Using ASCEM Modeling and Visualization to Inform Stakeholders of Contaminant Plume Evolution and Remediation Efficacy at F-Basin Savannah River, SC – 15156

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ABSTRACT

Communication with stakeholders, regulatory agencies, and the public is an essential part of implementing different remediation and monitoring activities, and developing site closure strategies at contaminated sites. Modeling of contaminant plume evolution plays a critical role in estimating the benefit, cost, and risk of particular options. At the same time, effective visualization of monitoring data and modeling results are particularly important for conveying the significance of the results and observations. In this paper, we present the results of the Advanced Simulation Capability for Environmental Management (ASCEM) project, including the discussion of the capabilities of newly developed ASCEM software package, along the its application to the F-Area Seepage Basins located in the U.S. Department of Energy Savannah River Site (SRS).

ASCEM software includes state-of-the-art numerical methods for simulating complex flow and reactive transport, as well as various toolsets such as a graphical user interface (GUI), visualization, data management, uncertainty quantification, and parameter estimation. Using this software, we have developed an advanced visualization of tritium plume migration coupled with a data management system, and simulated a three-dimensional model of flow and plume evolution on a high-performance computing platform. We evaluated the effect of engineered flow barriers on a nonreactive tritium plume, through advanced plume visualization and modeling of tritium plume migration. In addition, we developed a geochemical reaction network to describe complex geochemical processes at the site, and evaluated the impact of coupled hydrological and geochemical heterogeneity. These results are expected to support SRS's monitoring activities and operational decisions.

INTRODUCTION

The Savannah River Site (SRS) is located in south-central South Carolina, near Aiken, approximately 100 miles from the Atlantic Coast. It covers about 800 km2 (300 mi2) 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. The SRS F-Area seepage basins were constructed as unlined, earthen surface impoundments that (from 1955 through 1988) received ~7.1 billion liter of acidic, low-level waste solutions from the processing of irradiated uranium in the F-Area Separations facility [1]. Currently, an acidic contaminant plume extends from the basins ~600 m downgradient to the Four Mile Branch creek. The plume contains various radionuclides, such as uranium isotopes, strontium-90, iodine-129, technetium, tritium, and other contaminants, such as nitrate.

Various remediation activities have been conducted at the site, including capping of the basins (1991) and pump-and-treat (1997–2004). A hybrid funnel-and-gate system has been in operation since 2004, which includes low-permeable engineered flow barriers, and injection of alkaline solutions. The base injections are considered to be effective in neutralizing the acidic groundwater and in greatly increasing uranium retardation, since uranium mobility is significantly influenced by pH (because higher pH values increase uranium sorption). At the same time, the barriers slow down plume migration and increase decay and mixing before the plume reaches the Four Mile Branch creek, a downgradient stream that ultimately captures the plume. Monitored Natural Attenuation (MNA) is a desired closure strategy for the site, assuming that infiltration of rainwater will eventually increase the pH of the plume, causing much stronger retardation and dilution of the uranium plume.

The SRS F-Area is also a primary application site of the Advanced Field Research Initiative (AFRI) project under the U.S. Department of Energy (USDOE) Office of Environmental Management (EM), which is developing cost-effective approaches for long-term monitoring at the DOE sites. Such approaches are critical, since long-term monitoring of contaminated groundwater is in fact considered to be a large fraction of DOE's life-cycle cleanup costs, and the current practice of obtaining and analyzing the contaminant concentrations in groundwater samples at numerous wells over time is quite expensive. SRS's AFRI is, therefore, exploring alternative approaches that focus on measuring the controlling (or master) variables (such as pH, contaminant concentrations, and groundwater table), which are leading indicators for changes in the plume mobility and its spatial and temporal distribution. This will result in development of a more robust and cost-effective monitoring approach that could also serve as an early warning of plume migration, and will also provide the necessary information of modeling activities.

Communications with stakeholders and regulatory agencies are always necessary before implementing any remediation activities and monitoring strategies, as well as in developing site-closure strategies. Modeling is a critical component of these communications to inform stakeholders of potential benefits, costs, and risks of proposed activities. Long-term predictive understanding of plume migration is essential for such cost-benefit-risk estimations and decision-making. The challenge is that such predictions are often hindered by complex and coupled hydrological and geochemical processes associated with remediation treatments, the large computational requirement in simulating such complex processes, and the inherent uncertainty and heterogeneity in the natural system. Both expected outcomes and uncertainties in model predictions have to be communicated effectively for robust decision making. In addition, monitoring data and modeling results have to be visualized in a way that facilitates communications with both technical communities and the general public.

To tackle such challenges, the DOE-EM recently initiated the Advanced Simulation Capability for Environmental Management (ASCEM) [2]. ASCEM is an open source, modular computing framework that incorporates new advances and tools for predicting contaminant fate and transport in natural and engineered systems. ASCEM includes a state-of-art numerical code (Amanzi) for simulating complex flow and reactive transport, and numerous toolsets for data management, visualization, uncertainty quantification (UQ) and parameter estimation (PQ). In the Phase II Demonstration (2012), ASCEM developed a two-dimensional flow and reactive transport model at the F-Area, and performed uncertainty quantification studies [3, 4]. The demonstration showed that the ASCEM toolsets coupled with Amanzi's parallel processing capabilities could overcome the large computational burden required for such a large-scale uncertainty quantification study. This study also identified important parameters and processes required for accurate prediction.

The ASCEM application at the SRS F-Area has currently two main objectives. The first objective is to apply the ASCEM software to evaluate the effects of past and current engineering systems on flow and the geochemical conditions of the site, as well as to predict the time frame for transition to MNA. The UQ toolsets are used to compute the uncertainty range of those predictions for robust decision-making. The second objective is to support the ARFI efforts by assessing the efficacy of the long-term monitoring strategies through advanced visualization and modeling. Advanced plume visualization is necessary to monitor the plume evolution over time, and to communicate effectively with stakeholders. Modeling efforts are critical for estimating the plume extent, determining the optimal layouts of the monitoring network and also understanding the correlations between the master variables and contaminant concentrations of interest.

