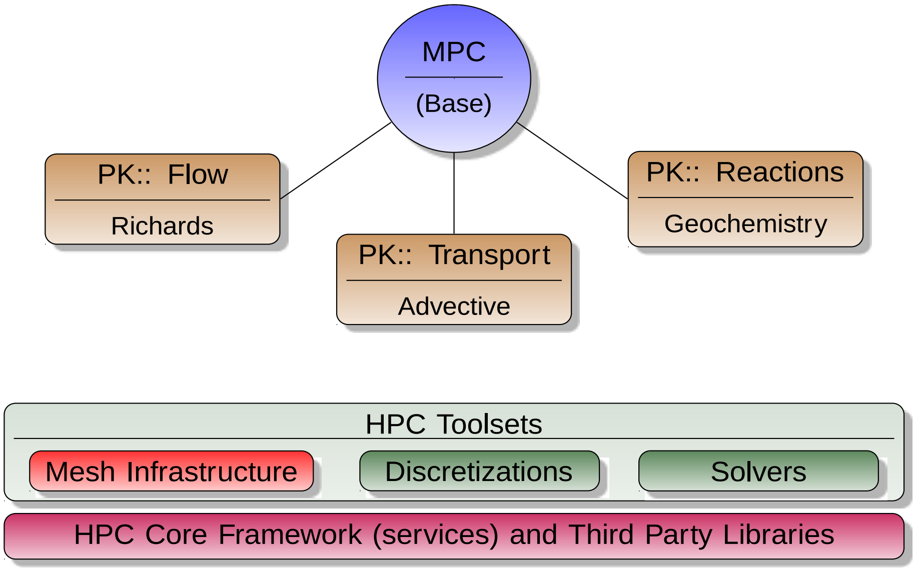


Fig. 5. Schematic showing a base Multi-Process Coordinator that has Process Kernels (PK) for flow, transport, and reaction modeling.

The Phase II Demonstration provided an excellent test-driven environment for the prioritization, development, and testing of new Amanzi features. At the highest level, Process Kernels have been added or their capabilities have been enhanced to support these demonstrations. In addition, new capabilities have been added to the MPC to manage these processes during simulation, control output for observations and visualization, and initiate input and output associated with parallel restarts. These high-level capabilities have been supported by significant advances in the underlying HPC Toolsets (e.g., mesh infrastructure, discretization, reactions), as well as the HPC Core Framework. The high-level input specifications ensure that a user can focus on the model description in geologic and geometric terms, without being overly concerned with the underlying computational approach.

In addition, a portable build system has been developed to enable the use of Amanzi on a wide variety of modern architectures. Automatic builds and tests run nightly and are documented for quality assurance.

CASE STUDIES OF CAPABILITIES FROM THE PHASE II DEMONSTRATION

Unlike the Phase I Demonstration, Phase II working group efforts were performed sequentially rather than in parallel. This approach allowed developers to focus on advances needed to meet specific objectives of one demonstration at a time. The approach also allowed each demonstration to build on previously developed capabilities. The focus of the DVZ Working Group was to demonstrate a relatively simple but complete beginning-to-end demonstration of ASCEM capabilities. The SRS F-Area Working Group demonstration focused on implementing some of the linked ASCEM capabilities under conditions of dense and complex environmental data, including reactive chemistry, source-term uncertainty, and linked vadose zone and saturated flow. The waste tank demonstration emphasized application of the adaptive mesh refinement capabilities for fine features associated with engineered structures. A few examples from the demonstrations are provided in the following sections.

