Advanced Simulation Capability for Environmental Management: Early Site Demonstration - 11560

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The U.S. Department of Energy's Office of Environmental Management (EM), Technology Innovation and Development (EM-32), 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. This modular and open-source, high-performance computing tool will facilitate integrated approaches to modeling and site characterization that enable robust and standardized assessments of performance and risk for EM cleanup and closure activities. As part of the initial development process, a series of demonstrations was defined to test ASCEM components and provide feedback to developers, engage end users in applications, and lead to an outcome that would benefit the sites. The demonstration was implemented for a sub-region of the Savannah River Site General Separations Area that includes the F-Area Seepage Basins. The physical domain included the unsaturated and saturated zones in the vicinity of the seepage basins and the Fourmile Branch. An unstructured mesh was used to fit the grid to the hydrostratigraphy and topography of the site. The calculations modeled variably saturated flow, and the resulting flow field was used in simulations of the advection of non-reactive species and the reactive-transport of uranium. As part of the demonstrations, data management, visualization, and uncertainty quantification tools were developed to analyze simulation results and existing site data. These new tools can be used to provide summary statistics, including information on which simulation parameters were most important in predicting uncertainty and visualizing the relationships between model input and output.

INTRODUCTION

The mission of the U.S. Department of Energy's (DOE's) Office of Environmental Management (EM) is to complete the safe cleanup of the environmental legacy from the nation's five decades of nuclear weapons and nuclear energy research. Contamination has been introduced into complex subsurface environments through intentional disposal through injection wells, disposal facilities, and settling ponds as well as through accidental spills and leaks from waste storage tanks and transfer lines. The subsurface environment is characterized by multiple hydrological, geochemical, and microbiological processes occurring at different scales, significant heterogeneity, and daunting measurement and observational constraints [1]. This EM cleanup, which is one of the most technically challenging and complex worldwide, is projected to take many decades to complete [2] and to cost as much as $305 billion [3].

ASCEM Phase I Demonstration

Recent workshops and panels have concluded that systematic gaps in the technical foundation supporting environmental decisions have led to ineffective remediation and that the complexity and magnitude of the DOE environmental problem justifies a long-term investment in remediation science and technology [4–6]. Based on these and other workshop reports, the DOE EM-32 Office of Groundwater and Soil Remediation Program identified various needs, including the development of numerical tools that can accurately predict the long-term behavior of subsurface contaminant plumes and engineered materials used for waste disposal.

The Advanced Simulation Capabilities for Environmental Management (ASCEM) initiative was established to develop a state-of-the-art scientific tool and transformational approach for integrating data and scientific understanding into a framework for remediation decisions. The ASCEM program will focus on advancing the approach for subsurface contaminant fate and transport simulations to support risk-informed environmental remediation and waste management decisions. This will be done by combining today's (1) petaflop supercomputing capabilities, (2) new and open-source, high-performance computing applications, (3) data analysis and integration approaches, and (4) increased understanding of subsurface hydrological-biogeochemical processes. It is envisioned that this will be updated as new insights and approaches are developed through the DOE Office of Science and other research agencies.

ASCEM is organized into (1) Multi-Process High Performance Computing (HPC), (2) Platform and Integrated Toolsets, a user interface with associated toolsets, and (3) Site Applications. The relationship between the thrust areas is illustrated in Figure 1. The HPC Thrust includes meshing approaches, new solvers for multi-physics coupled processes, advanced methods of discretization in time and space, capabilities to select and coordinate the use of problem-specific processes, and application-programming interfaces. The Platform Thrust includes tools 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 site demonstrations through "working groups" so that end users are engaged in development of ASCEM and it benefits DOE-EM's remediation obligations.

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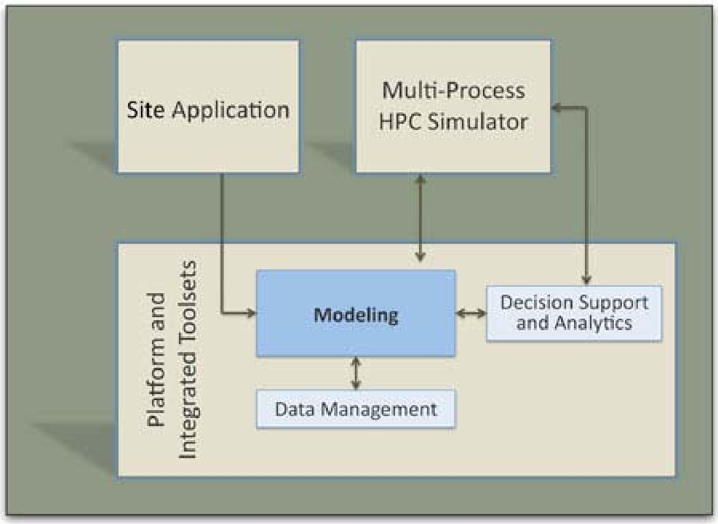

Figure 1. Illustration of the relationship between the three ASCEM technical thrust areas: HPC simulator, Platform and Toolsets, and Site Applications.

A series of ASCEM demonstrations will be performed in a phased manner to correspond with development of the Platform and HPC components as well as ASCEM releases. The ASCEM demonstrations are designed to advance, test, and illustrate ASCEM capabilities as well as engage end-users.