This paper focuses on presenting: (1) an advanced contaminant plume visualization coupled with the data management system, (2) a three-dimensional (3D) flow and transport model, (3) an improved geochemical sorption model, and (4) an evaluation of the effect of aquifer facies and geochemical heterogeneity on plume evolution. Specifically, using the plume visualization and three-dimensional flow-transport models, we evaluate the impact of the engineered barriers on the movement of nonreactive plumes (such as tritium plumes).

METHODOLOGY

ASCEM Visualization

The goal of the ASCEM plume visualization is to provide a unified and straightforward way for creating contaminant plume maps quickly and easily on the database user interface, and at the same time to enhance the productivity of data exploration. Figure 1 shows a diagram of major components in the coupled data-management and visualization system. The data-visualization infrastructure consists of four major components: (1) a comprehensive unified data management system, (2) visualization software (VisIt) on the NERSC (National Energy Research Scientific Computing Center) system, (3) Google Maps for displaying geospatial data, and (4) the web-based data browser. Users have quick access to various types of datasets through the web browser, and can create time-varying contour plots and movies of contaminant plumes on the same browser.

The ASCEM database provides a means for comprehensive storage for various datasets collected at the site, including contaminant concentrations at monitoring wells over time, water-table data, core-analysis data, and cone-penetrometer data. The database can take datasets from multiple sources and perform quality check to eventually provide one underlying infrastructure that serves the ASCEM data browser website. The ASCEM data-browser client utilizes Google Maps as its core interface, which allows users an intuitive look at geospatial regions of interest, and enables users to select well locations using a well-known visual layout. The selections can then be used to query the database system for data associated with a particular well, such as a time series of contaminant concentrations. The visualization services are provided by VisIt, which is a DOE supported visualization package designed to scale from desktop environments to super computing facilities such as the ones at NERSC (National Energy Research Scientific Computing Center) [5]. VisIt is an open-source, interactive, highly parallel, and scalable visualization, animation, and analysis tool. The open-source environment allows developers to customize the visualization to any specific applications. It accommodates a remote client system such that users can visualize their data on their data browser while utilizing the power of high-performance computing facilities.

As shown in Figure 1, in the ASCEM data-visualization system, a user first starts the data browser, where multiple data locations are shown within the Google Maps interface. After selecting a contour-plot option, the user can specify an aquifer and/or an analyte of interest, as well as the temporal range and concentration range for visualization. This selection is then passed down to the visualization server for querying the database, to get the required data that match the selection. The visualization server interpolates the obtained data to construct a custom contour surface with annotations and markers. The resulting image is then returned to the ASCEM data browser client. One of the core action items of the rendering phase is to interpolate the well-concentration data, which are often quite sparse over spatial regions. The visualization system provides several interpolation options, and currently supports both linear interpolation and inverse weight interpolation schemes [6]. Although the inverse weighted calculation is currently the default, the infrastructure can easily be extended to allow for implementation of more complex interpolation methods (e.g., kriging).

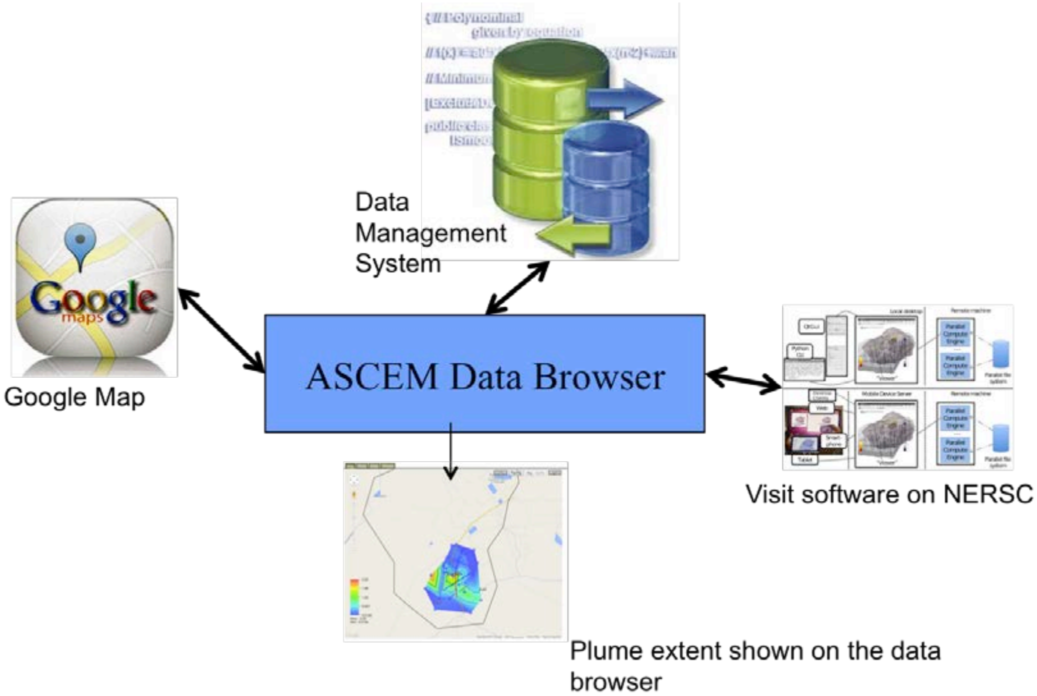

Figure 1. ASCEM data-visualization infrastructure

In addition to this web-based two-dimensional plume visualization, three-dimensional visualization is currently being developed. In a three-dimensional domain, the visualization system can add significantly more information to the monitoring data. It is possible to visualize the plumes in more than one aquifer in the same frame, which facilitates the comparison among different aquifers. Furthermore, additional pieces of information (such as topography, hydrostratigraphic interface depths, and depositional facies along wells) can be visualized. Three-dimensional visualization enhances the ability to explore datasets, such as correlations among different datasets, to enable a better understanding of a given system. Creating an animation over multiple time steps provides a more complete picture of the complexity of data, while being interactive at the same time.