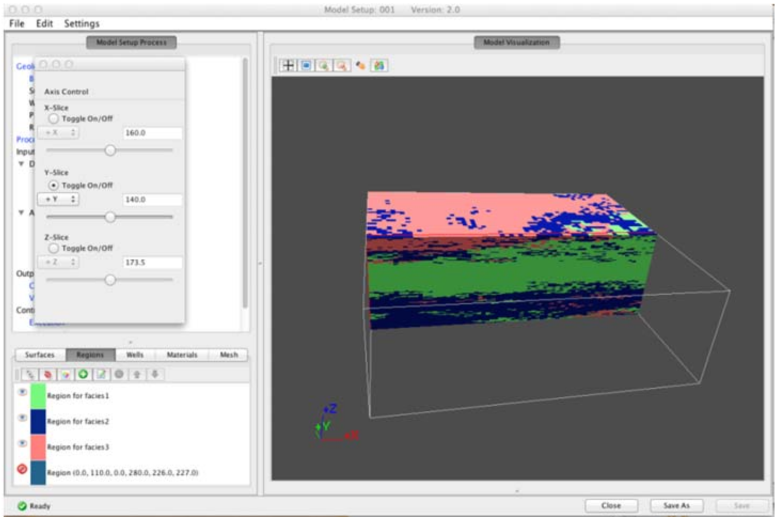
Deep Vadose Zone Demonstration

The DVZ AFRI at the Hanford Site provides an opportunity to demonstrate ASCEM capabilities needed to evaluate innovative treatment technologies for recalcitrant contaminants. For example, a technology currently under evaluation at the BC Cribs waste site is soil desiccation, an approach that minimizes Tc-99 movement in the vadose zone by removing pore water via the injection of dry air and vapor extraction. The first step in modeling the site is an analysis of contaminant transport. Future demonstration phases will include explicit representation of soil desiccation as well as other remediation approaches being developed by the DVZ AFRI or by the USDOE Richland Operations Office.

The primary objective of the Hanford Site DVZ Phase II Demonstration was to illustrate end-to-end integration of Platform and HPC components, from the Data Management and Model Setup and Analysis Toolsets to PE and UQ. The Platform Toolset was executed to import and manage data from the BC Cribs waste site, visualize multiple conceptual models, facilitate PE and uncertainty analysis, and set up and execute Amanzi simulations. Integration of Platform and HPC components is demonstrated through the model setup, execution and analysis of Amanzi simulations that evaluate flow and transport at the DVZ site. The use of parallel processing in the HPC toolset makes execution of multiple simulations feasible, and the Akuna Toolset streamlines this process. Illustrative examples of the model setup and analysis and visualization toolsets are included in this section.

The Model Setup and Analysis Toolset allows simulation input file generation in a fast and user-friendly way. When a new model is created in Akuna, the user is led through steps to define 1) a Geologic Model (e.g., domain extent and geologic layers); 2) Inputs (e.g. material properties, boundary and initial conditions); 3) Outputs (e.g., checkpoint and visualization data); and 4) Execution Controls (e.g., solver parameters, time step control periods). The geologic conceptualization of the BC Cribs involved multiple conceptual models generated outside of Akuna and lithofacies were assigned on a cell by cell basis via a file read. The other option for defining the geologic model involves defining stratigraphic layers (surfaces) and the Model Setup and Analysis Toolset fills in regions of the model in between the surfaces.

Hydraulic properties are assigned to each of the lithofacies through the Model Setup and Analysis Toolset. The structured grid for the BC Cribs domain was generated using Gridder, a structured mesh tool associated with the Akuna Toolset. Once the domain extent has been defined, the Mesh Generation window allows the user to create a structured mesh. The grid can be toggled on and off in the visualization window. The domain can also be interrogated using slices (Fig. 6).



X-Slice ○ Toggle On/Off +X 160.0

Y-Slice ● Toggle On/Off +Y 140.0

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Fig. 6. Viewer in the Model Setup and Analysis Tool showing the distribution of lithofacies.

Once model setup is complete, simulations are executed. Simulations can be performed as a forward simulation run, SA, PE, or UQ. In this demonstration, a simulation was first executed to validate the model setup, and to compare the simulated results with the measured data at Boreholes A and C before performing a PE. Parameter estimates were assigned from pedotransfer functions prior to the initial simulation. The Model Setup and Analysis Toolset created an input file and launched the simulator.

Akuna also provides on-going status of simulations (e.g., submitted, running, and completed). When the simulation completes successfully, a small green check mark appears next to the SR directory in the Akuna viewer window. In the BC Cribs Phase II Demonstration, the simulation completed using the initial values from pedotransfer functions showed a mismatch between simulated and measured data as shown for concentrations, which indicated the need for model calibration.