PHASE I DEMONSTRATION

In the first year of development, ASCEM focused on illustrating individual (stand-alone) capabilities within the HPC and Platform Thrusts. Later demonstrations will focus on integrating ASCEM capabilities. The Phase I demonstration illustrates testing of early concepts and tool development using common datasets from a specific site. The demonstration was implemented for a sub-region of the Savannah River Site (SRS) General Separations Area that includes the F-Area Seepage Basins. The SRS F-Area is a primary applied field research site for testing attenuation-based remedies for metals and radionuclides in groundwater. This effort is supported by the DOE EM-32 Office of Technology Innovation and Development. The site also offers an opportunity for significant leveraging of work by the DOE Office of Science. This ongoing research includes an extensive laboratory component focused on developing geologic facies-specific (layer-specific) surface complexation (reaction) models; approaches to identify and spatially distribute reactive facies using geophysical data [7]; process model development, sensitivity analysis, and mechanistic reactive transport model development [8]; and a formal evaluation of the benefit of increasing complexity on successful predictions of contaminant mobility over stewardship time frames. The EM-32 and Office of Science activities interface with the Savannah River National Laboratory (SRNL) team to explore the impact of a migrating, acidic plume, pH gradient. Also, the power of the concept of reactive facies as an organizing principle to integrate laboratory and field information about transport-relevant properties and mechanisms as needed to make reliable and computationally tractable predictions of uranium and iodine-129 at the plume scale will be explored.

The ASCEM demonstration at the SRS F-Area focused on the following Platform and HPC components:

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- **Data Management (Platform),** including development of data input, organization, and query tools, using a map-based interface with a focus on contaminant concentration and hydrostratigraphic variables.
- **Visualization (Platform)** of the hydrostratigraphy, water table, topography, wells, and migration of contaminant plumes through aquifers over time.
- **Uncertainty Quantification (Platform),** including evaluation of strategies and development of tools to evaluate the sensitivity of model output to parameter suites.
- **HPC Components,** including three-dimensional flow and reactive transport for uranium simulations in the unsaturated and saturated subsurface, and modeling advection of a non-reactive species.

SRS F-AREA DESCRIPTION

SRS is located in south-central South Carolina, near Aiken, approximately 100 miles from the Atlantic Coast. It covers about 800 square kilometers (300 square miles) and contains facilities constructed in the early 1950s to produce special radioactive isotopes (e.g., plutonium and tritium) for the U.S. nuclear weapons stockpile. SRS has approximately 172×10^6 m^3 of groundwater, soil, and debris contaminated with metals, radionuclides, and organics [9] as a result of onsite disposal practices. The SRS F-Area Seepage Basins consist of three unlined, earthen surface impoundments that received approximately 1.8 billion gallons (7.1 billion liters) of acidic, low-level waste solutions from the processing of irradiated uranium in the F-Area Separations facility from 1950 through 1989. The plume currently extends from the basins approximately 600 m downgradient to a stream (Figure 2) and contains a large number of contaminants. Based on risk to potential receptors, the most hazardous contaminants are uranium isotopes, strontium-90, iodine-129, technetium-99, tritium, and nitrate. Groundwater is currently acidic with pH values as low as 3.2 near the basins.

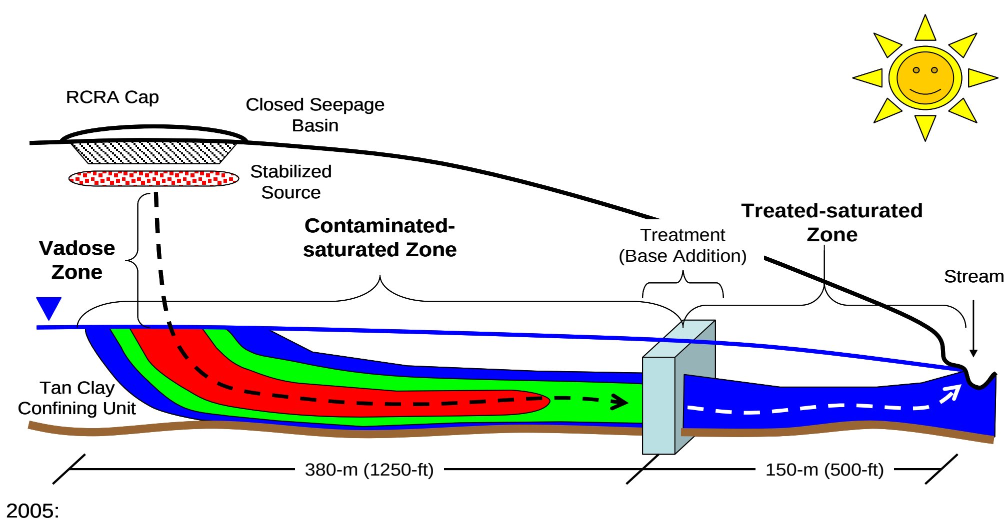

Figure 2. Schematic of the F-Area Groundwater Plume

The basins were closed and capped in 1991. A pump-and-treat remediation system began operation in 1997, and it was replaced in 2004 by a hybrid funnel-and-gate system installed about

300 m upgradient from the stream (see Figure 2). Alkaline solutions are now being injected into the gates in an attempt to neutralize the acidic groundwater downgradient of the seepage basins. Monitored Natural Attenuation (MNA) is a desired closure strategy for the site, based on the premise that rainwater will eventually neutralize the lingering mineral surface acidity, causing an increase in pH and stimulating natural immobilization of uranium in the trailing end of the plume. If the natural pH neutralization upgradient from the treatment system is insufficient, additional enhanced neutralization will be required. Critical to assessing the *in situ* treatment requirements over the long time frame is to develop an understanding of the long-term H^+ and uranium sorption at the site.

DATA MANAGEMENT

The objective of the Data Management demonstration was to illustrate capabilities to organize and manage data that are commonly used for subsurface flow and transport investigations. Specific capabilities were developed to manage two different types of data: (1) measured or simulated data, referred to as “transparent data” and (2) documents, graphs, pictures, and similar data objects, referred to as “opaque data.” Transparent data are measured or simulated data that can be searched and extracted, which for this demonstration include data from the concentration and depositional database.