Three-dimensional Flow and Transport Model

A 3D hydrological model was developed based on a previous flow model developed for a larger domain encompassing the overall General Separations Area at SRS [7]. The flow velocity field computed in the

GSA flow model was used to define a model domain that follows natural hydrogeologic boundaries (Figure 2a). The domain includes three hydrostratigraphic zones within the Upper Three Runs Aquifer: (1) an upper aquifer zone, (2) a Tan Clay Confining Zone, and (3) a lower aquifer zone. The domain also includes low-permeability engineered flow barriers, which are part of the funnel-and-gate system.

Los Alamos Grid Toolbox (LaGriT) [8] was used to develop an unstructured three-dimensional mesh of prism cells and to export it to the Exodus II format for Amanzi (Figure 2b-d). The mesh includes the regions and faces necessary to define the material properties, initial and boundary conditions. It is also designed to include fine discretization that conforms to the boundaries of the barriers, seepage basin and injection/extraction wells to accommodate setting material properties (e.g. permeability) and boundary conditions (sources and sinks for injection and extraction wells).

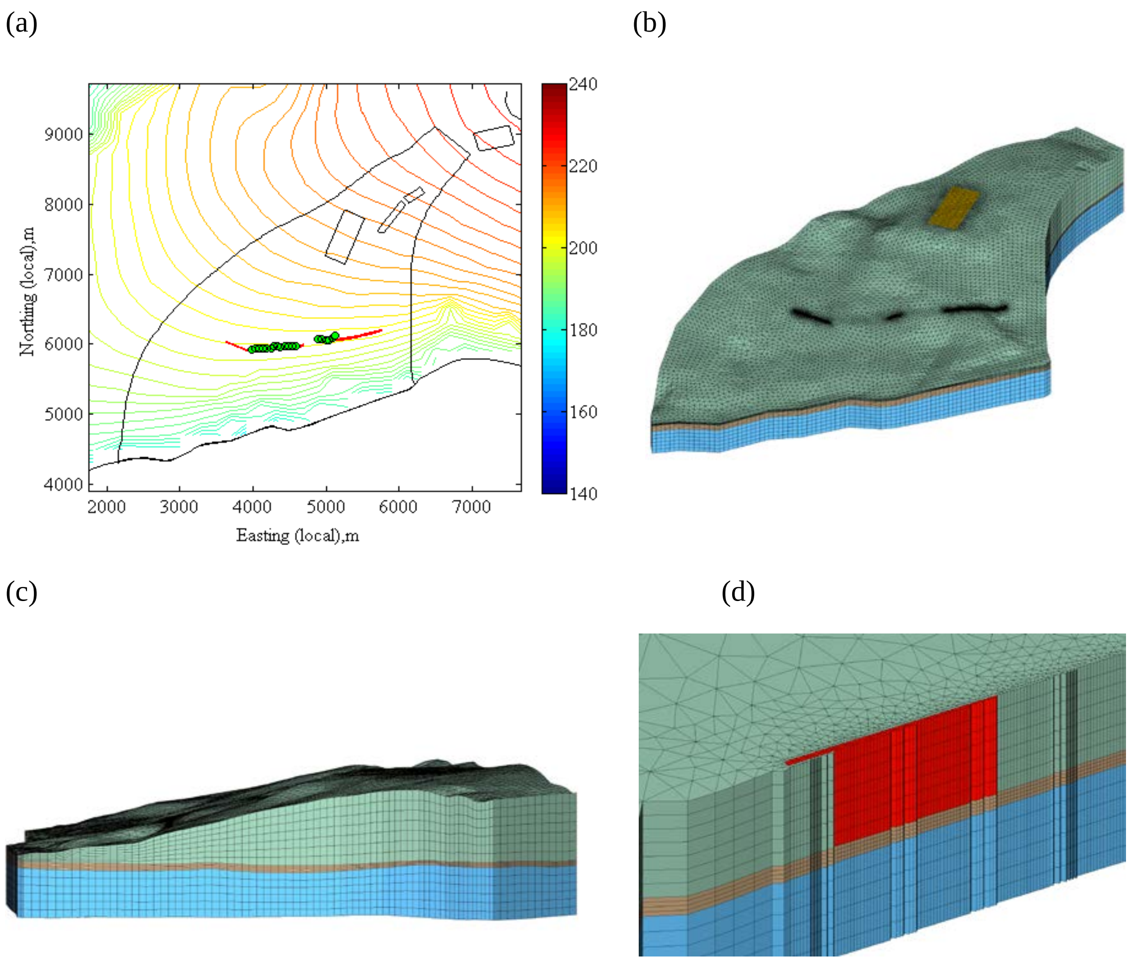

Figure 2. (a) Plan view of the 3D flow and transport domain, (b) 3D mesh generated including three hydrostratigraphic units, the F-Basin site (yellow) and each of three barriers (red), (c) the vertical view of the mesh created from the surface layers and derived sub-layers (top) and filled with triangular prism elements, and (d) cutaway of mesh showing one of the barriers (red) and layer materials. In (b), the top green material region is the upper aquifer, the middle brown layer is the Tan Clay confining zone, and the bottom blue region is the lower aquifer.

The modeling domain is represented by surface elevations coinciding with the tops of each hydrostratigraphic layer and ground surface. The elevations are interpolated onto a triangulated surface designed to conform to the boundary polygon and to fit the barrier features with high-resolution spacing. In addition, intermediate layers (5 for lower aquifer, 3 for the Tan Clay and 6 for the upper aquifer) are created that are proportionally spaced between the top and bottom of each layer. These layers are then stacked and filled with triangular prism cells (Figure 2c). Various versions of the mesh included variations in the horizontal mesh resolution and vertical layer resolution. Iterations between the flow solution and re-meshing resulted in improved designs. The final mesh used in this study has 371,518 cells and 199,494 vertices. Mesh edge lengths were smallest (highest resolution) at the barrier locations (Figure 2d) with edge lengths near .2 meters. The regions with no small features to capture have larger spacing with edge lengths between 20 and 50 meters (Figure 2b).

