Advanced Simulation Capability for Environmental Management Initial User Release (14134)

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ABSTRACT

The Office of Soil and Groundwater Remediation within the U.S. Department of Energy 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 under one framework. It is designed to facilitate integrated approaches to modeling and site characterization, and provide robust and standardized assessments of performance and risk for EM cleanup and closure activities. The project is linked with applied field research sites also funded by the EM Office of Soil and Groundwater Remediation.

The ASCEM project has continued development of capabilities, with emphasis on both the Platform and Integrated Toolsets (Platform) and the High-Performance Computing multi-process simulator (called Amanzi). Platform capabilities provide the user interface and toolsets (called Akuna) for end-to-end model development, starting with definition of the conceptual model, management of data and metadata for model input, sensitivity analysis, model calibration and uncertainty analysis, model execution on diverse computational platforms, and processing of model output, including visualization. Development of Platform capabilities focused on robust integration among the Akuna toolset and with Amanzi. The toolsets were thoroughly tested, including 1) integration testing of interfaces, and 2) user testing to ensure that the Akuna user interface is readily usable and intuitive. Akuna runs on a local computational environment for the user interface. Amanzi is designed to be executed on a wide range of computer architectures, from laptops to supercomputers, to access the appropriate level of computational power for the problem at hand. User testing included participants from the Site Applications Thrust with a broad spectrum of modeling experience. Development of Amanzi focused on improving robustness, increased functionality of process representations, toolsets for interaction with Akuna, and verification and model confidence building.

The ASCEM toolset and tutorials were released to an initial set of users for testing and evaluation. ASCEM development is divided into three phases following a risk-based graded approach to quality. The initial release represents the Research and Development (R&D) branch corresponding to the initial “Basic Phase.” The R&D branch release is available for testing but cannot be used for regulatory applications.

INTRODUCTION

In 2009, the National Research Council (NRC) of the National Academies reviewed 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* [1]. The NRC report outlined prioritization needs for the Soil and Groundwater 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, EM funded a number of initiatives in 2010, including a strategic initiative in the Office of Soil and Groundwater Remediation to develop the Advanced Simulation Capability for Environmental Management (ASCEM). ASCEM is a state-of-the-art scientific approach that uses an integration of toolsets to understand and predict 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 (Fig. 1). The toolset facilitates integrated approaches to modeling and site characterization that enable robust and standardized assessments of performance and risk for EM cleanup and closure activities.

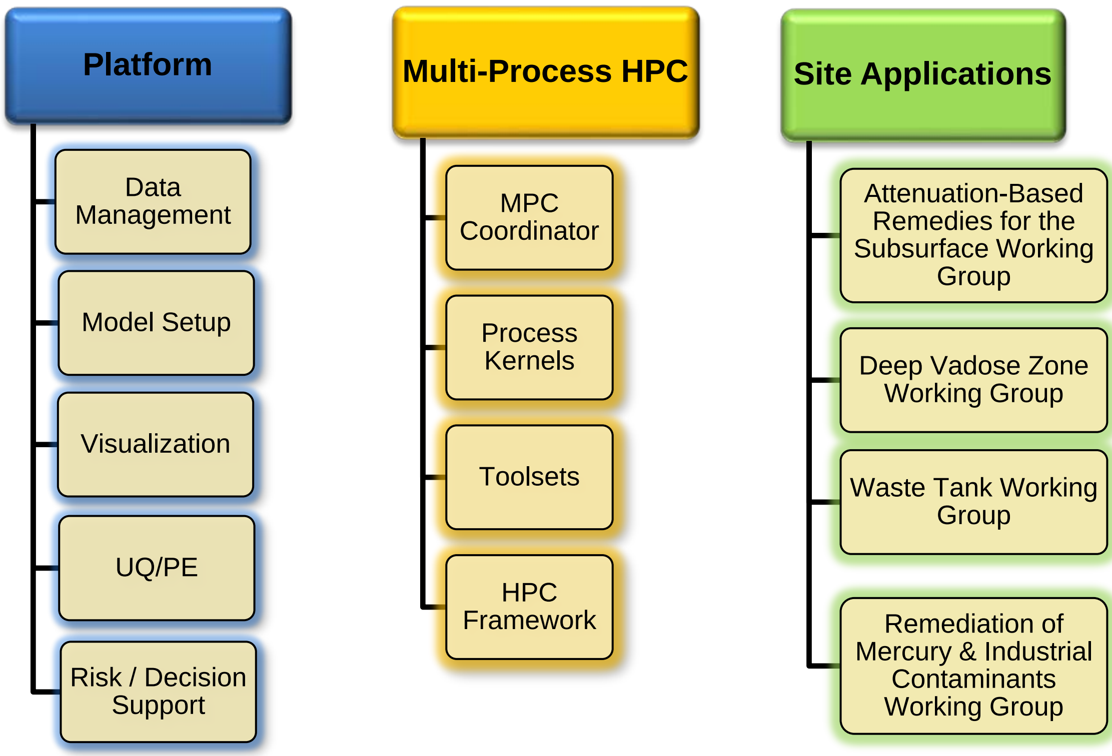

Fig. 1. ASCEM Project Organization.

The ASCEM project is a multi-national laboratory effort to develop a state-of-the-art scientific toolset to address a number of simulation challenges across the DOE EM complex, including the following:

- Standardization of performance and risk assessment analyses using integrated open-source toolsets (i.e., available at no cost to the user community).
- Development of a community model approach to engage the user community.
- Improved model support for decision-making and demonstrations of regulatory compliance through documentation of modeling approaches and data.
- Application of modeling approaches that use complex data and approaches in an understandable manner to explore challenging remediation and disposal problems in greater detail.