The demonstration required different tools for managing transparent and opaque data. The data were put into a relational database with flexible search capabilities. Web-based tools, such as Google maps, were adapted to enable the display of wells on maps to query the data and to display results in terms of graphs and tables. A web-based semantic wiki tool called Velo was customized to describe opaque data and to store and index metadata associated with wellbore data (such as descriptions of measurement variables or acquisition procedures). Inconsistency in wellbore nomenclature, wellbore coordinate systems, and measurement units is a common problem associated with subsurface databases.

Typical first steps in subsurface data exploration include plotting the location of wellbores and displaying associated measured parameters. Figure 3 displays the F-Area well locations on a map, which could be either a satellite image or (as shown) a road map with topography. In the figure, the wellbore color indicates the aquifer in which the wells were screened. From this map interface, a well or cluster of wells can be selected for further investigation by clicking on a single well or by drawing a rectangle around a cluster of wells. Once selected, measurements from the concentration database (analytes and other attributes) are displayed, illustrated as the list on the right hand side of the figure.

Plotting the temporal variations in measurements collected from a single wellbore and querying the measurement database are also common procedures used with subsurface data. Figure 4 shows how the Platform tools can be used to illustrate the time series of concentration values for one or several of the analytes. This display also provides the method detection limit (MDL) and practical quantitation limit (PQL) for each analyte. An interface tool was developed to display and query the database measurements.

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The tools were used to display geologic data and assess associated characteristics associated with a single or a cluster of wells. Figure 5 illustrates use of a map tool for displaying the percentage of mud, sand, and gravel as a function of depth. A user can also choose to only display wells and their attributes associated with a particular depositional environment.

The developed ASCEM data management tools allow users to easily plot, browse, filter, and output various types of data important for subsurface investigations and conceptual model development. A useful characteristic of the tools is that they can be used iteratively to display and query different subsets or characteristics of the databases.

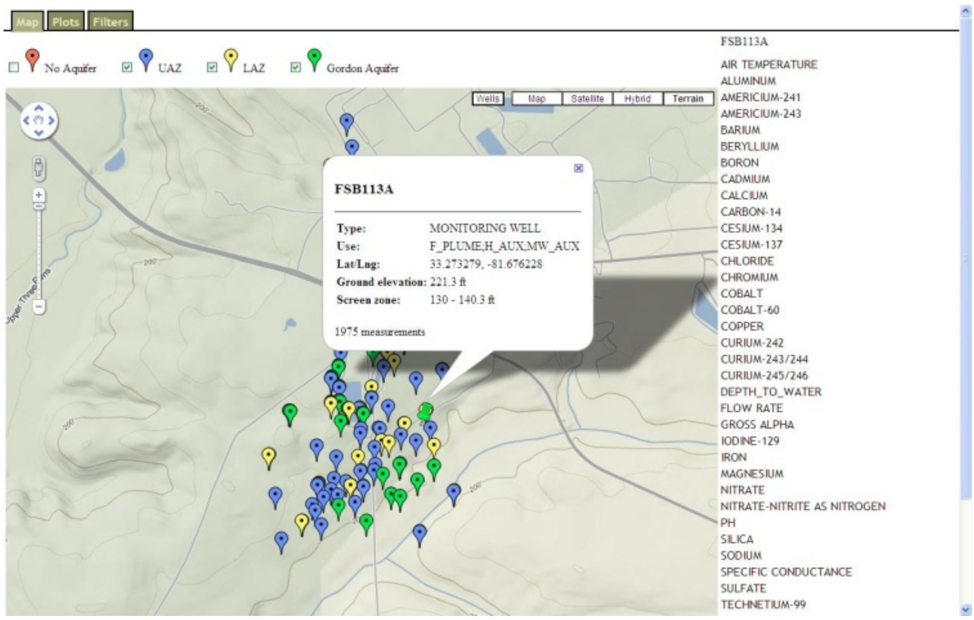
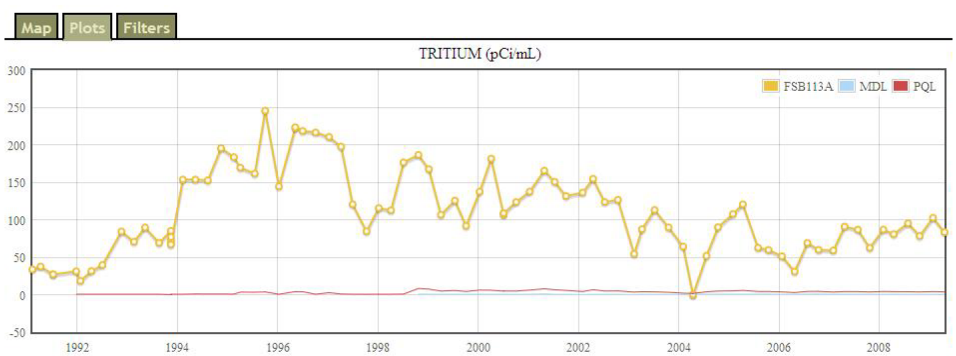


Figure 3. A map-based interface for browsing concentration data.



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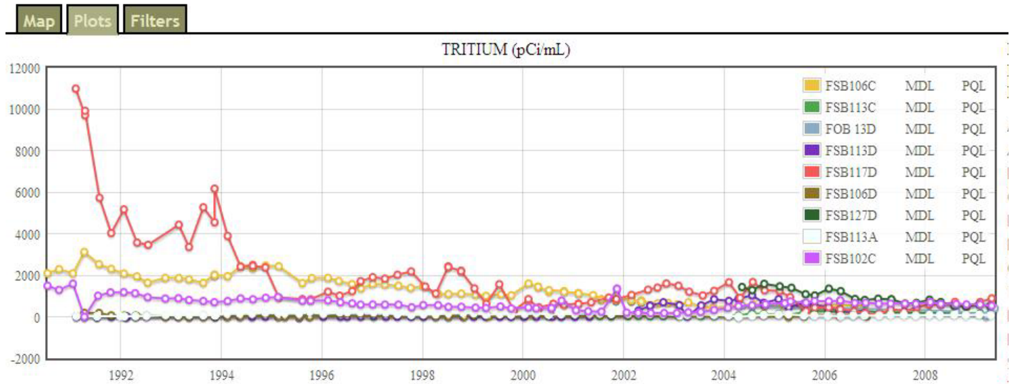

Figure 4. Examples of computed time series of tritium concentrations. Upper figure: tritium concentration from one well compared with the MDL and PQL concentrations. Lower figure: tritium concentrations from eight wells.