Three-dimensional flow and transport simulations were performed using Amanzi on the NERSC high-performance computing platform [9]. The Richards equation was used to model fluid flow in a variably saturated medium, and the solute transport was modeled with a linear advection-dispersion equation. A 3D unstructured prismatic mesh imposes severe requirements on discretization methods to achieve accurate discretization of the continuum PDEs. We used the mimetic finite difference method for the Richards and dispersion operators to preserve their fundamental mathematical and physical properties in discrete schemes [10]. To discretize the advection operator, we implemented monotone first-order and second-order MUSCL schemes with new limiters that improve accuracy on unstructured meshes [11].

We used the same aquifer properties as the 2D flow model developed by Bea et al. [3]. For the barriers, we assumed a permeability of $1\times10^{-17}m^2$ and a porosity of 0.05. Among six faces surrounding this domain, the upstream face has a fixed pressure boundary based on the measured water-table height, while the ground surface is a fixed recharge boundary with a moving seepage face to allow groundwater flow to upwell and discharge to the Four Mile Branch creek. The other faces are no-flow boundaries, since the downstream face corresponds to the stream, the bottom face is a relatively continuous low-permeability clay layer, and the other two faces are parallel to the flow.

Geochemistry Model Development

- Alternative Model to Describe H^+ Sorption

Bea et al. [3] developed a geochemical reaction network for the F-Area to simulate pH and uranium plume evolution for a background condition without any engineering treatments. The geochemistry model was developed based on the experimental data and sorption model development of Dong et al. [12]. The sorption model of Dong et al. [12] was developed with an inclusion of (so-called) electrostatic correction terms that quantitatively influence the mass laws describing the sorption reactions of H^+ and UO_2^{2+}. The purpose of these correction terms is to correct for the development of a positive electrical charge and potential on the surfaces of the sorbing minerals (kaolinite and goethite) at low pH values.

The Bea et al. reactive transport model results demonstrated that sorption of H+ (rather than H+ ion exchange as assumed in [4]) is very important in buffering pH values, retarding the initial advance of the acidic front in the F-area, and maintaining low pH values for a long period on the aquifer. For the current work, we are investigating the development of alternative models to that of Bea et al. [3] that will describe H+ and U sorption reactions such that they can be accommodated directly into Amanzi for future simulations, without the need for an electrostatic correction.

- Evaluation of Facies and Geochemical Heterogeneity on Plume Evolution

The impact of geochemical heterogeneity was evaluated in a reactive transport model through a onedimensional (1D) column, representing a flow line from the basin [13]. The width of the model is set equal to the basin length (219 m) and is oriented perpendicular to the F-3 basin. As preparation for implementing the geochemical model into Amanzi, we implemented a reactive transport model within TOUGHREACT [14] that follows the same conceptual modeling framework as Bea et al. [3].

After validating the 1D model using existing data from two well locations at SRS, we performed uncertainty analysis by varying hydrological and geochemical properties of the sediments. To represent the subsurface heterogeneity, we used two reactive facies, Lagoonal facies and Barrier Beach facies, which were identified and confirmed to have distinct reactive transport properties [15]. The average hydrological properties, geochemical reaction network, and initial and boundary conditions were similar to the model setup of Bea et al. [3]. The reaction network consisted of 15 primary species and four sites for sorption of H^+/U—namely, kaolinite (two sites), goethite, and quartz. As suggested earlier, uncertainty in these sorption properties, including the variation in mineral fractions, reactive facies distribution, etc., are evaluated using this 1D model. The ranges of these key physical and chemical factors relevant to two reactive facies are included in Sassen et al. [15].

RESULTS

Plume Visualization

Figure 3 shows an example of the web-based 2D plume visualization overlying the site map on the data browser. A series of concentration maps correspond to the snapshots of the movie displayed on the browser. The data-management functions can be seen as tabs above “Plots” for plotting a time series of concentrations, “Data” for displaying data values, and “Filter” for searching wells that have the datasets of interest. In this example, each plot shows a contour map of tritium concentrations. The blue circles are the well locations that have tritium concentration data; by clicking on each of them, users can quickly view a time series of concentration over time.

In Figure 3, we can observe the tritium-plume evolution, and evaluate the impact of the flow barriers on the tritium plume. The high-concentration part of the tritium plume migrates toward downstream in 1996, passing through the future location of the barriers (Figure 3a). Although the main part of the tritium plume was discharged to the stream by 2000 (not shown), the tritium concentrations are still significant and higher than maximum the contamination level of 20,000 pCi/L. After the flow barriers are constructed, the center of the tritium plume appears to stay in the upgradient of the barriers; it does not migrate towards the creek (Figure 3b-d). Although this observation is qualitative, it is very informative before moving on to more detailed analyses. We can do this kind of visualization with only a few clicks in the data browser.

In addition, this tool was useful for conceptual model development of flow and transport, to identify the plume extent in each aquifer and define a model domain. We can also quickly identify wells with observations necessary for model validation and calibration. This will be also useful for long-term monitoring efforts—for example, to monitor the plume evolution, evaluate the efficacy of engineering treatments, and identify high-concentration locations.