The ASCEM development process includes site application demonstrations to test and evaluate ASCEM components, engage end users in applications, and provide feedback to software developers. The approach for ASCEM demonstrations consists of testing components and integrated capabilities at an increasing number of DOE sites and with disparate datasets over time. These applications also provide the basis for increasing levels of quality assurance testing and documentation as well as tutorials for user releases that occur regularly.

CAPABILITY DEVELOPMENT

Significant development of capabilities has occurred on both the Platform (Akuna) and HPC (Amanzi) thrust areas of the project. The Platform and Integrated Toolsets Thrust includes a user interface (UI) and tools for site data management, model setup, model calibration and uncertainty analysis, and model results visualization. The HPC multi-process simulator capabilities include process model representations, toolsets for interaction with the Platform, model confidence testing, and verification for quality assurance.

Akuna

The Akuna Toolset is a collection of Java-based desktop graphical user interfaces (GUIs) to support a complete modeling workflow (Fig. 2), from model setup to simulation execution and analysis. The overall Platform requirements were defined in a specification of system requirements [2]. The toolset is an open-source, platform-independent user environment that is designed to perform basic model setup, including Core Platform, Model Setup and Analysis, Data Management, Sensitivity Analysis (SA), Parameter Estimation (PE), and Uncertainty Quantification (UQ). The model setup tool includes visualization of wells and lithologic contacts, generating model layers or loading surfaces produced by other geologic modeling software (e.g., EarthVision or Petrel), and specifying material properties, initial and boundary conditions, and model output. The model setup tool includes generation of both structured and unstructured model simulation grids. Integration with the National Aeronautics and Space Administration's (NASA's) WorldWind is included to facilitate conceptual model construction and provide a linkage with specific locations on a map.

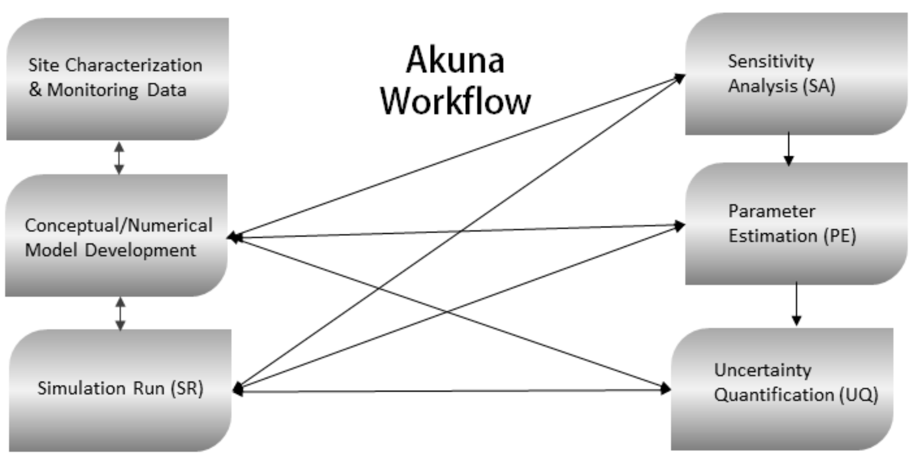

Fig. 2. Akuna workflow.

Akuna facilitates launching simulations on high-performance, parallel computers to perform SA, PE, UQ, and visualization of results. Automated job launching and monitoring capabilities allow users to easily manage simulation activities, making HPC accessible to users who might not be familiar with batch queue systems and usage protocols on supercomputers and other computing platforms. The user environment of Akuna is shown in Fig. 3. Akuna is tightly integrated with Amanzi, but can be used with any simulator. The Akuna UI is written in Java and is built on the Velo [3] knowledge management framework. The UI includes a browser that provides access to data, metadata, provenance, and tools associated with the workflow. The VisIt visualization tool [4] 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 [3]. Shared and private workspaces are supported for collaboration.

The Agni software, located on the computer server, executes modeling requests from the Akuna client and reports information back to the UI. 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 can support other simulators.

The Platform and Integrated Toolsets Thrust focused recent development activities on integration among the ASCEM toolset's Akuna, Agni, and Amanzi tools. A key element of this integration is a new Extensible Markup Language (XML) Amanzi input file specification and schema. An XML schema is a document that describes the structure of and rules that apply to an XML file. The XML input file provides a framework for automated validation of input files as well as a well-defined specification for file format used by the development team. A parallel specification for the Agni input file has also been developed. The tools that read and write files in Akuna, Agni, and Amanzi were refactored to accommodate the new specification and ensure that all three elements can interface robustly and effectively. The Akuna UI was updated to reflect changes in the input file specification and structure, and to address deficiencies identified in previous testing.

