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Benefits of numerical flow and transport modeling applied to CCR site characterization, remedial design, and closure

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INTRODUCTION

The complexity of coal combustion residual (CCR) sites and variability between sites creates special challenges when selecting ways to characterize, evaluate, and manage them. Numerical flow and transport modeling offers site operators, consultants, contractors, and regulators a powerful tool to assist in achieving these goals as well as a means of communicating complex ideas and findings between the respective parties. The continued advancement of numerical modeling methods and tools has steadily improved the capabilities and accuracy of numerical models while reducing costs associated with developing both large- and small-scale models.

Numerical modeling can be used throughout the life of a CCR project from initial site characterization to conceptual site model (CSM) development and refinement, to closure selection and design, and finally to closure performance monitoring. Furthermore, numerical models can be continuously updated with new data as the project progresses to improve the predictive capabilities of simulations and reduce uncertainty. Numerical modeling assists in planning data collection efforts and in identifying potential data gaps during site characterization. Numerical modeling can be used when developing and refining the CSM to inform and test its components while finding potential inconsistencies. Numerical modeling is a powerful tool for decision-makers when evaluating potential closure options by providing them with comparable predictive scenarios and visualizations so closure options can be understood and costs can be balanced with closure effectiveness. Numerical models can improve confidence in a selected closure option's ability to meet/maintain closure goals in the future as well as assist in the design process once closure is selected. Furthermore, if remediation is necessary to meet the goals for a CCR site, flow and transport modeling is an effective tool for evaluating potential remediation strategies.

FLOW AND TRANSPORT MODEL DEVELOPMENT

There are generally three phases of flow and transport modeling. The first is model development and construction, the second is model calibration, and the third is using the calibrated model to make predictions or answer questions about a site. Currently, there are a variety of potential modeling codes and graphical user interfaces (GUIs) that can be used to conduct flow and transport modeling. Some of the industry-accepted modeling codes include[2,3]

- MODFLOW (flow modeling)
- FEFLOW (flow modeling)
- MT3DMS (transport modeling)
- RT3D (transport modeling)

Some available GUIs for flow and transport modeling include:

- Groundwater Modeling System (GMS)
- Groundwater Vistas
- ModelMuse

For all work discussed in this paper, modeling was conducted using MODFLOW, in particularly the MODFLOW-NWT version[4], and MT3DMS[5].

Model development and construction generally involve the following steps:

- Determine an appropriate model domain.
- Construction of a geologic model representing the site.
- Construct the model numerical grid using the geologic model and selected model boundary.
- Populate the numerical grid with flow and transport parameters.
- Populate the numerical grid with the known hydrologic and hydraulic boundaries, source and sink boundaries, and constituent source terms.
- Calibrate the flow and transport models to measured data from the site.
- Develop predictive models using the calibrated flow and transport models to make predictions and evaluate aspects of the site.

When developing a flow and transport model a model domain must first be chosen. The model domain represents the size of the model including the lateral extent and depth below the surface. The model domain should be chosen such that it encompasses the area of investigation, and the boundaries of the model are far enough away from the area of investigation that mathematical error at the model boundaries does not affect model results. Often these boundaries will be chosen such that a natural hydrogeologic boundary, such as a river or a natural groundwater divide, is between the area of investigation and the model boundary. Once a model domain is chosen then a geologic model must be developed. The geologic model is the initial framework from which a numerical grid will be created in hydrogeologic flow and transport modeling. Geologic site data used to generate this model can come from several sources including but not limited to geologic boring logs, geophysical logs, surface mapping data, test pit data, etc.

Using the geologic model and model domain the numerical grid can be constructed (Figure 1). This numerical grid is the mathematical grid used to solve the underlying flow and transport equations (typically algebraic approximations of the original differential equations).

