Advanced Simulation Capability for Environmental Management: Development and Demonstrations (12532)

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ABSTRACT

The U.S. Department of Energy Office of Environmental Management (EM), Technology Innovation and Development 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 capabilities, which are organized into Platform and Integrated Toolsets and a High-Performance Computing Multiprocess Simulator. The Platform capabilities target a level of functionality to allow end-to-end model development, starting with definition of the conceptual model and management of data for model input. The High-Performance Computing capabilities target increased functionality of process model representations, toolsets for interaction with Platform, and verification and model confidence testing. The new capabilities are demonstrated through working groups, including one focused on the Hanford Site Deep Vadose Zone.

INTRODUCTION

The U.S. Department of Energy (DOE) Office of Environmental Management (EM) is responsible for completing the safe cleanup of the environmental legacy from the nation's five decades of nuclear weapons development and government-sponsored nuclear energy research. This charge is one of the most complex and technically challenging cleanup efforts in the world; it is projected to take decades and cost between $265–305 billion to complete [1]. The contamination was introduced into complex subsurface environments at a variety of sites [2] by disposal in injection wells, underground disposal facilities such as cribs and trenches, and evaporation or seepage ponds as well as accidental leaks from waste storage tanks, basins, and transfer lines.

Reviews by participants at workshops and national panels have concluded that gaps in the technical foundation supporting environmental decisions have led to ineffective remediation, and that the complexity and magnitude of the EM cleanup mission justifies long-term investment in science and technology [1, 3]. Based on these reports, the EM Technology Innovation and Development, Groundwater and Soil Remediation Program identified key needs, including the development of numerical tools to accurately predict the long-term behavior of subsurface contaminant plumes and degradation of engineered materials used for waste disposal. This investment was the basis for the Advanced Simulation Capability for Environmental Management (ASCEM) program.

The goal of ASCEM is to develop an approach and state-of-the-art scientific tools for integrating data, software, and scientific understanding. The program combines new and open-source high performance computing algorithms, models, data analysis and integration approaches, and an evolving understanding of subsurface hydrological-biogeochemical processes to enable EM cleanup. ASCEM will also provide other DOE programs with a code that will be applicable to a variety of subsurface flow and transport problems. ASCEM is envisioned as a community code that will be updated and augmented as new scientific insights are developed through DOE's research programs in the Office of Advanced Scientific Computing Research and the Office of Biological and Environmental Research, and other federal programs.

ASCEM is organized into three Thrust Areas: 1) High-Performance Computing Multiprocess Simulator; 2) Platform and Integrated Toolsets, and 3) Site Applications. The High-Performance Computing Thrust includes meshing approaches, new solvers for multiphysics coupled processes, advanced methods of discretization in time and space, and capabilities to select and coordinate the use of problem-specific processes. The Platform Thrust includes an integrated software infrastructure to facilitate model setup and analysis, parameter estimation and uncertainty quantification, risk assessment and decision support, information and data management, and visualization in a consistent and flexible user interface and modeling workflow. The Site Application Thrust coordinates and implements demonstrations through working groups to provide data and feedback to developers and to ensure the software is developed in a manner that will engage users and benefit EM's remediation obligations.

During the first year of ASCEM operations, the project completed an initial (Phase I) demonstration, largely undertaken from September through December 2010. The first demonstration was focused on illustrating individual (stand-alone) ASCEM capabilities. The demonstration was designed to provide an early snapshot of advances associated with four specific components of ASCEM: Data Management; Visualization; Uncertainty Quantification; and High-Performance Computing. Coordination of the Phase I effort was facilitated through a working group associated with the Savannah River Site F-Area. Information regarding the initial demonstration can be found in [4] and [5].

PHASE II DEVELOPMENT

Following completion of the Phase I demonstration, development of ASCEM components that will be implemented for the Phase II demonstration began in 2011. These capabilities are being developed for both Platform and High-Performance Computing and represent a subset of the overall capabilities that will eventually be developed and implemented.

Development of Platform capabilities, collectively named Akuna, was initiated to target a level of functionality defined by a series of use cases. The overall Platform requirements were defined in a specification of system requirements [6]. Use cases define the primary functionality for the Core Platform, Model Setup and Analysis, Data Management, Parameter Estimation, Uncertainty Quantification, and Visualization toolsets. The development is being undertaken in phases, consisting of an initial release (January 2012) and a second phase (April 2012). Use cases will be refined and implemented through these two phases.