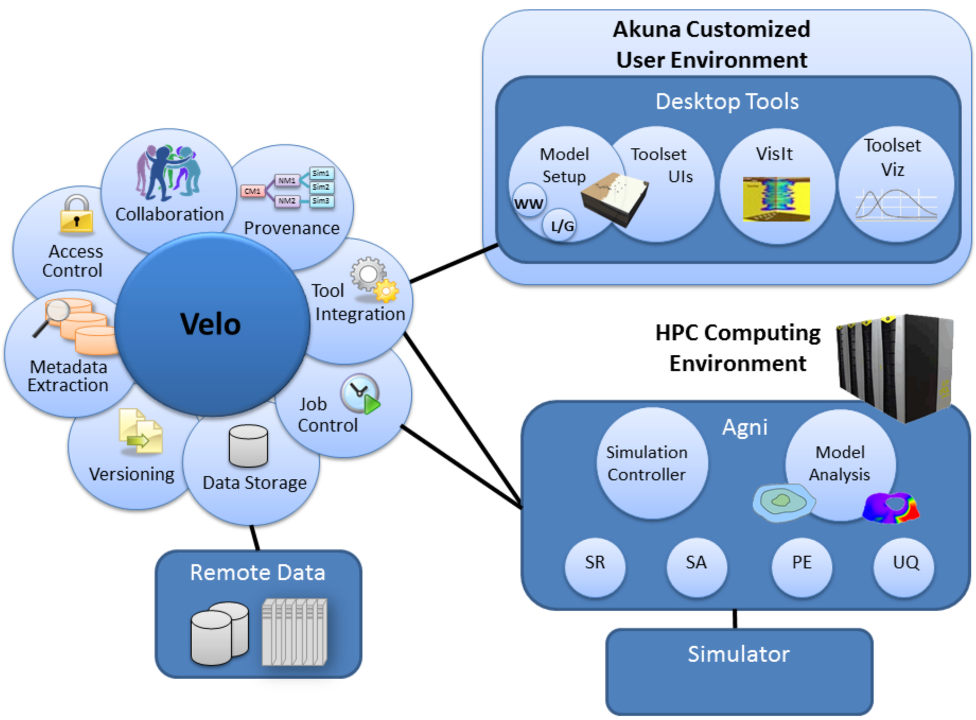

Fig. 3. Akuna user environment.

A second key element of integration was coordinated testing, encompassing two phases: 1) integration testing, to ensure that the interfaces described above work effectively, and 2) user testing, to ensure that the Akuna UI is readily usable and intuitive, and that any major bugs have been identified and addressed.

The following Akuna capabilities were developed for the initial user release:

- Implementation of the new XML file format and schema, with interactive file validation.
- Incorporation of all supported Amanzi capabilities in the Akuna UI model setup tool.
- Integration with Agni and Amanzi, including options to work directly with raw input files or build input files through the Akuna model setup UI.

Amanzi

The HPC multi-process 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 a graded and iterative approach to performance and risk assessment. Amanzi is designed to be implemented on a range of computer architectures, from laptops to supercomputers, to access the appropriate level of computational power for the problem at hand. High-level requirements, including the underlying mathematical formulations of the models, were developed [5] and a design document generated for Amanzi [6].

To initiate a simulation with Amanzi, a user starts with a conceptual model that 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. 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 defined. A mesh is a collection of discrete cells or grid blocks that represent 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 Amanzi reflects the steps in translating a conceptual model to a numerical model to produce simulation results (Fig. 4). Process kernels are high-level objects that represent processes such as flow, transport, and reactions. The Multi-Process Coordinator (MPC) manages the coupling of the process kernels and data. 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. The HPC Core Framework provides low-level services such as data structures to operate on parallel computers, input and output, and error handling.

The HPC Thrust focused recent development activities on improving performance and robustness of Amanzi, as well as enhancing capabilities for the initial release. The new XML schema was developed for the input specification to improve the robustness of the Akuna/Amanzi coupling as well as to significantly enhance the usability of Amanzi. Development and testing were performed on fully unstructured polyhedral meshes. In addition, more-flexible interfaces to nonlinear and linear solvers were developed, the mimetic finite difference schemes were made more robust and optimized, and more-efficient two-point flux based schemes were added. An interface and library named Alquimia was developed to allow Amanzi to use existing, mature geochemistry software as process kernels. This application programming interface (API) provides access to advanced features of these established tools, such as complex geochemical conditions at boundaries and advanced high-ionic strength chemistry models (e.g., Pitzer) for waste tank scenarios and engineered barriers. In addition, the API encourages more active collaboration with geochemists and computational geoscientists who have already implemented specialized reaction networks and models that they would like to use with Amanzi's flexible flow and transport capability.

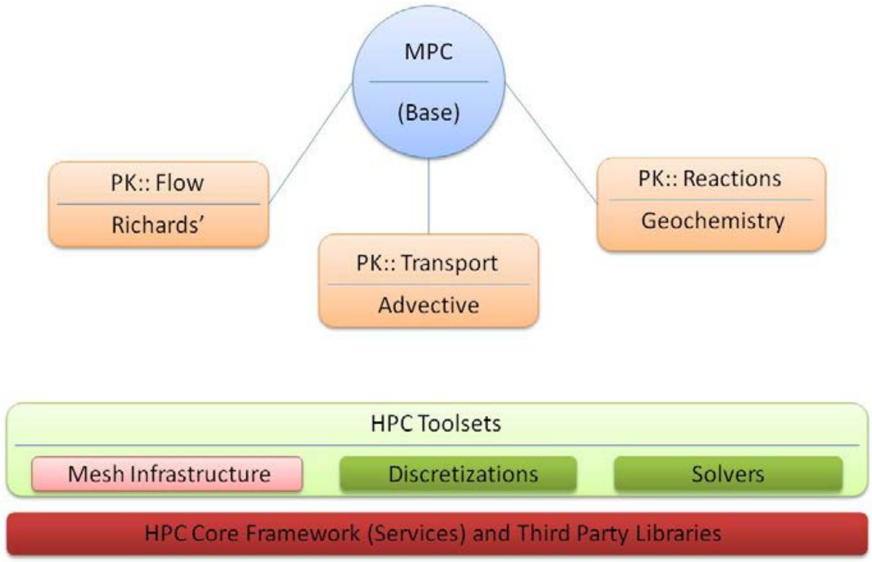

Fig. 4. Schematic showing the MPC that has process kernels for flow, transport, and reaction modeling.