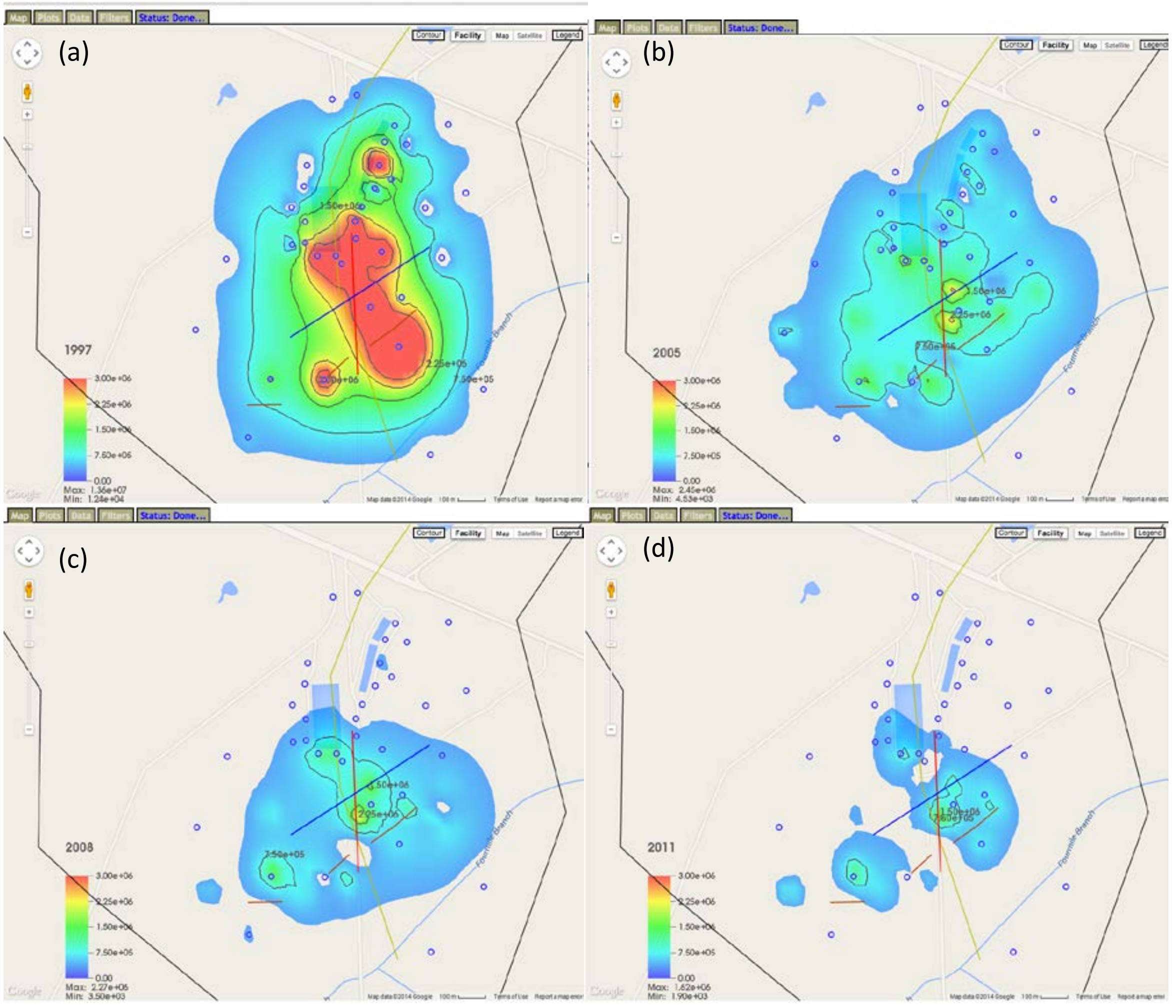

Figure 3. Web-based 2D plume visualization on the ASCEM data management website. A colored contour map of the tritium concentrations (in pCi/L) is created on top of the Google Map of the SRS F-Area: (a) 1997, (b) 2005, (c) 2008 and (d) 2011.

Figure 4 shows the 3D visualization capability currently being developed to visualize various types of datasets available at the site in a single viewer on the VisIt software. Tritium concentrations in each aquifer are projected onto the aquifer interface. The figure also includes the ground surface topography, aquifer interfaces, depositional facies along the wells, observation-well layout, and plume extents in different aquifers. This is a powerful tool for visualizing complex and disparate heterogeneous datasets at the site, and for performing visual exploration, such as comparing different types of datasets. Eventually, the 3D visualization will be accessible within the ASCEM GUI, Akuna, so that the users can compare the observed and simulated plumes easily after simulations.

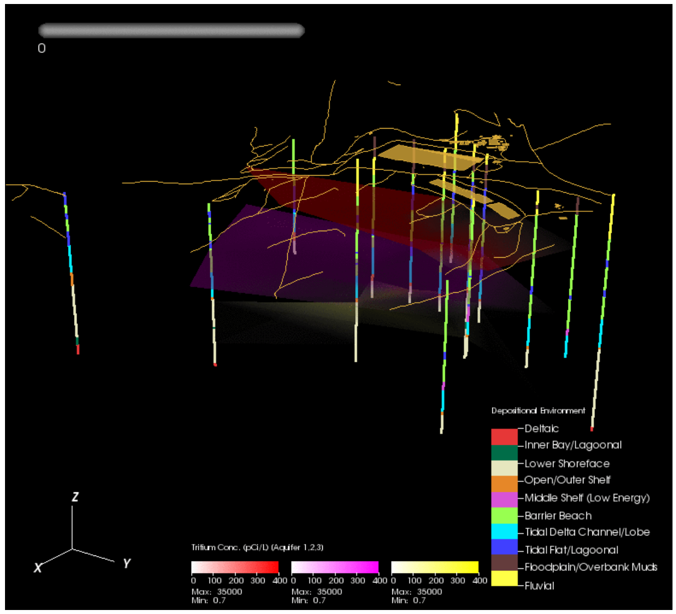

Figure 4. 3D tritium plume visualization along with various types of datasets. The visualization includes the surface topography along with roads and building footprints, the depositional facies along the wells and the plume contour maps in three aquifers projected on to their hydrostratigraphic interfaces.