The Core Platform allows users to create and manage modeling projects, launch simulations, and share data and modeling results with a team. In the Model Setup and Analysis toolset, a user will be able to import files to define geologic layers; import files that describe the site geology (opaque data such as well information or geologist logs); import and define structured and unstructured meshes for simulations; assign material properties; define boundary and initial conditions; and define input and output for simulations, including specification of the physics model. The Data Management component allows users to import and browse data sets for analysis and data extraction as well as allow storage and retrieval of simulation results. The Parameter Estimation module allows users to perform model calibration and data inversions. Interaction is allowed with the Core Platform to perform parameter estimation by Bayesian integration of disparate data sets without running the Multiprocess Simulator. The Uncertainty Quantification toolset includes design and execution of Monte Carlo analyses and visualization of results. Capabilities to execute global sensitivity analyses, perform maximum and minimum predictions, and compare alternative conceptual models are also included in the Uncertainty Quantification toolset. Development of the Visualization toolset focuses on interfaces with data management systems to facilitate site data investigation. The user will be able to visualize three-dimensional output from the multiprocess High-Performance Computing Simulator, as well as visualize parameter estimation and uncertainty quantification results.

Advances in high-performance computing capabilities were initiated through development of process models, the High-Performance Computing Core Framework and toolsets, as well as through verification and validation testing. The capabilities of the ASCEM simulator, called Amanzi, include transient flow with the Richards equation [7] using both structured and unstructured grids. The meshing capabilities support complex geometries such as pinched-out layers and fine-scale features. For the Phase II development effort, Amanzi is scalable to 1000-plus processors. Enhanced transport capabilities are implemented to reduce numerical dispersion. Additional geochemical processes extend the range of sites for which reaction networks can be modeled, including sorption processes and radioactive decay. An interface between Akuna and Amanzi, which is being developed as part of the Phase II activities enables effective management of both single and multiple forward runs. Additional capabilities include the ability to restart parallel runs (to ensure parallel runs can be repeated or that work is not lost if a run is stopped), a build system for compiling on different desktop systems and supercomputers, and selective output for supporting the Parameter Estimation, Uncertainty Quantification, Risk Assessment, and Decision Support toolboxes in the Platform. A test suite—including data from the demonstration sites—supports development team efforts and code compilation capabilities. Automated builds and tests provide documentation for quality assurance.

At the end of fiscal year 2012, ASCEM capabilities will be assembled into User Release V 1.0 and will be distributed to a small subset of the EM end-user community for testing and evaluation. This release will not be suitable for regulatory analyses; a qualified code is expected to be released in subsequent years.

PHASE II DEMONSTRATION

The Phase II Demonstration is focused on integration across capabilities and applications to address specific, site-related questions. Complexity will be added in future iterative demonstrations as ASCEM capabilities are developed. This approach is expected to provide tractability in the demonstrations and facilitate the transfer of insights and methods that are being developed.

The Phase II demonstration will be performed in conjunction with three working group efforts, conducted in series to allow each one to build on developed capabilities. The Deep Vadose Zone Working Group is the first to complete the Phase II demonstration. The focus of this working group is to demonstrate a beginning-to-end integration of ASCEM capabilities for model development and execution. The ASCEM Deep Vadose Zone Working Group is linked to the Deep Vadose Zone Applied Field Research Initiative at the Hanford Site. Two other demonstrations will be underway at that time, focused on attenuation-based remedies at the Savannah River Site F Area and a waste tank performance assessment. The focus of the F Area working group is to implement some of the linked ASCEM capabilities under conditions of increased data availability and model complexity, including reactive chemistry, source-term uncertainty, and linked vadose zone and saturated flow. The waste tank performance assessment working group emphasizes visual analysis tools for model sensitivity as well as high-performance computing.