Amanzi documentation includes a user guide describing how to obtain, install, and use the simulator. The user guide features a tutorial that provides an overview of key elements of the new XML input specification through working examples, as well as a collection of well-established verification tests for transient and steady-state flow and transport. The user guide is continually rebuilt as new tutorials and tests are added, and the documentation of each test is rebuilt with output from the current build of Amanzi. This automated approach helps developers ensure that Amanzi is functioning properly and synchronizes updates to the user guide with the most recent code developments and modifications.

APPLICATION AND TESTING

The Site Applications Thrust contributed testing and application of the ASCEM toolsets to EM-relevant problems. Activities focused on the F Area Seepage Basins at the Savannah River Site (SRS) for evaluating attenuation-based remedies, BC Cribs at the Hanford Site representing the deep vadose zone, representative waste tank problems, and the Nevada Nuclear Security Site (NNSS).

For the SRS F Area, the team prepared plans for the next phase of developing a model of the site. The working group 1) developed new conceptual models of the site including the past and current engineering treatments performed for remediation (e.g., pump and treat, funnel-and-gate system) and facies-based subsurface heterogeneity, 2) identified capabilities that need to be developed to carry out the demonstration, 3) acquired new site datasets needed for demonstration, particularly those associated with engineering treatments (i.e., barrier geometry), and 4) developed a detailed plan for the demonstration based on the feedback from the Platform and HPC teams. The new capabilities include more efficient three-dimensional simulations, improved robustness to include engineered structures having sharp contrasts in hydraulic properties, heterogeneity of flow and reactive-transport properties, wellbore-delivered remediation treatments, random field generation of flow and reactive-transport property fields, and incorporation of geochemistry interface (Alquimia). The demonstration plan also includes communication with the F Area operations staff to assess existing and new remediation strategies. This plan will be implemented in future demonstration efforts for ASCEM.

The deep vadose zone at the Hanford Site continued to be used to demonstrate and test ASCEM capabilities needed to evaluate innovative treatment technologies for difficult contaminants. At BC Cribs, soil desiccation, an approach that reduces moisture content and slows vadose zone flow and Tc-99 transport, is being evaluated. This demonstration provides the basis for tutorials included in the recent user release of ASCEM.

The ASCEM project has been working with the NNSS to evaluate the Underground Test Area Program. The capability is being developed to predict and characterize reactive flow and transport in the fractured volcanic tuff on Pahute Mesa, where a large underground radionuclide inventory resides. The Amanzi code was enhanced by adding specific capacity and specific discharge capabilities, allowing evaluation of existing pumping tests conducted at the site. A series of benchmark simulations were performed on the University of Nevada, Las Vegas computing system.

For the user release, the Site Applications Thrust developed benchmarking and tutorial problems, focused on setting up suites of modeling tasks (i.e., model setup, simulation, UQ, visualization) using the F Area Seepage Basins and BC Cribs at the Hanford Site. The ASCEM toolset and tutorials were released to an initial set of users for testing and evaluation. To meet quality assurance (NQA-1) requirements, ASCEM development follows a risk-based graded approach that uses three phases of development. The release represents the Research and Development (R&D) branch corresponding to the initial NQA-1 "Basic Phase." The R&D branch release cannot be used for regulatory applications. The ASCEM website (http://ascemdoe.org) provides information on future release dates.

DEMONSTRATION OF ASCEM USER RELEASE AT BC CRIBS

The first step in modeling the BC Cribs site (Fig. 5) is analysis of baseline conditions and Tc-99 transport to the water table. As described in a demonstration report [7] and in Seitz et al. [8], the Hanford Site BC Cribs simulation was used to demonstrate end-to-end integration of Platform and HPC components, from the Data Management and Model Setup and Analysis Toolsets to PE and UQ.

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 using the Model Setup and Analysis Toolset to fill in regions of the model between the surfaces (Fig. 6). 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 adapted for 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. 7).

The simulations included boundary conditions of greater than 38 million liters of liquid wastes released at the six cribs from 1956 to 1958, with initial Tc-99 concentrations of 10^6 pCi/L. A recharge boundary condition was represented at the surface and the lower boundary of the model domain (Fig. 8) was the water table. Initial simulations were performed using a recharge boundary condition of 3.5 mm/y to obtain steady-state conditions prior to crib discharges. A recharge rate of 63 mm/y was used to represent conditions from 1956 to 2008. For the UQ analysis, the rate was uniformly varied from 0.1 to 75 mm/y.