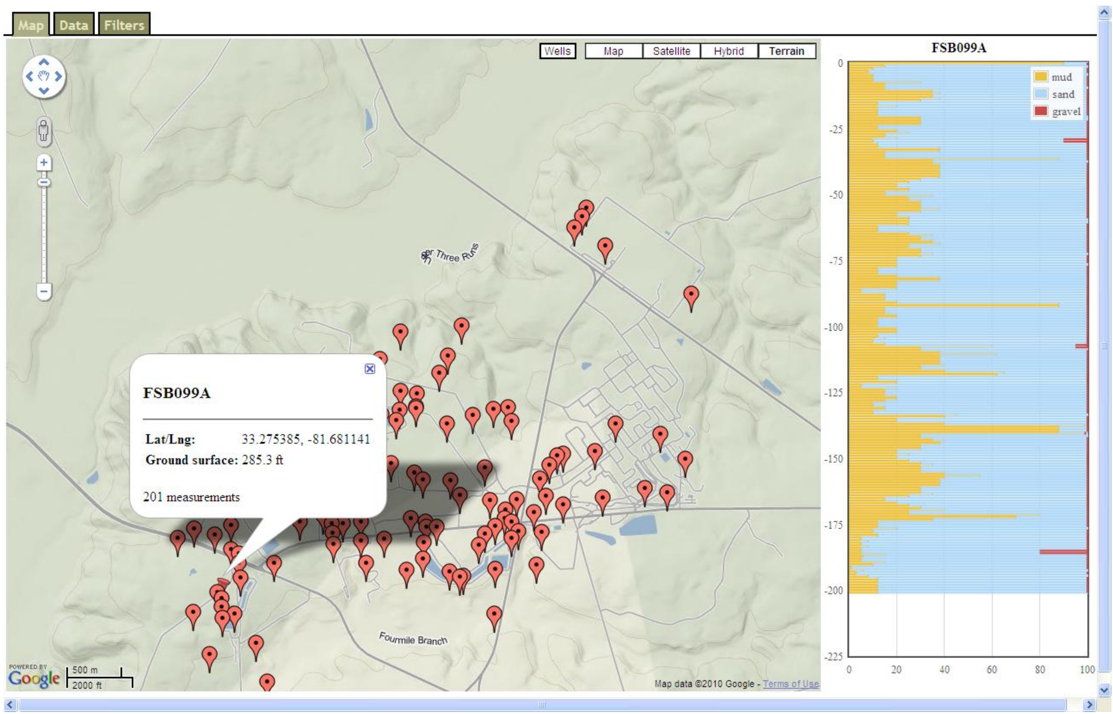

Figure 5. A map-based interface for browsing lithological data, showing (on the right) the percent mud, sand, and gravel as a function of depth.

VISUALIZATION

The objective of Platform visualization was to develop and demonstrate the visual exploration and analysis of a diverse range of conceptual and numerical model data common to subsurface science. This component of the Phase I demonstration focused on capabilities to visualize various aspects of developing the conceptual model and evaluating model results. Concentration,

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depositional, and Geographic Information System (GIS) databases were to support the Visualization demonstration.

An existing tool was modified and implemented to advance the Visualization component. VisIt is an open-source interactive parallel visualization and graphical analysis tool for viewing scientific data on Unix and PC platforms. It was developed with funding from the DOE Office of Science and the DOE National Nuclear Security Administration. The visualization demonstration at the SRS F-Area addressed (1) the layout of observation wells, (2) surface topography, roads and buildings, (3) the depths of lithostratigraphic units, (4) the groundwater depth, (5) the depths of hydrostratigraphic units, and (6) spatial and temporal variations of contaminant concentration values in groundwater. A custom data loader was developed to import the well-based datasets.

Two different approaches to visualize the spatiotemporal evolution of contaminant plumes were tested. Figure 6 shows the use of a triangulation approach to illustrate the temporal evolution of the uranium-238 plume at the F-Area site. A user can view the plume evolution by dragging a slider bar at the top of the figure to the right; in Figure 6, the concentration distributions for the years 1994 and 2009 are illustrated. Because the concentration data were collected at non-uniform time intervals, concentration data are presented as annually averaged values. Figure 7 shows the application of the developed inverse-distance and the isocontouring approach for computing and displaying the temporal evolution of the uranium-238 plume volume.