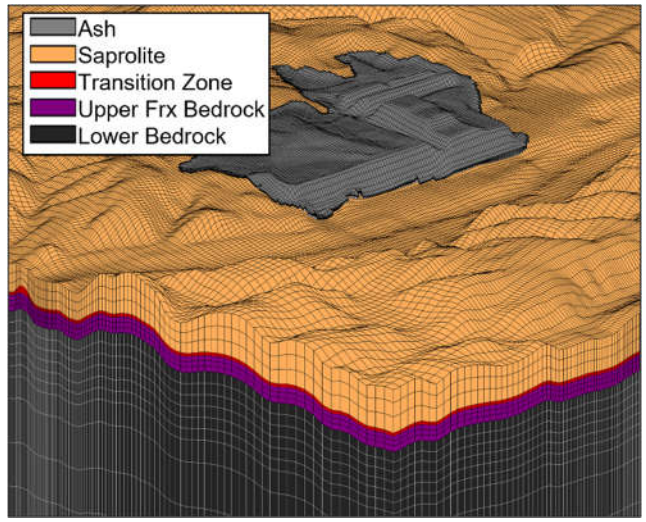

Figure 1. Flow and transport model grid

After the grid is constructed, it is populated with appropriate flow and transport parameters. Flow and transport parameters will include such parameters as hydraulic conductivity, effective porosity, storage coefficients (specific storage/specific yield), soil-water partition coefficients (K_d), dispersion coefficients, etc. The model grid is also populated with the known hydrologic and hydraulic boundaries, source and sink boundaries, source terms, etc. (Figure 2). These boundaries can include but are not limited to streams, lakes, ponds, wells, sources of groundwater recharge (natural and anthropogenic), and source zones.

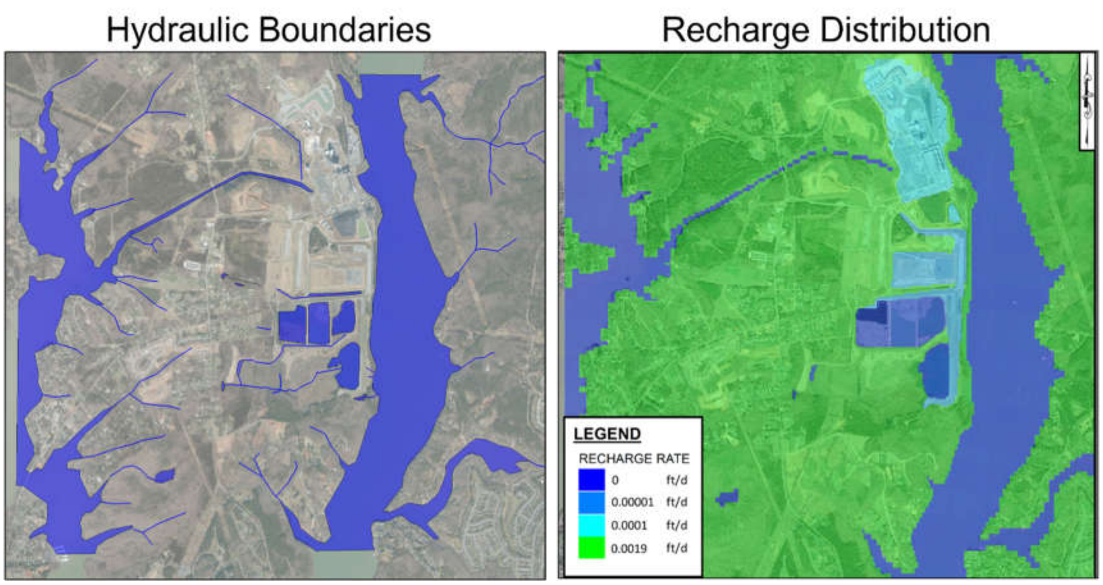

Figure 2. Hydraulic boundaries and recharge distribution model inputs

It should be noted that some of this input data may be unknown or poorly constrained because of a lack of data. For example, at CCR sites, data on sources such as historical placement and concentrations of source material is often limited or non-existent. Because of this potential lack of data, the model inputs often need to be adjusted during the calibration process to better match observed data. The calibration process involves matching the predicted hydraulic heads, flow rates, constituent of interest (COI) concentrations, etc. to data collected in the field (Figure 3). Generally, this is done manually by adjusting parameters and boundaries in the model until the predicted data matches the observed data to an acceptable level of accuracy. This process can also be automated using various tools such as parameter estimation tools such as PEST.[3] Often, how well a model matches observed data is quantified statistically using either the mean residual of the model or more often the root mean squared error (RMSE) or normalized root mean square error (NRMSE). The RMSE and NRMSE give a statistical calculation of how well a model is able to predict a known set of variables. A NRMSE less than 10 percent is the typical industry-accepted standard for a good model fit.