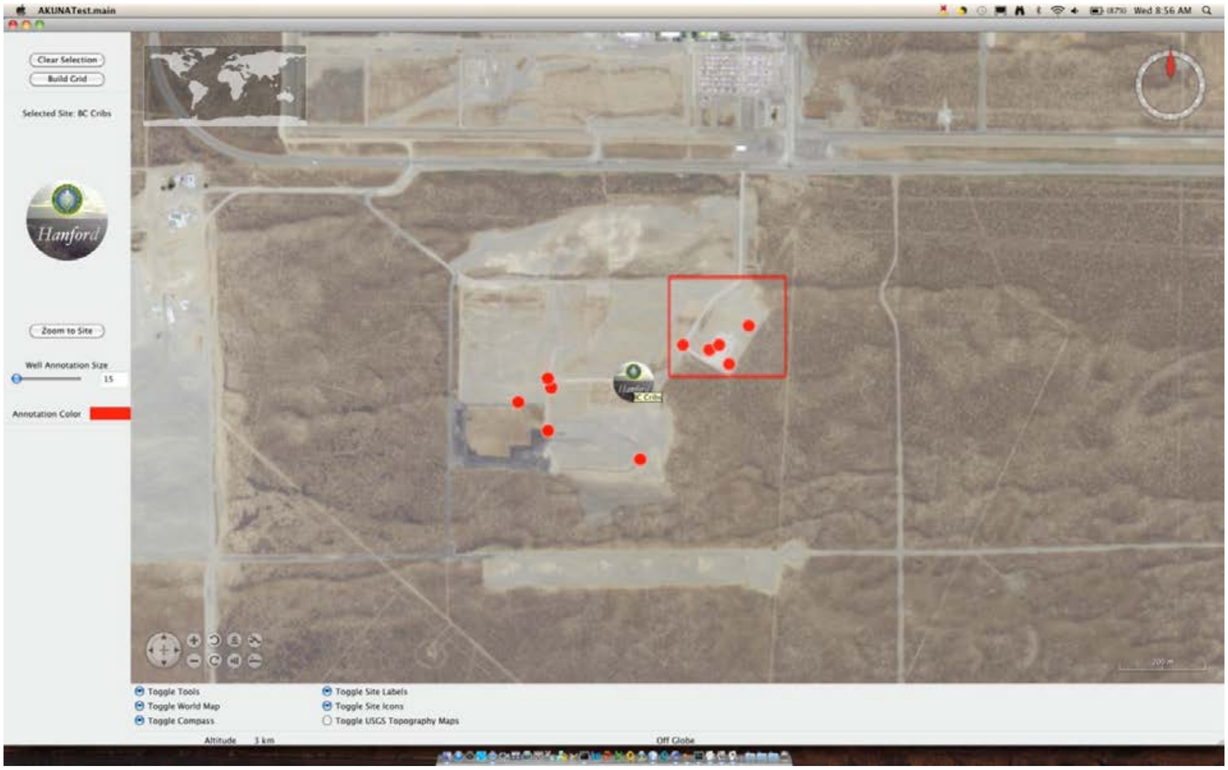

Fig. 5. Hanford BC Cribs viewed in Akuna.

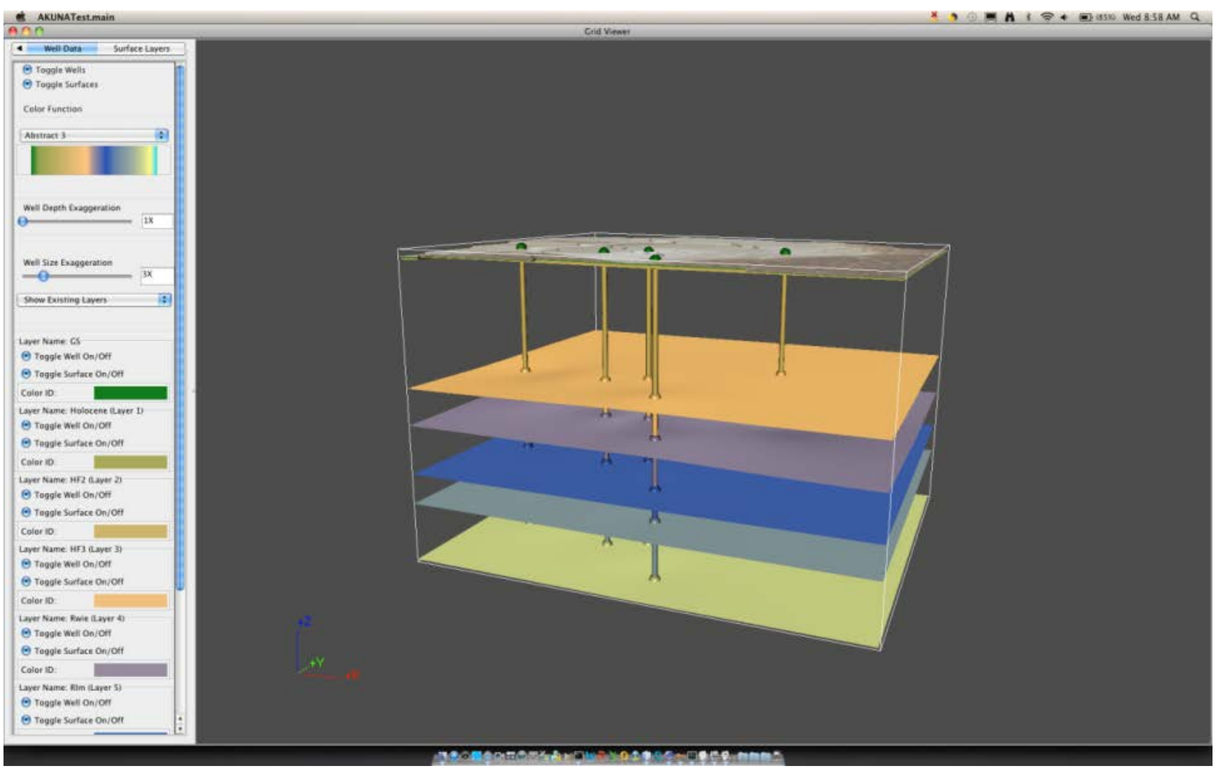

Fig. 6. Major stratigraphy viewed in the Model Setup and Analysis Toolset.