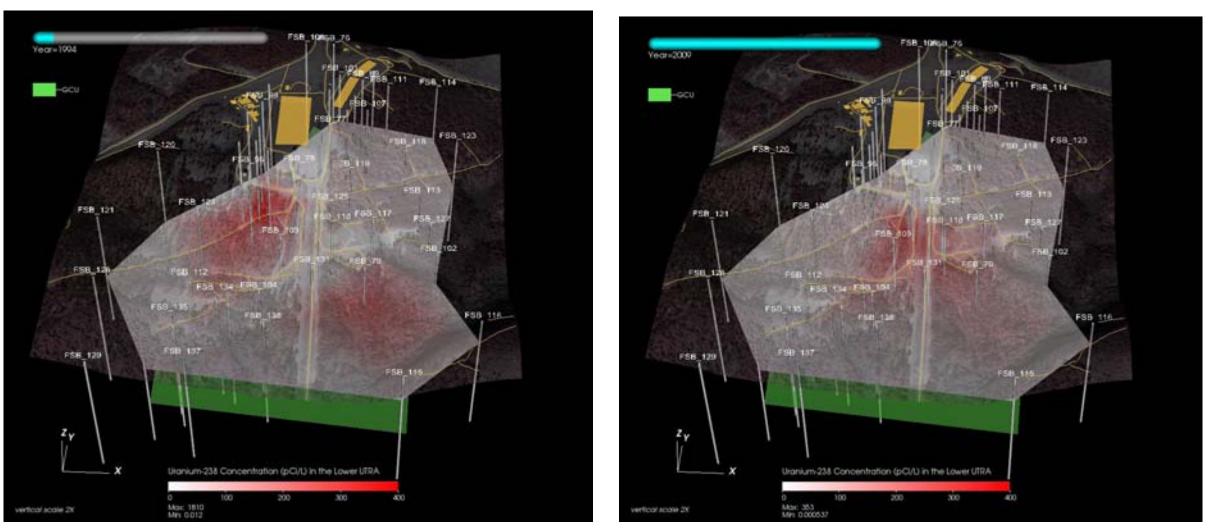

Figure 6. Examples of the images of uranium-238 concentration evolution over time (left-1994, and right-2009) displayed along with infrastructure and the depth of the Gordon Confining Unit (GCU).

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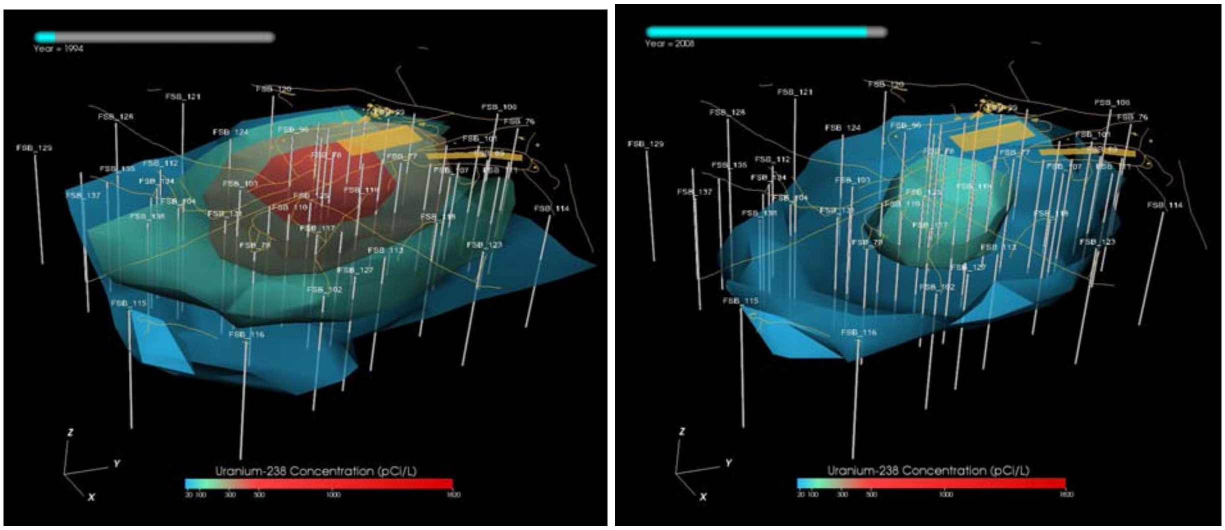

Figure 7. Examples of the evolution of four isosurfaces of the interpolated uranium-238 concentration over time steps (left-1994, and right-2008) displayed along with infrastructure.

UNCERTAINTY QUANTIFICATION

The objective of the Uncertainty Quantification (UQ) demonstration was to illustrate approaches to facilitate uncertainty analyses, including parameter selection, defining model outputs, and performing the analysis. The development effort focused on three different approaches and several analysis types implemented within the UQ toolset. The different approaches included (1) local sensitivity analysis, (2) global sensitivity analysis, and (3) probabilistic predictions (including Monte Carlo methods). Existing UQ software was incorporated into the toolset, including PEST [10]. For all approaches, the analysis was based on the assumption that a conceptual model existed with specified parameter inputs and model outputs that could be compared to physical observations.

UQ capabilities were illustrated using a Morris one-at-a-time method, which produces a measure of sensitivity for each input parameter. The method was applied to a model developed for the SRS F-Area as a test case. The geochemical reactions used for the analysis (and for the next HPC section) are preliminary. This model simulates the migration of acidic wastes through 1000 m of aquifer where the contaminants experience a relatively large number of chemical reactions. The parameters varied in the analysis included the basin infiltration rate, infiltrating water chemistry, sorption site surface area, and mineral precipitation/dissolution surface area. The analysis was facilitated by the graphical user interface (GUI) for the UQ toolset (Figure 8).