Understanding the spatial distribution of contaminants is important to identifying potential remedial actions at the BC Cribs. Visualizing the spatial distribution of Tc-99 also contributes to an understanding of how heterogeneities impact contaminant transport simulations. When a simulation has successfully completed, the Visualization Toolset using VisIt is launched from Akuna. For the BC Cribs demonstration, the spatial distribution of Tc-99 after the discharges to the cribs terminated (1960) is shown in Fig. 7. Horizontal cross-sections through each row of cribs, as well as a vertical cross-section through Borehole A, are also shown in Fig. 7. In general, the main advantage of the Akuna modeling framework lies in its ease for model setup, execution and analysis, from PE through uncertainty analysis.

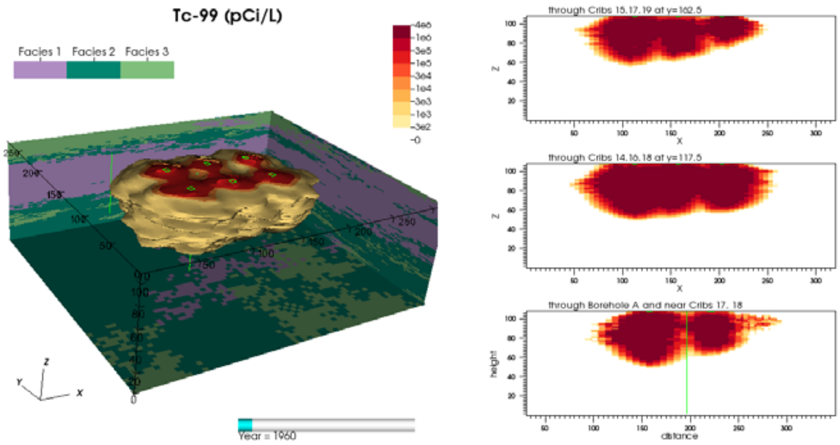


Fig. 7. Spatial Distribution of Tc-99 after the releases from the cribs using VisIt software.

F-Area Seepage Basin Demonstration

The study of the SRS F-Area Seepage Basins provides an opportunity to implement linked ASCEM capabilities, including those applied during the Phase II DVZ Demonstration. The SRS F-Area is characterized by complex geochemical conditions with large, dense, and disparate heterogeneous data sets. Specific information about the F-Area site geology, hydrogeology, geochemistry, contaminants, available data, leveraging activities, and early advances in the development of ASCEM components can be found in the Phase I Demonstration Report [7]. Building on previous advances, additional ASCEM capabilities are needed to help provide an efficient and cost-effective transition from active to passive remediation, using MNA and enhanced attenuation. For example, the site currently operates a base-injection remediation treatment but lacks the technical underpinning to quantify the duration that this treatment is necessary or if other treatment delivery strategies or natural attenuation would be equally or more effective.

The Phase II Demonstration at the SRS F-Area site incorporates source zone loading, infiltration, and complex geochemistry. Of particular interest was the impact of the uncertain input parameters on trailing uranium plume concentration gradients, which are drivers for the remedial treatments at the site. As such, Phase II focused on using UQ tools to assess how uncertainty associated with recharge, contaminant source characteristics, and geochemical reactions affect long-term predictions of plume transport to the base injection barrier. This topic is generally of interest, because recharge and basin seepage are common components of many DOE contaminated sites, but their effects on groundwater plume mobility are rarely considered in a quantitative manner. In addition to the emphasis on UQ, data management, HPC and visualization components of ASCEM were expanded and implemented during the Phase II Demonstration. This summary focuses on the UQ capabilities.

The F Area demonstration was designed to highlight the utility of Amanzi for gaining a predictive understanding of long-term plume transport in complex systems, as is needed to guide remediation decisions and closure strategies. The overall goal of the Phase II Demonstration UQ component was to demonstrate the application of Akuna and Amanzi to seamlessly integrate uncertainty analysis tools to assess the impact of the seepage from the basin (i.e., source of contamination), key uncertain hydraulic parameters, and geochemical reaction parameters on long-term acidic uranium plume transport. The UQ analysis was based on simulations along the 2-D centerline of the uranium plume originating at the F Area Seepage Basin. The analysis included Monte Carlo simulations and global SA. Agni generated multiple sets of parameters from the prescribed probability distribution, distributed the simulations over multiple processors, and analyzed the outputs. Measured and simulated breakthrough curves of pH and the U(VI) concentrations were simulated at the downstream monitoring wells (FSB95DR, FSB110D).