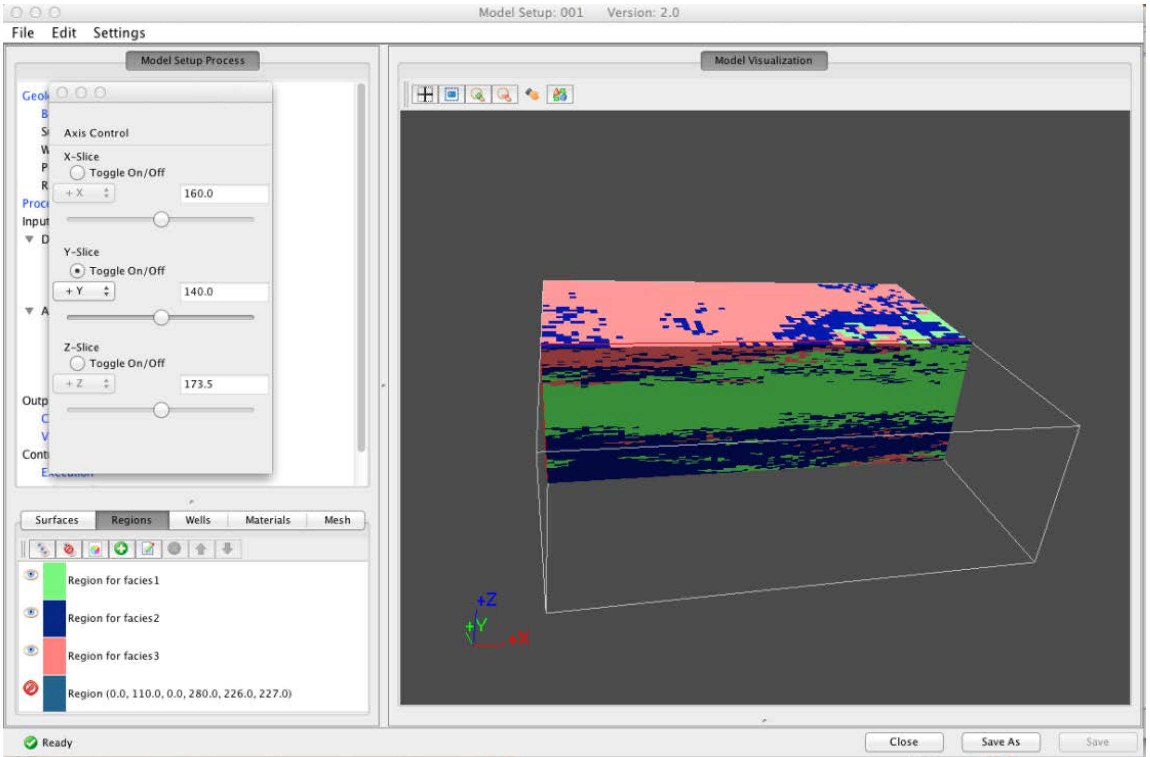

Fig. 7. Viewer in the Model Setup and Analysis Toolset showing the distribution of lithofacies.

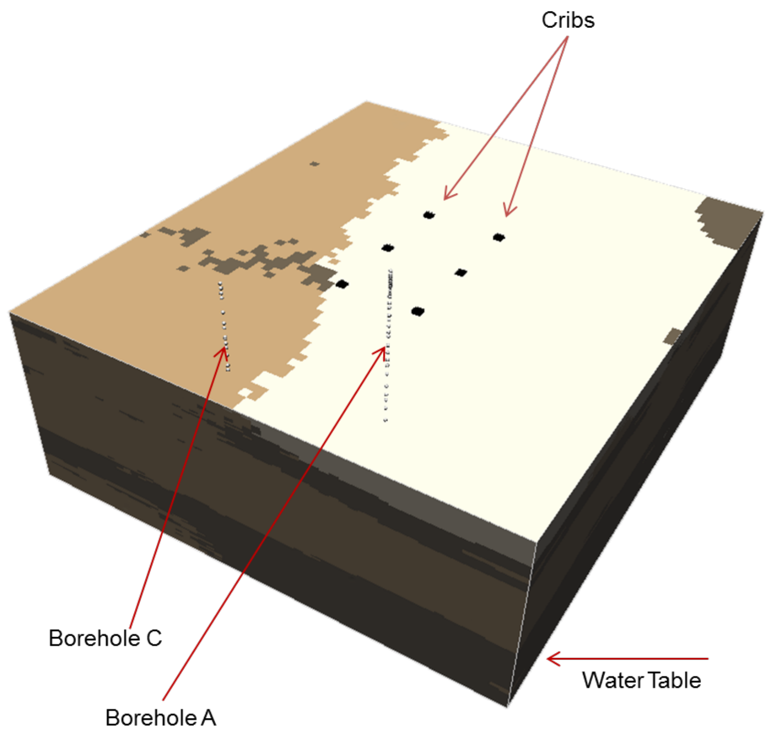

Fig. 8. BC Cribs model domain.

For the BC Cribs demonstration, a simulation was 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. Initial parameters for the calibration were assigned from pedotransfer functions. In the BC Cribs demonstration, the simulation completed using the initial values from pedotransfer functions showed a mismatch between simulated and measured data as shown for concentrations, indicating the need for model calibration (PE). The results of PE for all 10 conceptual models are shown in Fig. 9. Most of the conceptual models show a good match with the moisture content and Tc-99 concentrations, although some discrepancies occur because the observed data are too sparse to uniquely determine hydraulic properties.