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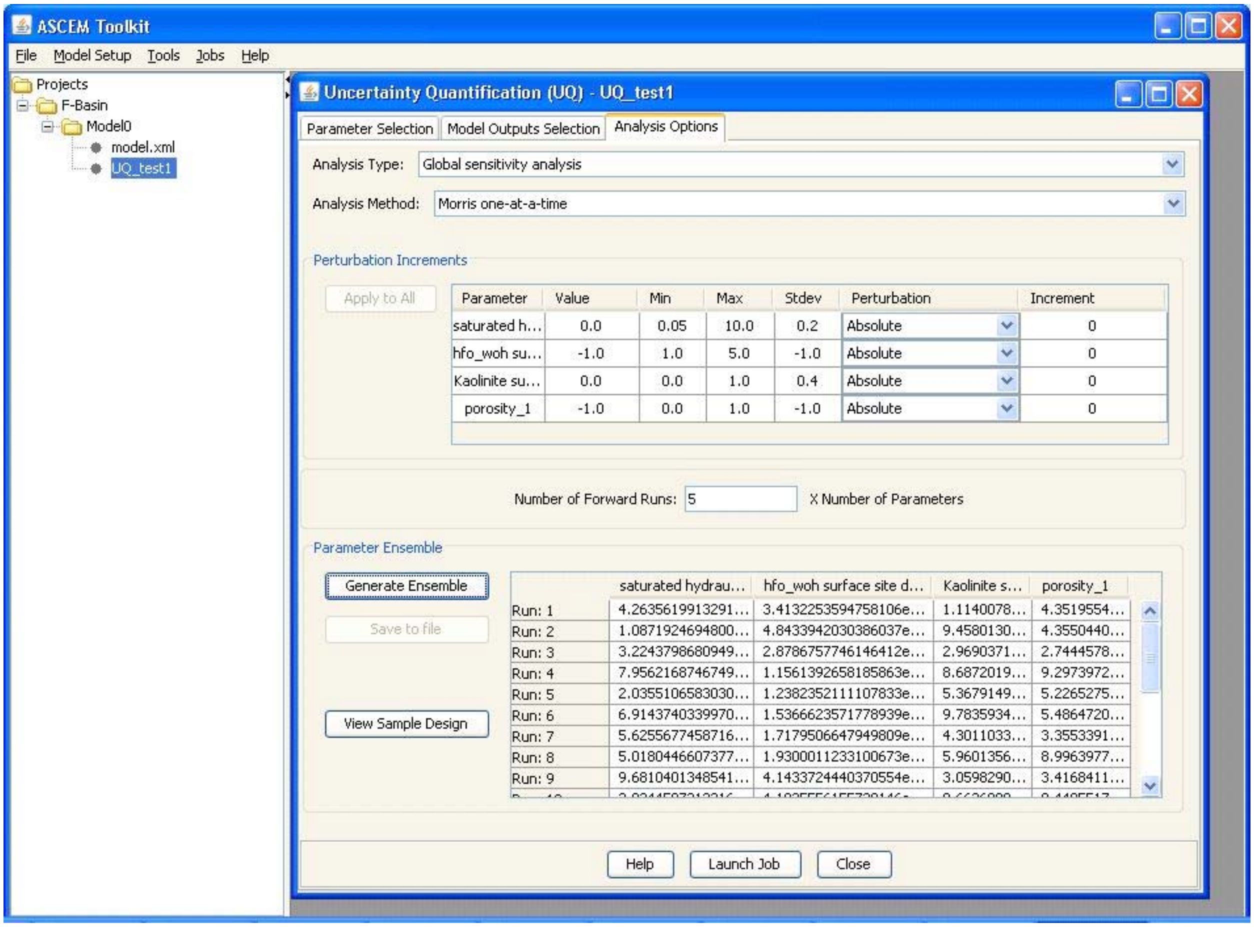

Figure 8. Screenshot of GUI for carrying out a global sensitivity analysis using the one-at-a-time method of Morris [11]. Here the user has already selected parameters and model outputs.

The user is prompted to select the size of the forward-run ensemble for the analysis. In the demonstration, outputs from an ensemble of 220 forward model runs were used to compute sensitivities. For each output, sensitivities were estimated—one for each model input parameter. Figure 9 shows the sensitivity of each model input to Al pH, SO_4, Al, and UO_2 (for each solute, the sum of concentrations at seven locations and times is output). The vertical axes are the mean sensitivity coefficients of the computed concentrations at seven location/times related to the 21 sampled parameters. Even though 21 input parameters were considered in the example, each of the outputs was controlled by a subset of input parameters.

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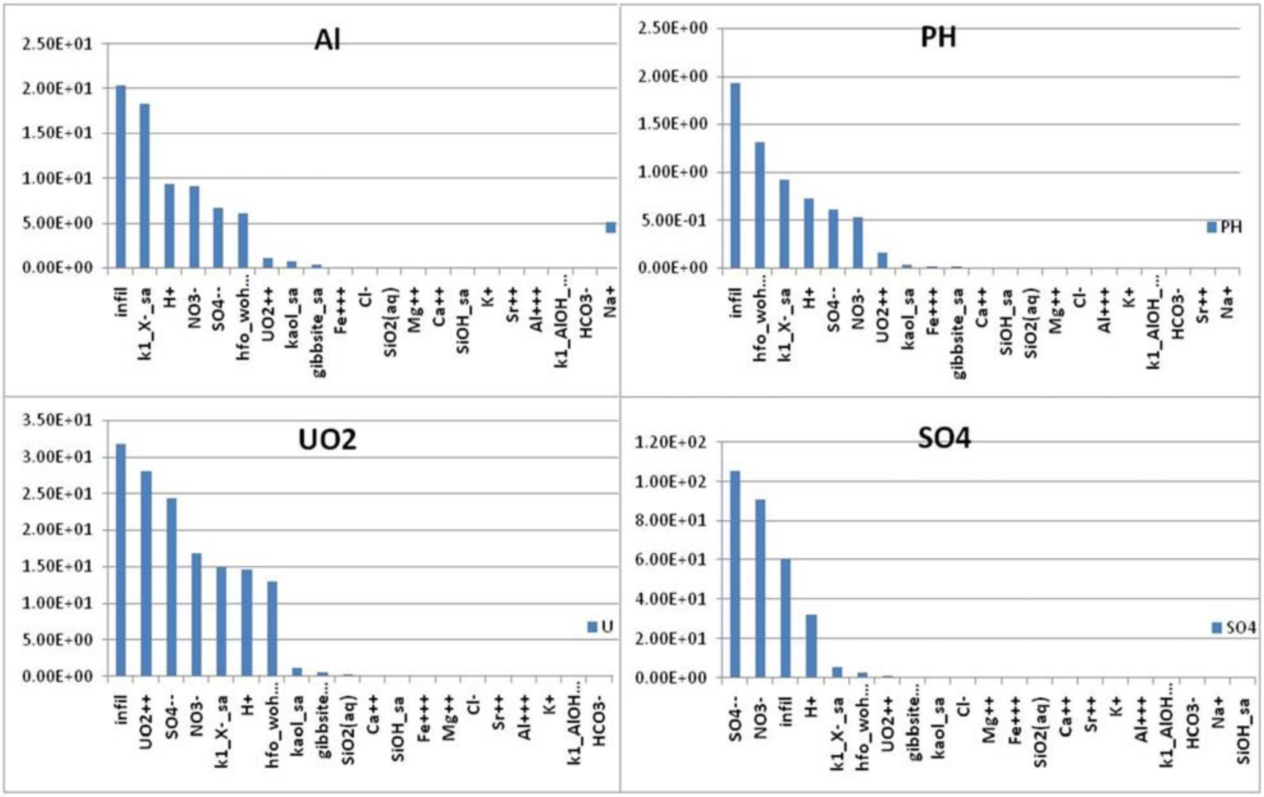