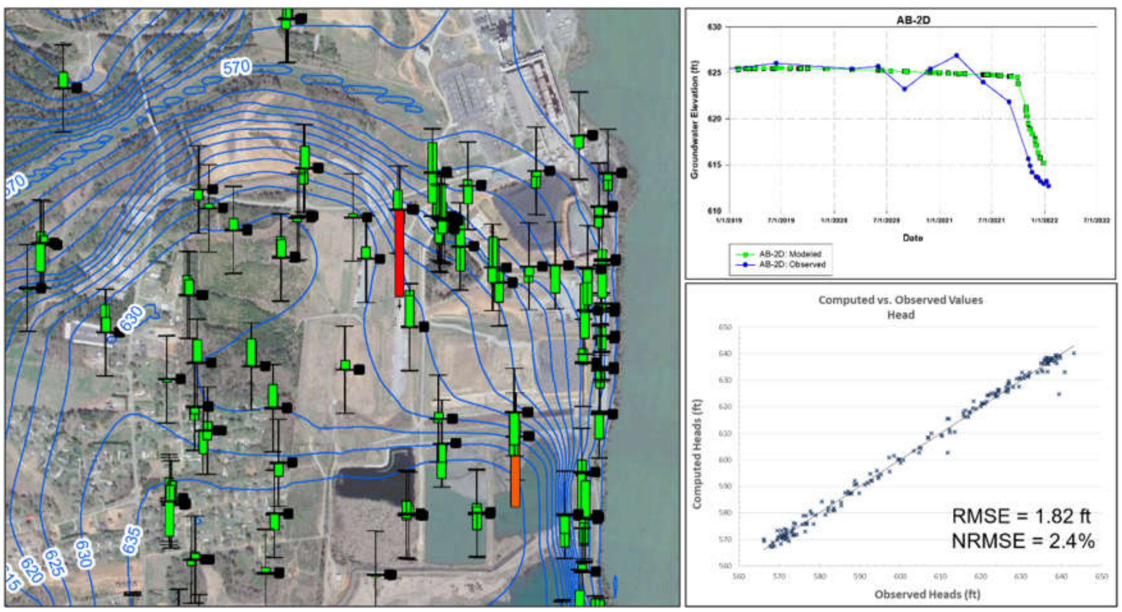

Figure 3. Flow model calibration results (error bars on plan view map show residuals between measured and predicted water levels; green: residual < 4ft, orange: 4ft < residual < 8ft, red: residual > 8ft)

Once a flow and transport model has been developed and calibrated, it can be a useful tool to evaluate various aspects related to CCR sites. Four examples of evaluations performed using flow and transport models are presented below and come from work performed at several CCR sites. These examples include applications of the models to help evaluate the flow system of CCR units, evaluate potential remediation strategies, evaluate methods for reducing saturated CCR material, and help design underdrain systems for CCR landfills.

MODEL APPLICATIONS – FLOW SYSTEM DEMONSTRATION

The first application discussed is the use of flow modeling to evaluate the behavior of the flow system at a CCR site located in the Piedmont region of the United States. Understanding the important aspects of a flow system is critical to understanding the expected behavior of CCR COIs and their transport in the subsurface. The general flow behavior at a site may not be obvious when initially evaluating a site, and flow models are valuable tools to identify key characteristics of the flow system. The CCR unit in question was built within a perennial stream valley. It was constructed by damming up the perennial stream valley and sluicing ash into the dammed-up valley. Originally it was anticipated that ash pore water was infiltrating into the groundwater system throughout most of the CCR unit (Figure 4).