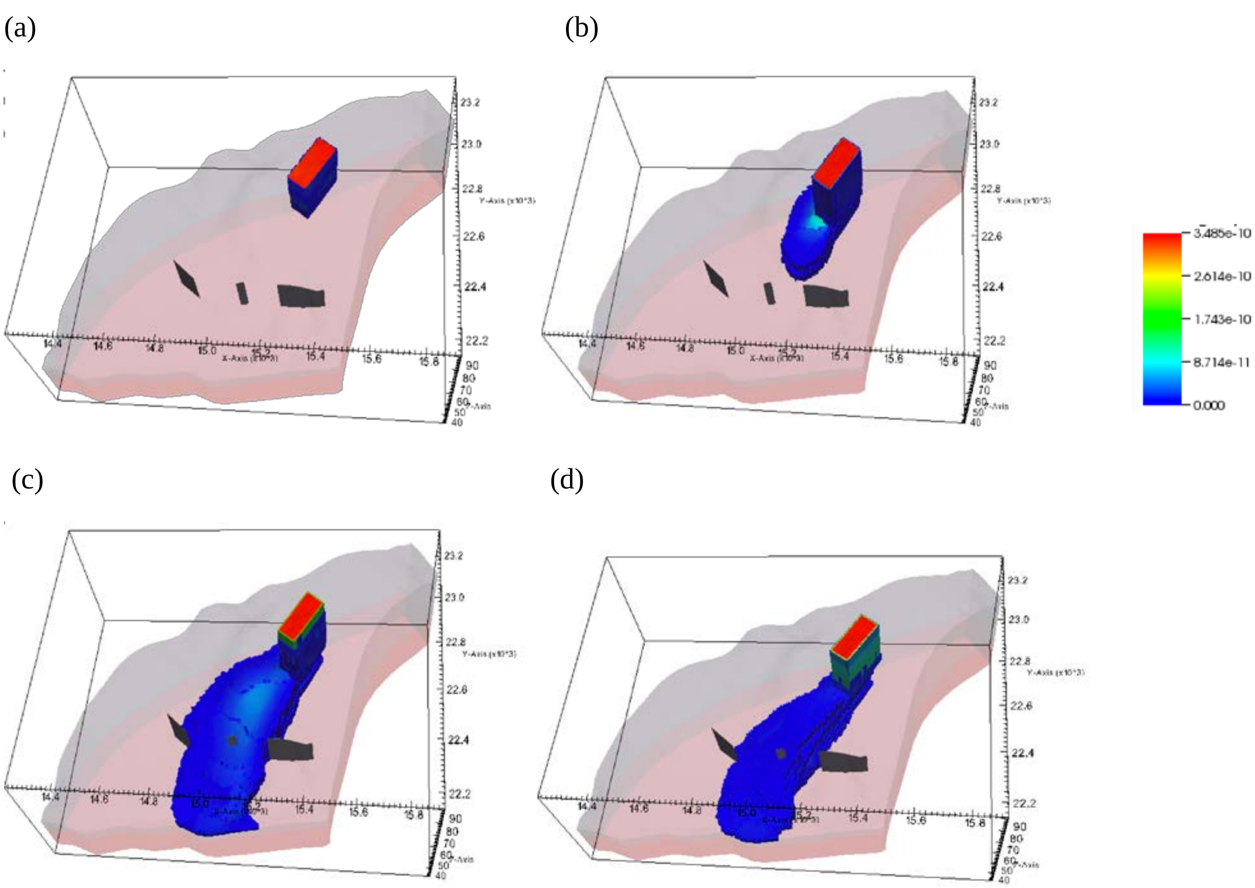

Figure 5. Simulated tritium plume evolution in the 3D flow and transport model: (a) 1955, (b) 1968, (c) 2005 and (d) 2025. The concentration unit is mol/L. The threshold of 1×10^{-12}mol/L is used to draw the plume boundary, and the brown vertical structures depict the barriers.

Three-Dimensional Flow and Transport model

Figure 5 shows the 3D plume evolution of the tritium plume visualized using the VisIt software. This simulation included the barriers and capping of the seepage basin. Although the barriers were installed in 2004, this simulation included the barriers from the beginning, to confirm Amanzi's ability to handle sharp permeability contrasts near the barriers, as well as to evaluate the effect of such barriers on the nonreactive tritium plume (in addition to diverting the plume into the funnel gates). In Figure 5, the plume initially moves straight down until it hits the water table (Figure 5a), and then migrates laterally within the upper aquifer (Figure 5b). As the plume spreads and migrates downgradient towards the creek, it hits the barrier (Figure 5c). Figure 5c shows that the barriers are successful in blocking the plume and directing it into the gates. Eventually, the plume starts decreasing in size, due to the effect of radioactive decay (Figure 5c). Note that significant tritium is trapped in the vadose zone even in 2025, which suggests the long-term effect of capping the basin.

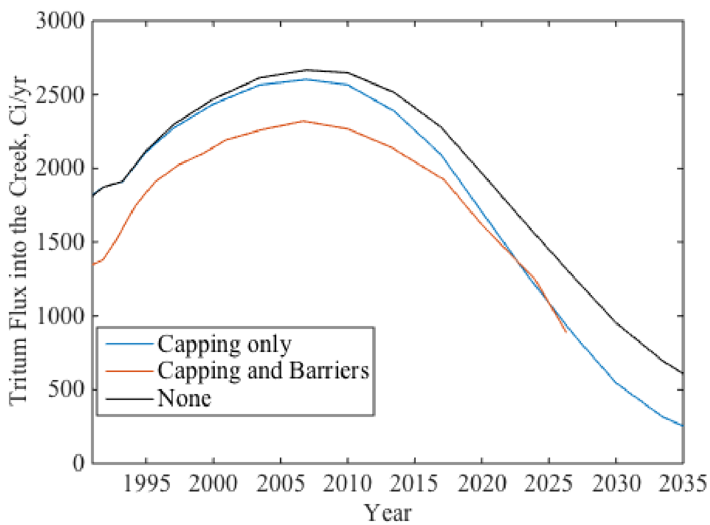

Figure 6. Simulated tritium flux into the Four Mile Branch Creek. Different remedial options are compared: basin capping only, capping and barriers.