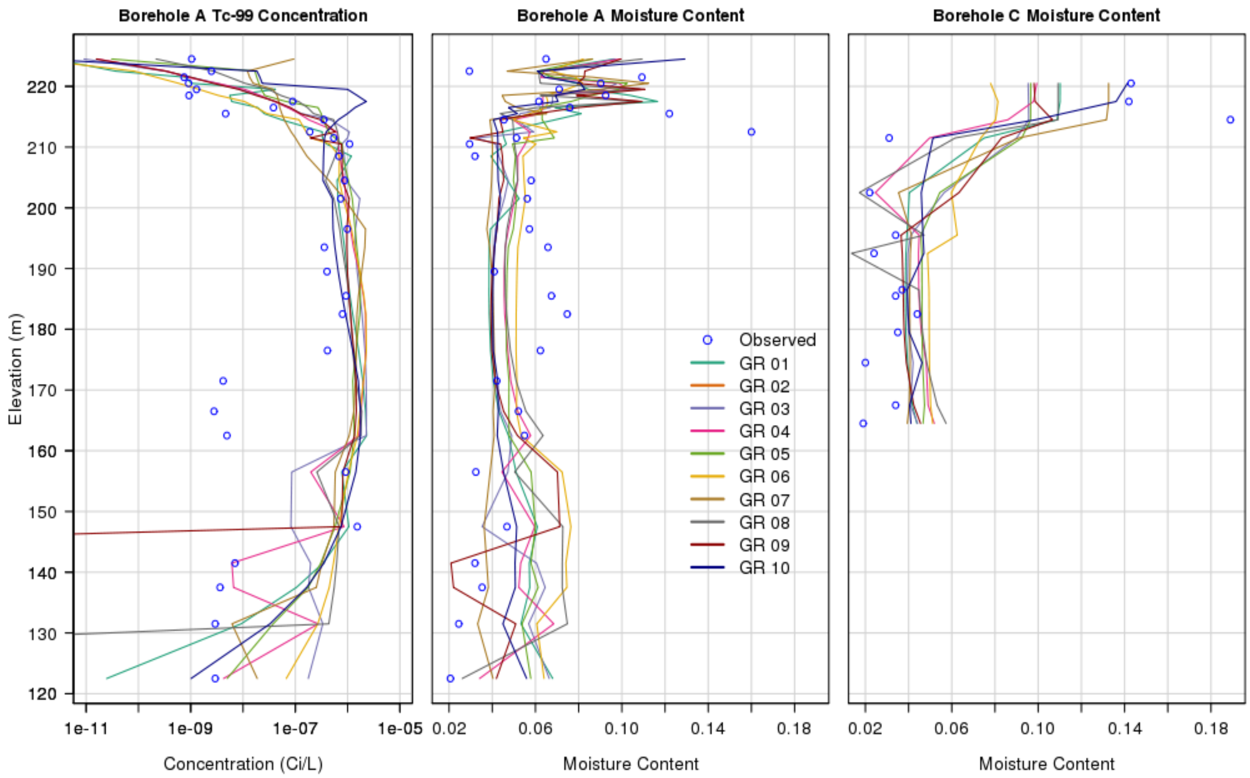

Fig. 9. Results of PE for all 10 conceptual models of the BC Cribs.

As documented in the demonstration report [7] and by Seitz et al. [8], visualizing the spatial distribution of Tc-99 transport contributes to an understanding of how heterogeneities affect contaminant transport in the vadose zone. The spatial distribution of Tc-99 after the discharges to the cribs terminated (1960) is shown in Fig. 10. Horizontal cross-sections through each row of cribs, as well as a vertical cross-section through Borehole A, are also shown (Fig. 10).

The UQ analysis included uniformvariation of the recharge rate from 1 to 75 mm/y, covering a range of potential remediation scenarios, from no action to soil desiccation with implementation of surface barriers. Metrics for the UQ analysis included peak concentrations and arrival time at the water table, times at which a threshold concentration is exceeded, and time period of exceedance. Execution of UQ required 96 processor cores each simulation, for a total of 9600. The UQ analysis demonstrated that time to peak concentration shows a slight correlation with the recharge rate and that the magnitude of the peak concentrations varies with rate (Fig. 11).