Using the Monte Carlo approach, Agni generated a total of 150 sets of different parameters from independent normal distributions, using Latin Hypercube sampling, and distributed the hundreds of simulations over 3600 cores (24 cores per each simulation) on the NERSC supercomputer, Hopper. The simulations using Amanzi took approximately 4 hours in wall time (which was the longest simulation time among the runs) and approximately 14,400 computer hours. Fig. 8 shows the Monte Carlo simulation results at the two different monitoring wells for pH and uranium concentrations. The observed breakthrough curves are fairly close to the predicted mean breakthrough curves, and within the confidence bounds (mean +/- 2 standard deviation), except for some scattered observation points.

The Amanzi simulations illustrate that during the basin operations, pH values rapidly decrease as the acidic plume arrives. All the pH curves reach a plateau due to saturation of the sorption sites. After the basin closure, the pH rebound is strongly delayed mainly due to the effect of hydrogen (H^+) buffering. Although some curves predict that the pH could exceed the value of 5 by the year 2055, the majority of curves predict a slower pH rebound. Fig. 8c and 8d show that the breakthrough curves of U(VI) concentrations are the reverse of those for pH. Similar to pH, the plateau of U(VI) concentrations can be seen during the basin operation. After the basin closure, uranium concentrations decrease significantly, although the mean curve does not drop below the MCL of 1.3E-7 mol/L.

The Agni global SA, using the Morris method, was performed to identify the key controls on the plume mobility. The sensitivity of pH and U(VI) concentrations were evaluated over time at two well locations. Fig. 9 illustrates complex patterns of the impact of different parameters on pH and U(VI) concentrations at different locations and times during and following the basin closure. Table I is a summary of the most influential parameters, including aquifer permeability, geochemical and source parameters. For pH, the cation exchange capacity (CEC) and source pH have a large impact on U(VI) concentrations at both locations during the operation, whereas after the basin closure, the permeability values become important. For the U(VI) concentrations, the sorption site density and the U(VI) source concentration are the key parameters during basin operation, and permeability of the clay layer becomes important after basin closure. This information is useful for those involved in decision making and design of long-term monitoring, sampling, and remediation strategies.