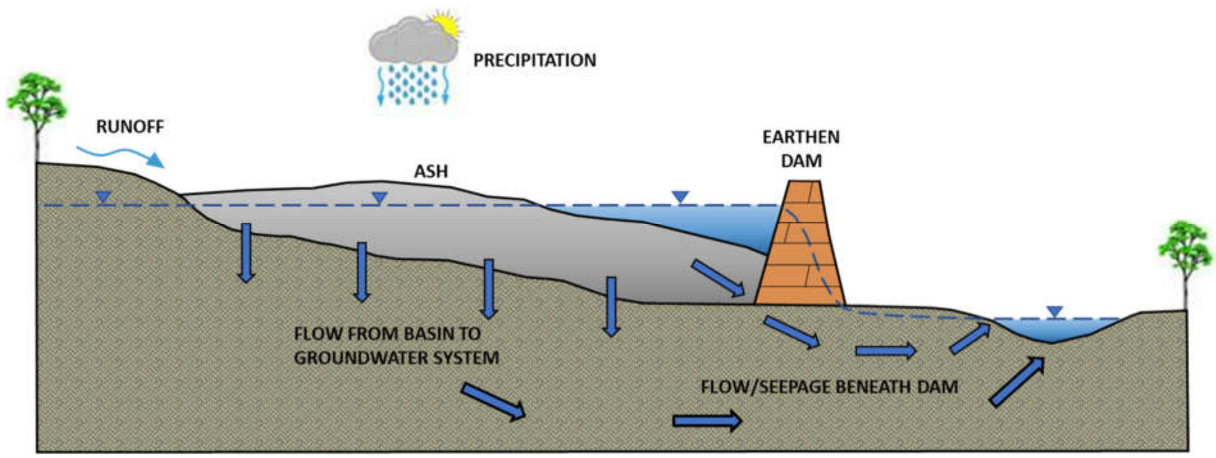

Figure 4. Initial conceptual model of the perennial stream valley CCR unit flow system

The initial conceptual model for this type of flow system was that water would enter the CCR unit from precipitation, runoff, and sluice water from ash placement and then infiltrate vertically downward into the underlying aquifer and eventually flow to the local discharge feature (typically a river or reservoir). In this system, it would be expected that COIs related to CCR material would be observed within portions of the aquifer overlain by CCR material.

However, COI data collected at the site indicated that CCR-related COIs appeared to be absent in the groundwater system below much of the CCR material where it was expected to be. To better understand the actual characteristics of the flow system, a groundwater flow model was used to evaluate how flow occurs within the CCR unit and underlying aquifer (Figure 5).