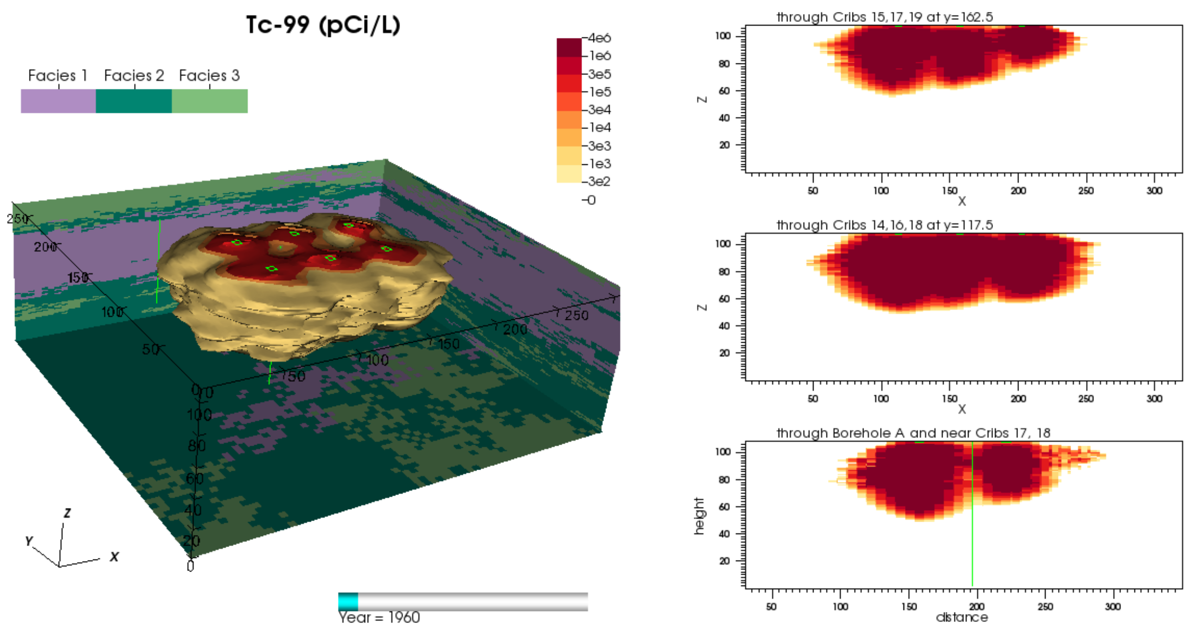

Fig. 10. Spatial distribution of Tc-99 after the releases from the cribs using VisIt software.

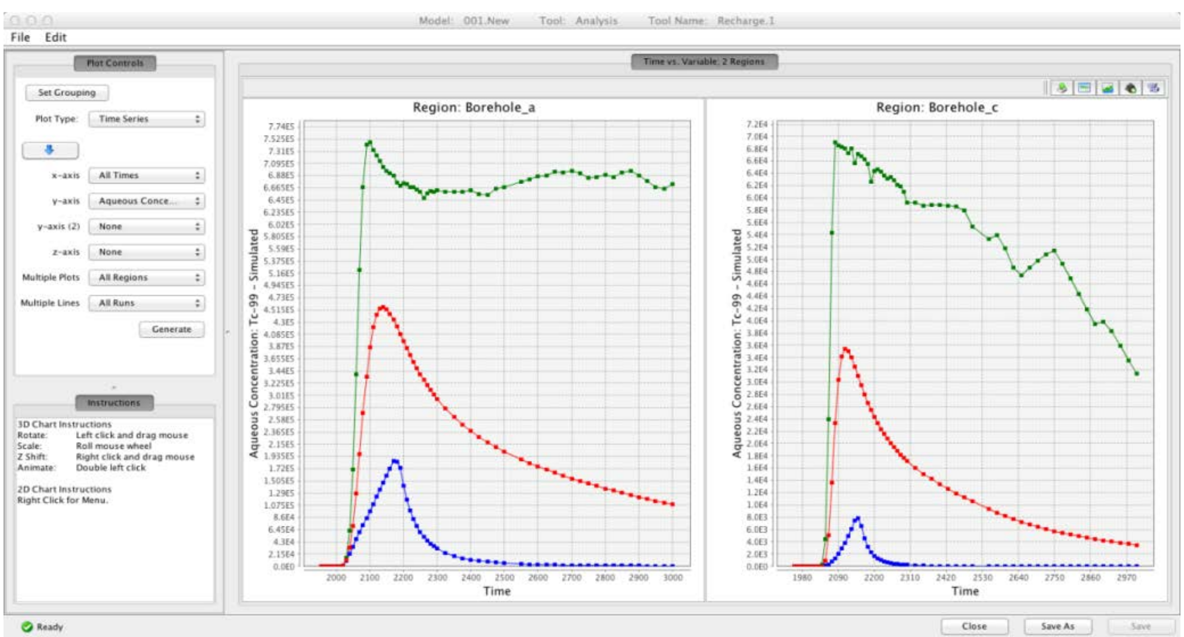

Fig. 11. Mean and 95% confidence intervals for the BC Cribs UQ analysis.

CONCLUSIONS

ASCEM's modular and open source toolsets facilitate integrated approaches to modeling and site characterization that enable robust and standardized assessments of performance and risk for EM cleanup and closure activities. ASCEM 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 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 goals for ASCEM were to complete capability development and testing to support release of the R&D branch of the toolsets. ASCEM has been released to an initial set of end users. The release will be made available at a future date for evaluation and feedback. This release is available for research applications, but cannot be used for regulatory analyses. The project is continuing development and testing to facilitate release of an applied version of ASCEM in 2014 and a version that meets NQA-1 quality assurance requirements in 2015 that can be used to support regulatory applications. The project is seeking feedback from end users to guide continued development and engage the EM modeling community.

The ASCEM project has successfully developed a robust set of capabilities in the Akuna and Amanzi toolsets. Additional capabilities will continue to be added and future demonstrations will increase in complexity. The project will begin to partner with the user community to engage in collaborative demonstrations across the EM complex. The applied phase of the project will involve refinement and quality assurance of the toolsets to enable the use of ASCEM to provide technical underpinnings for site cleanup efforts and performance assessments. The ASCEM capabilities are expected to help EM provide efficient and cost-effective implementation of remediation endpoint strategies. Through working groups and end user engagement, ASCEM will sequentially test and demonstrate capabilities that will enable it to be used to guide DOE in developing paths to completing the DOE cleanup mission.

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