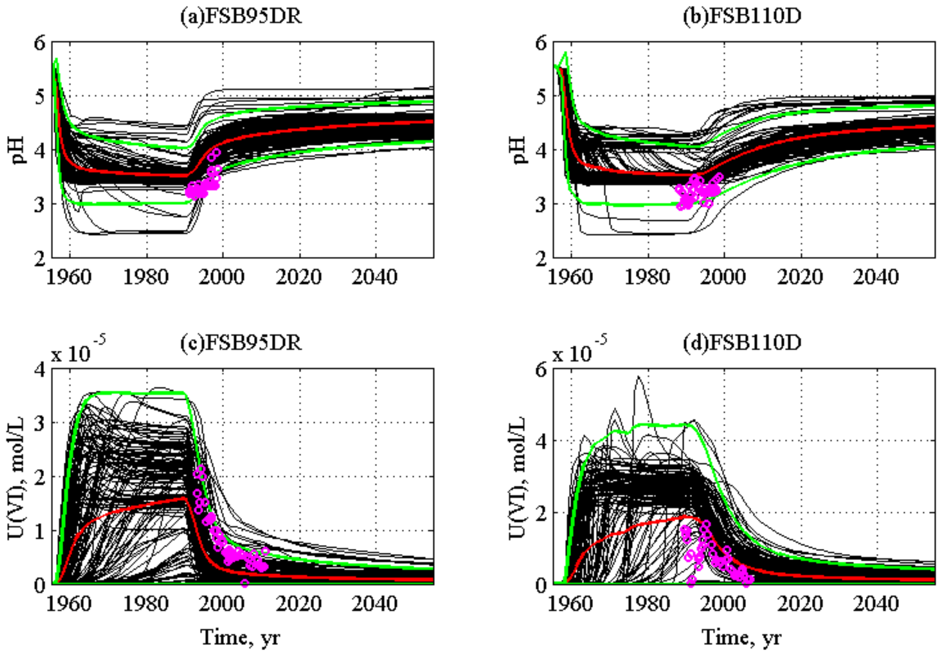


Fig. 8. Monte Carlo simulation results: breakthrough curves and uncertainty ranges: a) pH at monitoring well FSB95D, b) pH at monitoring well FSB110D, c) U(VI) concentration at FSB95D, and d) U(VI) at FSB110D. The black lines are the predicted breakthrough curves, red lines are the mean predicted curves, green lines are the mean +/- 2 standard deviations, and the magenta dots are observations.

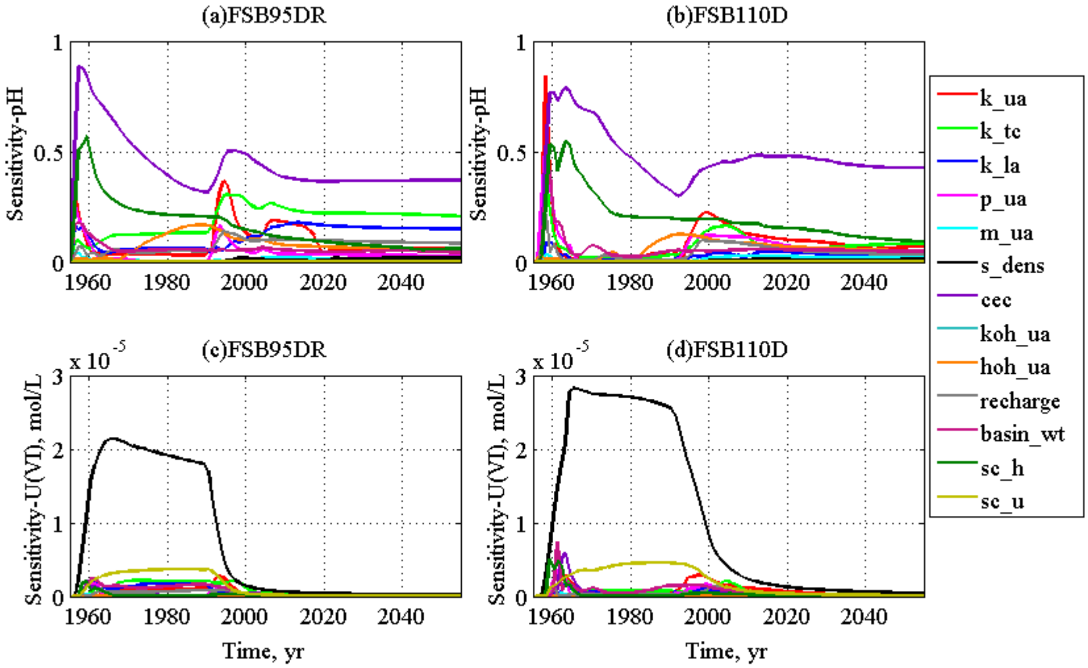


Fig. 9. Global sensitivity analysis results using Agni-Amanzi: time profile of sensitivity: a) pH at FSB95D, b) pH at FSB110D, c) U(VI) at FSB95D, and d) U(VI) at FSB110D.

TABLE I. Parameters controlling pH and U plume mobility at locations close to and far from the basin, assessed at 1985 (during operation) and 2055 (100 years from the beginning of the basin operation).

Location Close to Basin				**Remote Monitoring Well**		
pH		1985	2055		1985	2055
	1	CEC	CEC	1	CEC	CEC
	2	Source pH	TCZ permeability	2	Source pH	Source pH
	3	Goethite specific surface area	LUTRA permeability	3	Goethite specific surface area	TCZ permeability
U		1985	2055		1985	2055
	1	Sorption site density	Sorption site density	1	Sorption site density	Sorption site density
	2	Source U	TCZ permeability	2	Source U	TCZ permeability
	3	TCZ permeability	Source U	3	Basin discharge	Source U