Deep Vadose Zone Working Group

The Deep Vadose Zone Applied Field Research Initiative at the Hanford Site provides an opportunity to demonstrate ASCEM capabilities needed to help EM to evaluate innovative treatment technologies for recalcitrant contaminants in the deep vadose zone. Contaminant remediation in the deep vadose zone poses unique challenges because conventional remediation technologies are ineffective. The primary contaminant of concern at the BC Cribs is Tc-99, a long-lived radionuclide with a half-life of 2.13×10^5 years. The technology currently under evaluation 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 extraction of water vapor [8]. The technology is being evaluated as part of a treatability test at the BC Cribs, located in the 200 East Area of the Central Plateau at the Hanford Site (Figure 1). Other remediation approaches that may be evaluated in the future include foam delivery of amendments or ammonia gas treatment of uranium at the BC Trenches, adjacent to the BC Cribs.

The Hanford formation in the Central Plateau is known to contain relatively thin fine-textured lenses that could enhance lateral spreading of water and contaminants and reduce the vertical movement of contaminants [9]. Because the affected vadose zone is more than 100 m thick, thorough characterization using traditional sampling and implementation is cost and resource prohibitive. Given that flow and transport in porous media is determined by its structure, especially the connectivity of heterogeneous conductivities, this presents a large source of uncertainty in the conceptual model of the BC Cribs site. Additional uncertainties also exist in its contaminant release history. Therefore, uncertainties in source terms and permeabilities are investigated in the Phase II demonstration.

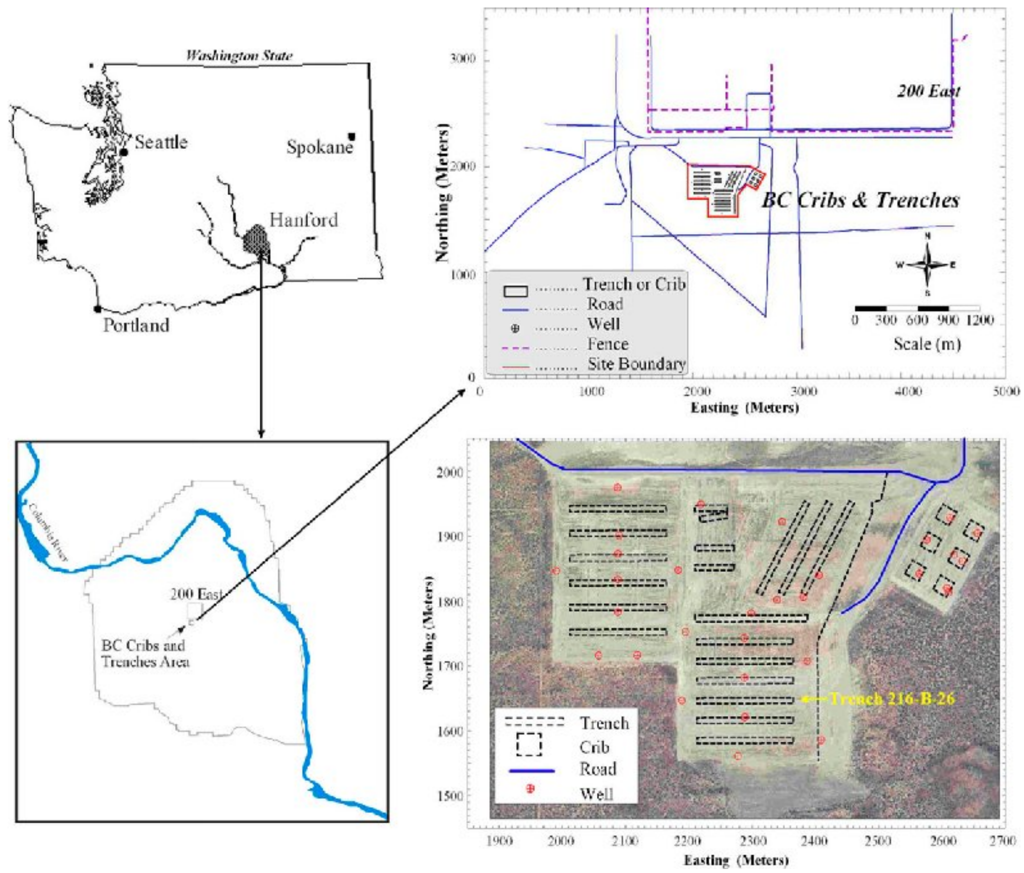


Fig 1. BC Cribs and Trenches at the Hanford Site (from [10]).