Figure 9. Morris one-at-a-time sensitivities for four different outputs. The computed sensitivities give the change in output over the range for each parameter.

HIGH PERFORMANCE COMPUTING

The objective of the ASCEM Multi-Process HPC Simulator demonstration was to highlight progress on early prototypes of selected components of the HPC Simulator with a conceptual model of the SRS F-Area. Members of the HPC team and the F-Area Site Working Group developed a conceptual model of the F-Area for the HPC Simulator. Scoping studies were conducted using an existing simulator to determine the computational domain, and the HPC team worked with the Platform Thrust area to develop unstructured hexahedral meshes with different resolutions. Figure 10 illustrates one of the grids that was generated for the demonstration.

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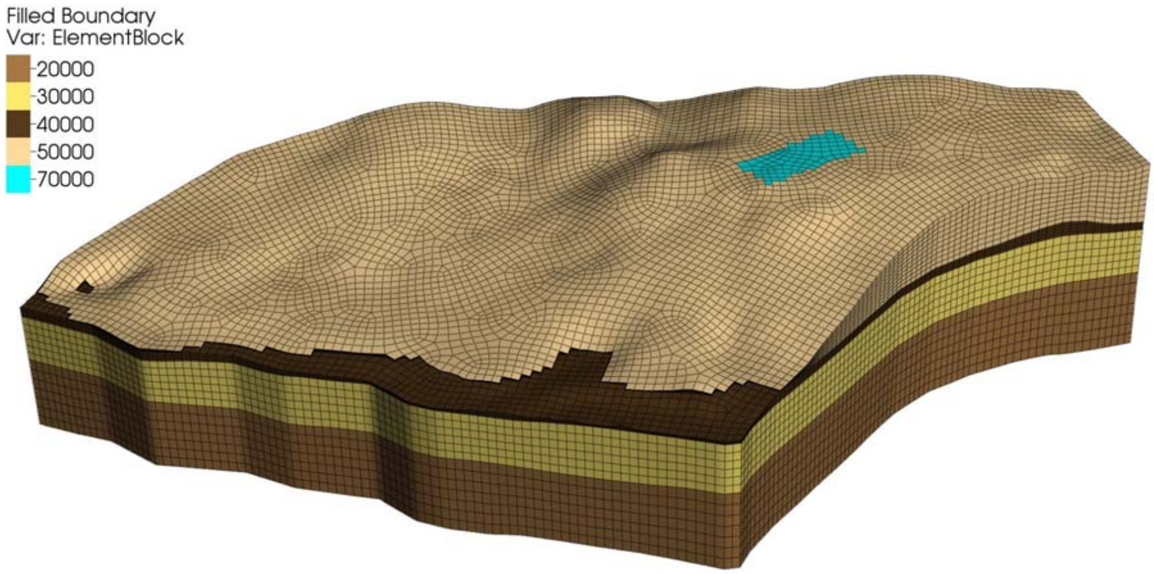

Figure 10. Unstructured hexahedral mesh of the F-Area subregion along with four hydrostratigraphic units included in the model.

The computational domain was discretized and implemented in the flow-and-transport simulator to produce a steady-state flow field and corresponding transport (Figure 11).