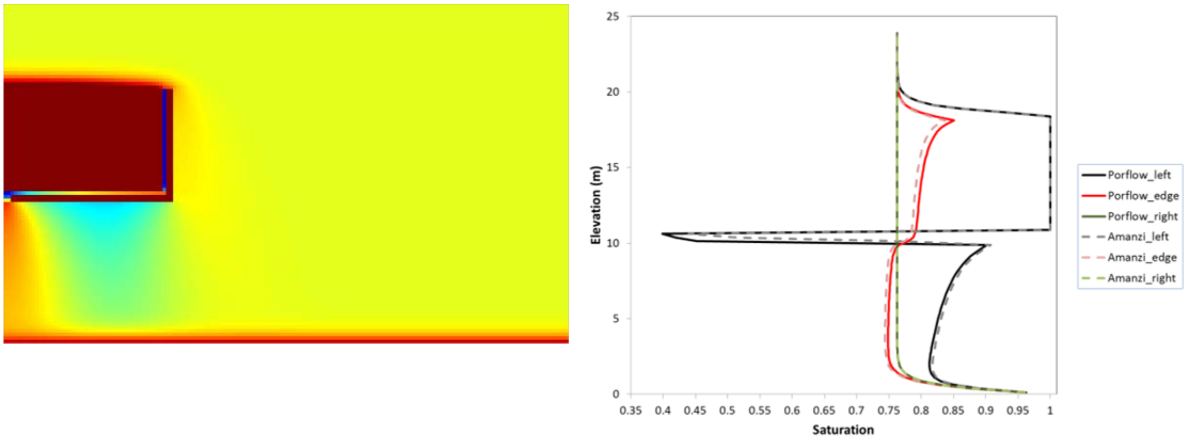
Waste Tank Performance Assessment

The Waste Tank Performance Assessment (PA) Working Group provides an opportunity to test and demonstrate ASCEM capabilities needed for EM performance assessments of waste tank closures and low-level waste in engineered containment systems. These types of systems are a prominent component of the EM program across the DOE complex and relevant to many waste disposal, remedial action, decontamination and decommissioning, and long-term stewardship activities. Engineered barriers and waste forms also present unique process and platform requirements in comparison to geologic systems in the form of geometries, materials and associated properties, and physical and chemical processes.

The Phase II Demonstration built upon the Phase I Demonstration and focused on the use of AMR to efficiently and accurately resolve fine-scale features such as steel liners and fast-flow paths that are routinely encountered in PAs of engineered containment systems for radiological waste disposal. AMR offers the prospect of increased computational efficiency and/or simulation accuracy by selectively refining only those regions of the domain occupied by small-scale features. Current practice typically involves a coarse uniform mesh resolution that cannot accurately resolve features, or a non-uniform orthogonal mesh that introduces large grid cell aspect ratios and size disparities, and corresponding numerical inaccuracies. The demonstration scenario involved radionuclide release from a closed waste tank that is representative of conditions at the SRS and Hanford Site.

Key ASCEM components engaged in the Phase II Demonstration include AMR and radioactive decay and progeny ingrowth capabilities within the HPC Toolset. The goal of AMR was to resolve fine-scale features of the tank closure scenario, including thin barriers and fast-flow paths, to avoid model simulation biases and uncertainties compared to typical practice. Radionuclide decay and linear sorption were included to demonstrate basic models for use in graded modeling approaches favored by USDOE. Graded approaches refer to using multiple levels of modelling detail as needed for screening, probabilistic analyses, or other purposes.

The demonstration focused on a benchmarking simulation of steady-state, unsaturated flow based on the Richards equation for a representative tank using a uniform grid. Two scenarios were considered: an "Intact" case for which the fast-flow path is not present, and a "Fast-Flow" case. The fast flow path required fine-scale discretization. The PORFLOW code was used for benchmarking (http://www.acricfd.com/software/porflow). For the Intact case, the two codes produced practically identical saturation fields and, for the Fast-Flow case, the results were very similar (Fig. 10).



(a) (b)

Fig. 10. Amanzi simulated results for ‘fast-flow’ case: a) saturation field (saturated is red and unsaturated is blue), and b) benchmarking comparison for selected vertical profiles.