The primary objective of the Hanford Site Deep Vadose Zone Phase II demonstration is to illustrate integration of Platform and High-Performance Computing components, from the Data Management and Model Setup and Analysis toolsets to Parameter Estimation and Uncertainty Quantification. Phase II focuses on a two-dimensional cross section through the BC Cribs waste site to establish baseline conditions that can be used to perform a relative comparison of concentration distributions and fluxes to those with soil desiccation so that its effectiveness can be evaluated. These simulations are used to examine effects of heterogeneity on the estimates of the contaminant flux to the groundwater. The Platform components include the following:

1) **Data Management**. The Data Management component stores sparse characterization data describing the geology, moisture content and subsurface contaminant concentrations and makes them accessible to the ASCEM modeling capabilities. These data include moisture content and borehole concentration data from the BC Cribs.

2) **Model Setup.** The Model Setup and Analysis toolset translates conceptual models to numerical modeling grids and generates input files for Amanzi (see Figure 2). Specifically, these tasks include generating grids, assigning material properties by zone, and generating input files for boundary and initial conditions, simulation controls, and output specification.

3) **Core Platform.** The Core Platform component performs job launching and monitoring tasks, as well as storing input and output data, and integrating user interface and toolsets.

4) **Parameter Estimation.** The Parameter Estimation toolset identifies permeabilities and source terms using water content and concentration data from the BC Cribs. Parameter estimation simulations are executed for approximately 50 years (1956–2006) and are integrated with Model Setup and Data Management toolsets.

5) **Uncertainty Quantification.** The Uncertainty Quantification toolset assesses parameter uncertainty on contaminant transport at the BC Cribs using Monte Carlo simulation. The conceptual model uncertainty is characterized by different representations of subsurface permeability—one with a geostatistical distribution of lithofacies, and another with a geostatistical distribution of permeabilities (Figure 3). Forward simulations of long-term transport of contaminants to the groundwater are performed with Amanzi. The uncertainty analysis focuses on identifying the heterogeneities significantly impacting peak concentrations and arrival times at the groundwater.

6) **Visualization.** The Visualization toolset provides visualization of high-performance computing and uncertainty quantification outputs from multiple realizations. These visualizations include spatial distributions of contaminant concentrations and breakthrough curves of contaminant concentrations at the water table (Figure 4).