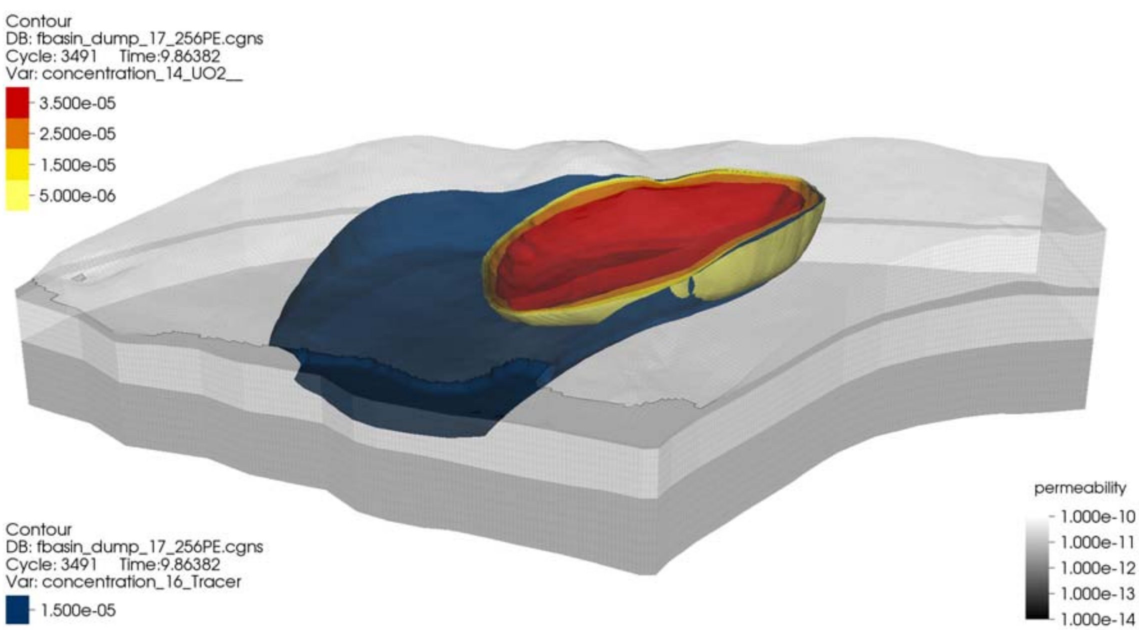

Figure 11. Iso-surfaces of the uranium plume (yellow and red) and a non-reactive tracer (blue) are shown at 9.86 years for the unstructured mesh F-Area seepage basin model described above. The reactive transport model was used, and the retardation of the uranium plume relative to the non-reactive tracer is evident, as the tracer has already reached the Fourmile Branch.

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A reaction toolset was developed that provides classes to depict chemical species and reactions for reactive transport. This toolset consists of an object within which a chemical reaction is solved, much like a batch reaction in a laboratory beaker. A simple interface for the reaction toolset was developed to support the modular design of the HPC simulator. The necessary chemical constraints and parameters (e.g., time step size, tolerances) are all that is required to solve a geochemistry step. To facilitate the use of the geochemistry toolset, routines were developed for reading and writing geochemical data, debugging, and verification/validation exercises.

A reactive transport simulation was performed in parallel on 516 processors. For the F-Area, the geochemistry module had 17 primary aqueous (or basis) species: Na^{+}, Ca^{+2}, Fe^{+2}, K^{+}, Al^{+3}, H^{+}, $N_{2(aq)}$, NO_3^{-}, HCO_3^{-}, Cl^{-}, SO_4^{-2}, HPO_4^{-2}, F^{-}, $SiO_{2(aq)}$, UO_2^{+2}, $O_{2(aq)}$, a tracer along with 103 secondary aqueous complexes, 11 kinetically reacting minerals, and 8 equilibrium surface complexes on three surface sites (>SiOH, >FeOH, >AlOH). All reactions but mineral precipitation-dissolution were equilibrium-based.

DISCUSSION

Significant progress in advancing all four of the defined ASCEM capabilities was realized during the Phase I (Savannah F-Area) Demonstration. The Data Management component adapted and implemented a relational database as well as other open-source, web-based tools to allow users to easily ingest, browse, filter, graph, query, and output various types of data common to subsurface investigations. Tools were developed to handle both transparent data (such as wellbore concentration and lithology data) and opaque data (such as historical documents). A useful characteristic of the Data Management tools is that they can be used iteratively to display and query different subsets of the database based on sub region, characteristic, or parameter range specifications. The Visualization component of the Phase I Demonstration modified and extended open-source VisIt software to visualize data or features common to environmental remediation efforts, such as wellbore geometry, depositional information, hydrostratigraphic surfaces and topography, and the evolution of contaminant plumes. These tools provide distinct advantages, such as the ability to 1) visualize many different types of data (point, surfaces, volumes) in an uncluttered fashion, 2) jointly visualize physical features and contaminant concentrations, and 3) use slider bars to navigate through temporal datasets (for example, to view the evolution of a subsurface contaminant plume within a physical framework). For the Uncertainty Quantification component, ASCEM capabilities were developed to allow a user to choose model parameters and model outputs and to perform UQ analysis using a variety of different analysis approaches and types. An ASCEM GUI was developed as a framework for the UQ capabilities, which takes advantage of many open-source UQ analysis approaches. A novelty of the ASCEM UQ capabilities is that the various methods are not available in a single software analysis package elsewhere; bringing them together under the ASCEM UQ tool represents a major advance. Substantial progress was made on developing early prototypes of selected toolsets within the ASCEM multi-process HPC simulator. Advances were realized using both the unstructured mesh and a structured mesh approach. For the unstructured approach, parallel, hexahedral mesh and parallel, single-phase, flow and reactive transport capabilities were developed. All of the targeted F-Area geochemistry was implemented and run as a single phase with the unstructured mesh approach. Future efforts will explore techniques to seamlessly use capabilities from multiple frameworks.

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Collaboration hurdles were (and continue to be) surmounted as the large, multi-disciplinary ASCEM team develops optimal mechanisms and shared vocabulary needed to coordinate and communicate efforts, respectively. The working group mechanism was found to be useful for aiding communication about the demonstration and for making sure that the development of ASCEM capabilities is relevant to DOE-EM's remediation effort. During subsequent demonstrations, the working groups will also be valuable for engaging site personnel in the ASCEM effort and for beta testing developing ASCEM capabilities. During the initial demonstration, various collaborative tools were used to assist ASCEM development teams. As subsequent demonstrations will focus on data sharing and component integration, it will be critical to develop a common framework for collaboration across the ASCEM team.

The initial demonstration was designed to provide an early snapshot of specific ASCEM capabilities by describing advances associated with the defined Phase I, F-Area effort as well as additional, opportunistic developments. It is the first of a series of ASCEM demonstrations that will be performed in a phased manner to correspond with the development of the Platform and HPC Thrust components and with ASCEM releases. The project is developing a long-range plan that will outline future demonstrations and will consider associated demonstrations, tutorials, and documentation.

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