Figure 6 compares the efficacy of different remedial options based on the tritium flux into the creek after the basin closure. Although we have not conducted a sophisticated calibration of our flow model, we verified the modeling results using a comparison with the results of field studies of the tritium flux: the computed tritium flux is within the same range as that measured at the site—from 1000 to 3000 Ci/yr. As we expect from Figure 5, capping of the basin has reduced the flux significantly over the long time period. The effect is small at the beginning, since the plume front is attributed to the tritium mass entering the groundwater during the operation before the basin is capped. In later years, the basin cap retards the tritium migration in the vadose zone below the basin, so that a significant mass of tritium decays out in the vadose zone. The barriers reduce the tritium flux, particularly in the first 30 years, since the barriers reduce flow velocities and increase mixing with the background groundwater. The effect is reduced in later years, possibly because, as the plume size decreases, the main part of the plume goes through the funnel gates (i.e., the open part of the barriers), as is shown in Figure 5d.

These results highlight the capability of Amanzi to simulate a complex flow process involving seepage, waste discharge, and barriers. This is the first time that Amanzi has been used to simulate a large-scale 3D plume evolution, including variable topography and sharp permeability contrasts, and also to compare the effect of different remedial options. This activity has also contributed significantly to debugging the code and to improving its robustness. Currently, parameter estimation and calibration is under way, using the ASCEM toolsets to improve the match to the observation data and predictions.

Geochemistry Model Development

As described above, our current geochemical model refinement includes the development of a H^+ sorption model that does not include electrostatic correction terms in the mass laws that describe the sorption reactions. Our initial approach has been to develop the model for the pH range 3–5.5; this is in part because groundwater in the acidic plume at the F-area is mostly in this pH range, but also because experimental data were collected in this pH range during the LBNL SFA Phase I program (Dong and Wan, unpublished data).

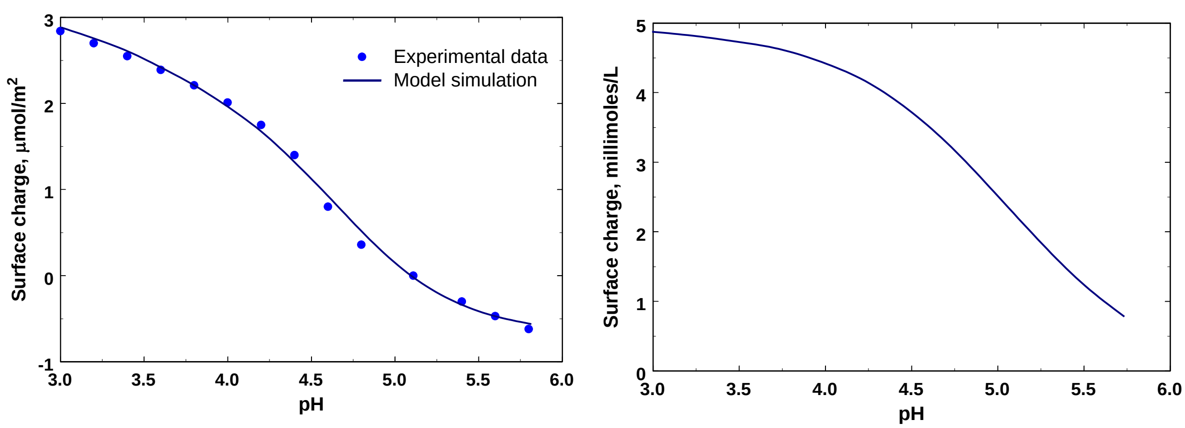

Figure 7. (a) Comparison of average experimental data for acid-base titration of F-area sediments in laboratory batch experiments and an H+ sorption model without electrostatic correction terms in the mass law for sorption reactions. (b) Extrapolation of the laboratory-calibrated H^+ sorption model to field conditions without any parameter adjustments.

Figure 7a shows averaged experimental data from acid-base titrations of nine separate F-area sediments. Surface charge in the experiments (per unit surface area of sediments) is calculated as the excess acid required to decrease the pH of a sediment-water suspension beyond what is required to decrease the groundwater only to the same pH value. The new H^+ sorption model consists of three surface sites with different site densities (per unit surface area), each with different acidity constants. Figure 7a illustrates the excellent agreement between the model prediction and the laboratory data. Figure 7b shows a prediction of the moles of charged surface sites per liter of groundwater in the aquifer using the new H^+ sorption model, assuming the same porosity value for the aquifer used in Bea et al. [3]; the average surface area for F-area sediments is 2.36 m^2/g [12]. At each pH value, the concentrations for positively charged surface sites are much greater than the concentration of dissolved H^+ in the groundwater, demonstrating why the aquifer surfaces are able to buffer the pH at low values for a long period of time [3, 13]. The result in Figure 7b is a straightforward extrapolation that needs to be tested further to confirm that the model is properly calibrated for field conditions; extrapolation from laboratory experiments with

<2 mm sediments to the whole aquifer often requires some corrections for upscaling.

In upcoming work, the model will be extended to the pH range 5.5–8.0, so that the base injection remediation scheme can be included in reactive transport modeling. In addition, the nonelectrostatic U sorption model used in the ASCEM Phase II demonstration will be updated to be consistent with the new H^+ sorption model. The new H^+/U sorption model will then be incorporated into the simulation and coupled with the 3D flow and transport model.