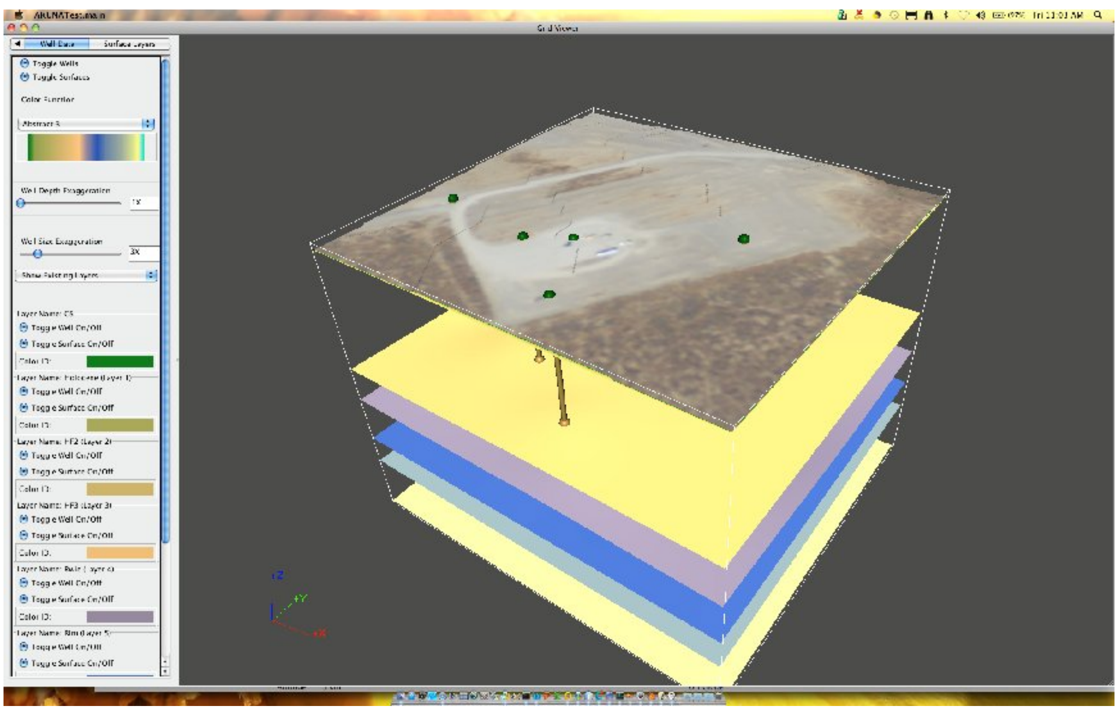
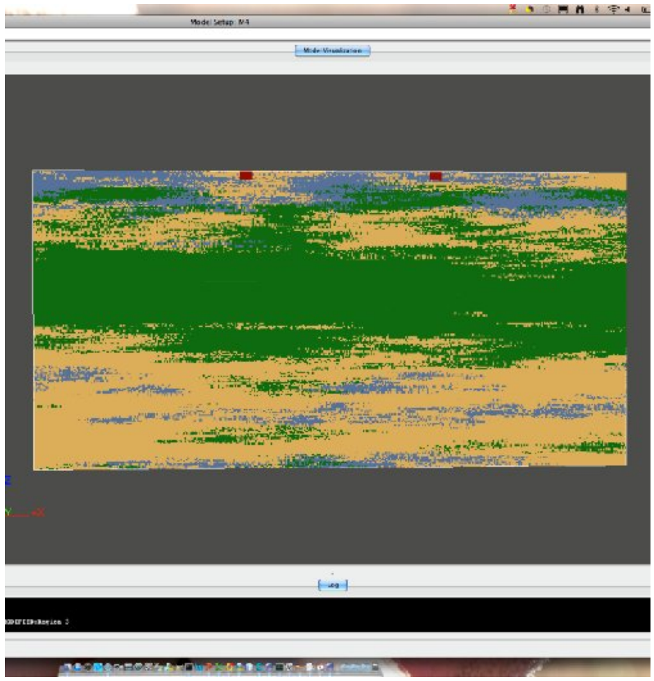


Fig 2. Screen shot of Model Setup Toolset in Akuna illustrating definition of model layers.

a)



b)

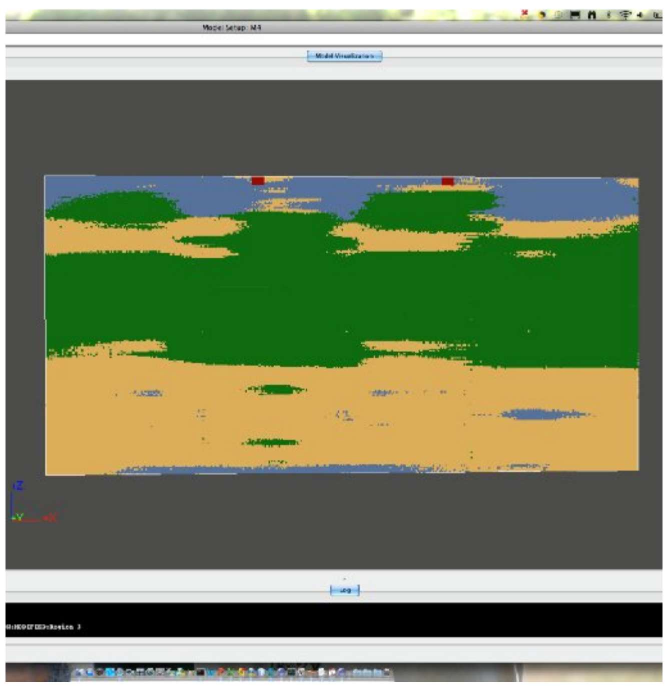


Fig 3. Screen shots from Model Setup illustrating cross sections with a) stochastic assignment of lithofacies; and b) stochastic assignment of permeability.