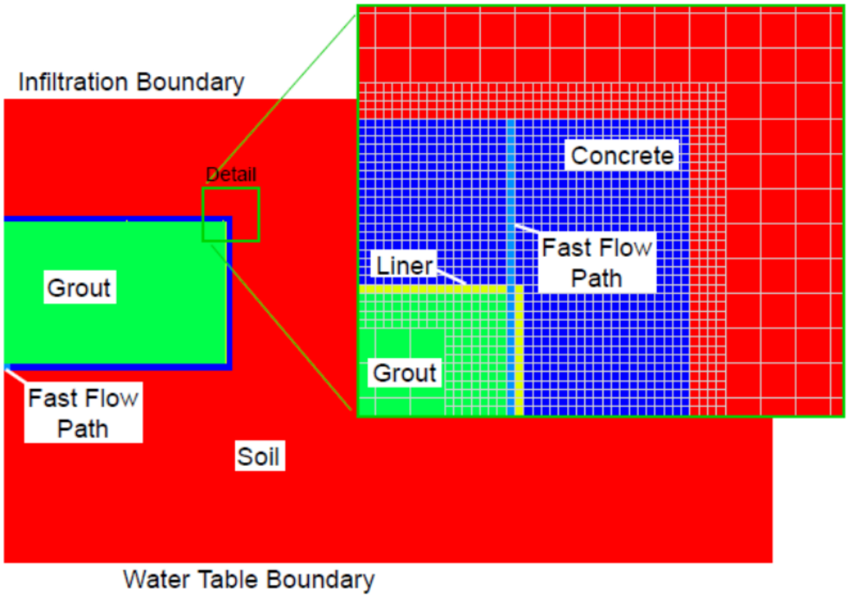


Fig. 11. Tank geometry for Amanzi benchmarking using an AMR grid.

The results in Fig. 10 were generated using a uniform 0.25 meter computational mesh. To demonstrate the AMR capabilities of Amanzi, a similar benchmark simulation for the refined geometry depicted in Fig. 11 was pursued. Although the two benchmarking problems share the same features, the second geometry was greatly refined to reflect the true physical dimensions of key features. In particular, the thick steel liner and fast-flow path were reduced to a thickness of 1 and 2 centimeters respectively from 25 cm, the resolution of the uniform grid. As anticipated, achieving convergence of unsaturated flow on an AMR grid for highly-contrasting fine-scale features was challenging. These challenges drove algorithm development for Amanzi during Phase II that focused primarily on two key areas: problem geometry specification, and computational efficiency through robust solver performance.

Currently, the HPC Thrust is pursuing numerical advances in solving the non-linear coupled system that arises from representing Richards equation on the AMR grid. These include a non-linear multigrid strategy to better couple the AMR refinement levels together, and a wider range of methods to solve the non-symmetric linear systems that arise. Other areas for enhancement include the incorporation of time-dependent material properties (to better represent the transient system throughout the lifespan of the engineered systems), and incorporation of the radioactive decay models into Amanzi for solute transport.

In future demonstrations, Amanzi will be used to simulate flow and releases of radionuclides from a grouted waste tank to the underlying water table over hundreds to thousands of years to complete the primary Waste Tank PA demonstration begun in Phase II. Physical phenomena to be considered in the simulation include transient, variably saturated moisture transport using Richards equation, and transport of dissolved radionuclides through advection and diffusion. The transport simulation will incorporate first-order decay and progeny ingrowth, linear sorption (K_d), and solubility controls under isothermal conditions. Infiltration and selected material properties will be prescribed to vary through time. Parallel runs on up to 1000 cores are anticipated. Collaboration with the Cementitious Barriers Partnership has also started for development of linkages for a loosely coupled near-field simulation of processes within a barrier including ASCEM far-field simulation of processes in the surrounding environment.

DISCUSSION

The goals for the Phase II demonstration were to showcase the continuing development of new capabilities for Akuna and Amanzi and integration of those capabilities in an end-to-end simulation involving the different toolsets. These goals were accomplished using three different demonstrations: DVZ at Hanford, F Area Seepage Basins at Savannah River, and a representative tank closure PA. The simulations involve a range of different environmental conditions, contaminants and also engineered systems. Thus, the suite of demonstrations provide the opportunity to highlight a number of different capabilities in the toolsets.