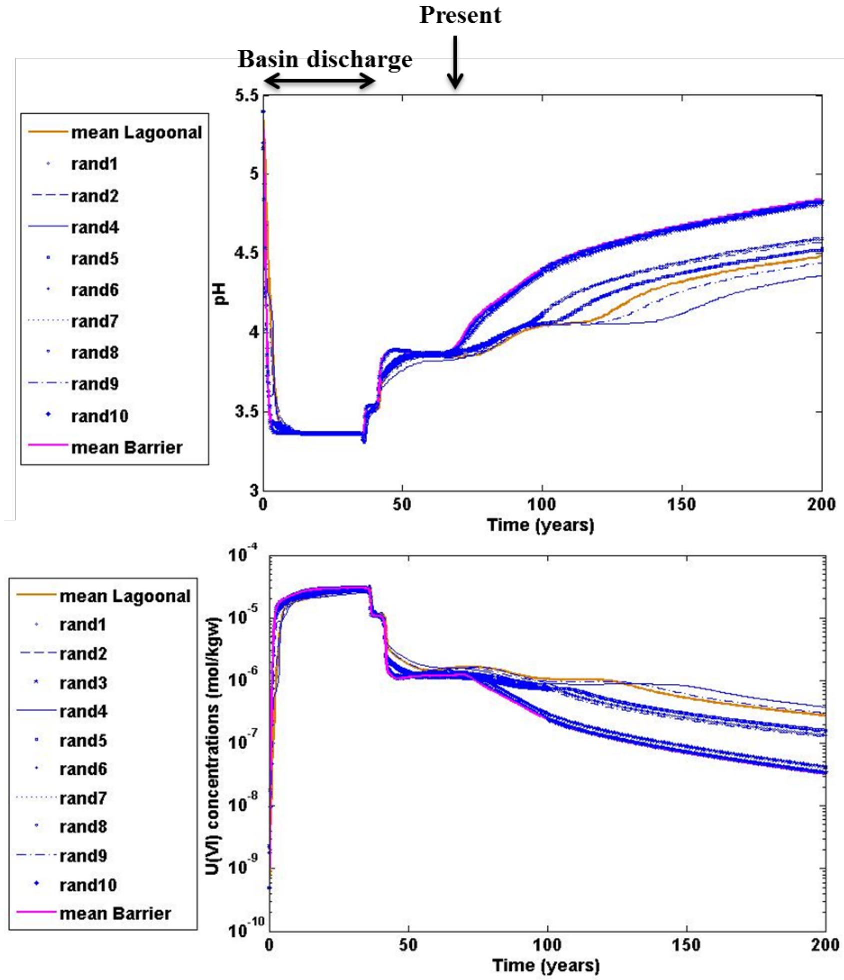

Figure 8: Uncertainty quantification simulations showing pH and uranium concentration profiles for well FSB95D using variable facies and geochemical parameters.

To explore the effect of aquifer heterogeneity on long-term plume mobility at SRS, we simulated reactive transport using a series of random fields of reactive facies and geochemical properties. The simulations used ten random fields and two homogeneous cases, each of which had properties of either the Lagoonal or Beach Barrier facies [15]. Figure 8 shows the predicted pH and uranium concentration at a downstream well over 200 years. If the current recharge and other site conditions persist, pH will rebound and uranium concentrations will continue to decrease. In Figure 8, the subsurface heterogeneity has a larger impact at later time, 75 years after basin operation ceased. Interestingly, even with a small number of samples, we see that random samples do not necessarily confine themselves to the range defined by the two homogeneous cases (i.e., average values predicted by Lagoonal and Barrier Beach facies).

This result suggests the importance of including subsurface heterogeneity when we predict plume evolution over a long time frame. Such long-term prediction would be essential for developing site closure strategies and evaluating the timing of transitioning to MNA. Although this model is simplified and does not include any remediation activities, the model predicts that, in several cases, the groundwater remains acidic and uranium concentrations are above MCL (30 mg/L or 1.26×10^{-7} mol/kgw). It suggests the need for the funnel-gate-system to actively control pH at the site for an extended time. Our future work will include spatial heterogeneity within 3D flow and reactive simulations, and will evaluate the effectiveness of engineering treatments in a more accurate manner.

CONCLUSIONS

In this study, we successfully applied the ASCEM software to reactive transport modeling and plume visualization at the SRS F-Area. Coupling of the ASCEM visualization toolset and database interface facilitated data exploration, and created the plume contour map and animation in a quick and intuitive manner. Amanzi was able to model 3D complex flow and conservative transport, including engineered flow barriers and a seepage face, and accommodate the sharp permeability contrast associated with the barriers. An H^+ sorption model was developed (for direct incorporation into Amanzi), which will describe pH buffering by the aquifer sediments; the impact of subsurface sediment heterogeneity was demonstrated to have very significant impact on predictions of long-term plume evolution.

Through the visualization and modeling, we confirmed that the flow barriers are potentially effective in decreasing the concentration of nonreactive contaminants such as tritium. Since tritium cannot be easily removed or remediated from wastewater or groundwater, these results are encouraging and potentially important for many other sites, such as the DOE Hanford site, and the Fukushima Daiichi Nuclear Power Plant in Japan, and many others.

Further testing, parameter calibration, and uncertainty quantification are currently under way to further advance the capability of the ASCEM software package. Additional developments are also currently under way to improve the geochemical model describing the base-injection, and also to couple the geochemical model into the 3D flow and transport model. In addition, geostatistics and random-field generation capabilities are currently being implemented in the software.

The SRS F-Area site will serve as an excellent demonstration site for such new capabilities. The impact of different geochemical models and heterogeneity will be evaluated using the integrated 3D model developed in this study. The integrated 3D flow and reactive transport model will also be used to support AFRI’s monitoring activities, by investigating the correlations between contaminant concentrations and master geological, geophysical, and hydrogeological parameters, and developing site closure strategies by estimating the optimal time frame of transitioning to MNA.

This study provides an example of implementation of the ASCEM tools to typical DOE modeling challenges. The site application drives the software development by adding complexity and new features required to deal with real sites. The flexible and open-source nature of the software facilitated evolution of the capabilities in a short time period. ASCEM capabilities are expected to help DOE EM provide efficient and cost-effective transition to site-closure end states, and guide DOE’s site decision making in developing long-term paths toward completing the DOE cleanup mission.

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