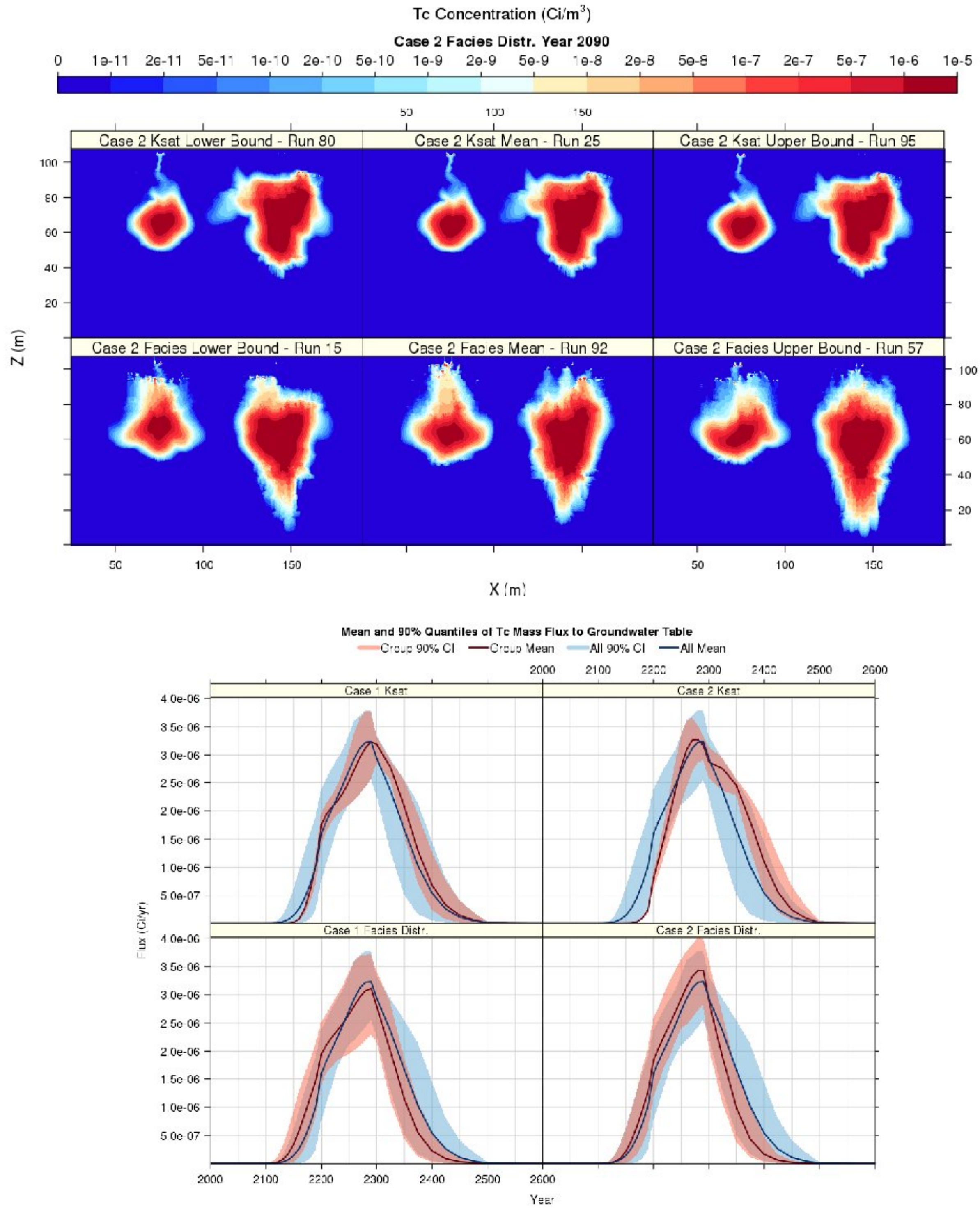


Fig 4. Visualization of contaminant distributions and breakthrough curves for an uncertainty quantification analysis at BC Cribs.

CONCLUSIONS

The ASCEM program focused on planning during the first year and executing a prototype toolset for an early demonstration of individual components. Subsequently, ASCEM has focused on developing and demonstrating an integrated set of capabilities, making progress toward a version of the capabilities that can be used to engage end users. Demonstration of capabilities continues to be implemented through working groups. Three different working groups, one focused on EM problems in the deep vadose zone, another investigating attenuation mechanisms for metals and radionuclides, and a third focusing on waste tank performance assessment, continue to make progress. The project experience has been that the working group mechanism continues to be useful for helping guide development and prepare the capabilities for end users.

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