The simulations of the DVZ (BC Cribs site) for Phase II were performed for the purpose of demonstrating the end-to-end integrated capabilities of ASCEM to establish baseline conditions expected under a “no-action” alternative. Because small-scale subsurface heterogeneities are known to be a major factor influencing transport at the site, heterogeneous lithofacies distributions were considered in the analysis. Although the PE effort provided a less than perfect match between measured and simulated values of moisture content and concentration, the new parameter estimates showed a significant improvement in matching historical data over the initial estimates. Modeling is an iterative process, and improvements in historical data matching are expected as the conceptual model is revised (e.g., boundary conditions, lithofacies distributions, etc.), and new capabilities are incorporated into the Akuna tools. These capabilities could include tools such as global search algorithms and the use of pilot points for PE and optimization.

The results of the DVZ demonstration show the importance of examining uncertainty with respect to subsurface heterogeneities, as well as any other sources of uncertainty that may impact mass transport to the water table. Using Akuna to generate breakthrough curves, histograms and scatter plots for UQ facilitated a rapid analysis and identification of trends.

The SRS F-Area Demonstration focused on using the newly developed ASCEM HPC and UQ capabilities to assess how uncertainty associated with contaminant source, geochemical reactions, and flow characteristics can impact the predictions of the long-term behavior of pH and U plumes in the region up gradient of the injection barrier at the SRS F-Area. The Amanzi simulations of the unsaturated-saturated flow and contaminant transport (based on the numerical solution of the Richards equation and including a non-electrostatic sorption model) compared well with field observations. The UQ analysis was also used to identify the key hydraulic and geochemical parameters that control plume behavior at different distances from the basin and over time. Gaining such an understanding is a critical prerequisite for making sound and sustainable risk management, remediation, and closure decisions. The UQ analysis included Monte Carlo simulations of coupled vadose zone and groundwater flow along with reactive transport simulations that take into account complex geochemical reactions, which are rarely performed over large spatial extents and long time frames. The Amanzi parallel processing capabilities have overcome this hurdle, thereby advancing capabilities to provide a stronger foundation upon which to make remediation decisions.

In summary, the SRS F Area demonstration showed that the ASCEM UQ Agni-Amanzi coupling could provide uncertainty ranges that can provide further insights for practitioners and managers involved in decision-making, risk assessment, and site management. The SRS F-Area Demonstration provides an opportunity to develop and test ASCEM capabilities, which are needed to help EM, Savannah River National Solutions (SRNS) and Savannah River National Laboratory (SRNL) provide an efficient and cost effective transition from active to passive cleanup of uranium-contaminated groundwater, using the MNA and enhanced attenuation technologies, which will ultimately be useful throughout the DOE complex.

The waste tank closure demonstration is in the early stages relative to the other demonstrations, but has provided a successful framework to highlight the ability to apply AMR to represent fine features and large contrasts in material properties. The effort to date has largely focused on the development of the modeling capability in Amanzi to be able to address the challenges associated with the non-linearity and large contrasts in material properties associated with engineered features. Moving forward the intent is to first include contaminant transport including radioactive decay, using levels of modeling detail more commonly associated with PA applications (e.g., linear sorption, solubility). Eventually, the intent is to specifically address multiphase processes and chemical reactions and oxidation of engineered features over time.

CONCLUSIONS

The ASCEM project has successfully implemented many different capabilities in the Platform and HPC toolsets. The Phase II demonstration provided a number of examples of implementation of the ASCEM tools for applications representative of typical DOE modeling challenges. Additional capabilities continue to be added to the tools and the demonstrations are expected to continue to add complexity as the capabilities are included in the tools. The Phase III ASCEM Demonstration marks the beginning of the applied phase of the project, where capabilities and quality assurance of the toolsets are refined to a point where they can be demonstrated to guide site cleanup efforts and be tested by end users. The first user release (Version 1.0) is planned for early in 2013. Working group activities and interactions with end users will be a new focus of the Site Applications Thrust to begin integrating ASCEM into the EM community and gaining broader feedback on needed performance and capabilities.

The ASCEM capabilities are expected to help EM 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 DOE site decision making to develop long-term paths to completing the DOE cleanup mission.

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