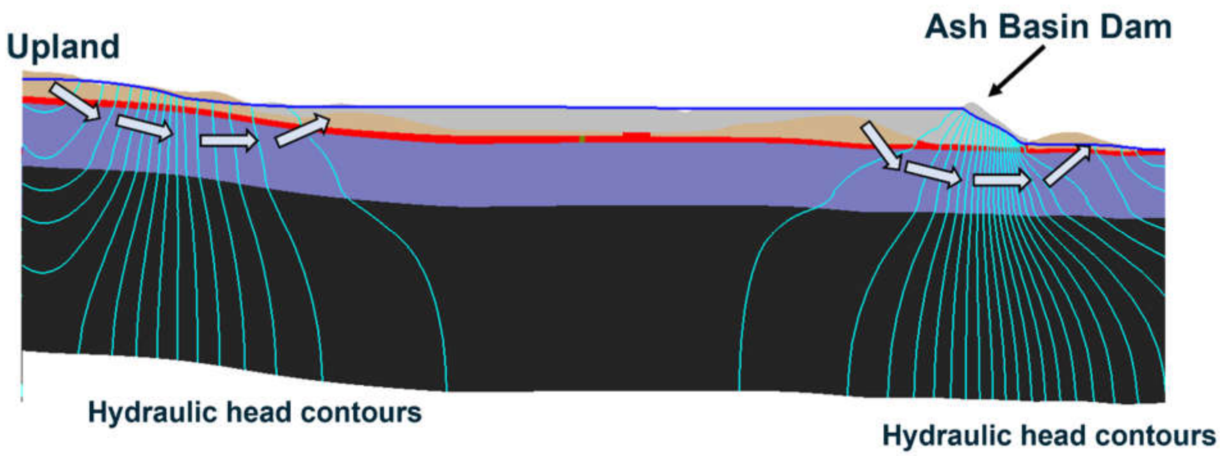

Figure 5. Modeled flow system within and below the CCR unit

These results indicated that groundwater from the underlying aquifer discharges into the CCR unit from the uplands, which would have been historical discharge locations along the perennial stream, then flows generally horizontally within the CCR unit and underlying aquifer through portions of the unit with little water transfer between the two, and finally, water from the CCR unit flows downward into the underlying aquifer near the dam to discharge to the local drainage feature. The findings from the flow model resulted in a revision in the conceptual model for these types of systems from what is shown in Figure 4, to the conceptual model depicted in Figure 6.

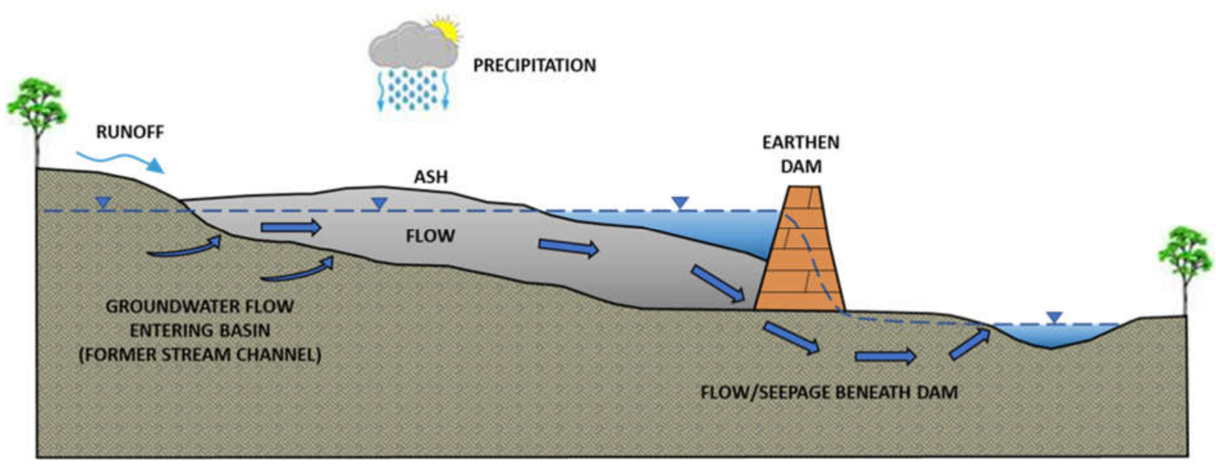

Figure 6. Revised conceptual model of the perennial stream valley CCR unit flow system

The revised understanding of the flow system has critical implications for the best approach to evaluating the potential effect of CCR-related COIs on the surrounding and underlying aquifer. Based on these results, additional resources (time and money) were directed to site assessment activities in areas where COIs were anticipated based on the simulated flow fields. This also reduced resources spent on assessing areas where COIs were not anticipated.

MODEL APPLICATIONS – REMEDIATION SELECTION

For some CCR units, remediation activities may be necessary so that the CCR unit is in compliance with federal or state regulations. Selecting an appropriate remediation strategy that is both successful and cost-effective is critical to meet regulatory and stakeholder goals for projects where remediation is necessary. Flow and transport modeling can be a powerful tool for selecting appropriate remediation for a given site. Often times monitored natural attenuation (MNA) is a preferred option because of the reduced costs compared to many of the more active forms of remediation. Results from flow and transport models can be a good first indicator of whether MNA may be viable for a given site.

Modeling results from two sites within the Piedmont region were compared to determine if the results could help identify whether MNA is a potential option or whether a more active remediation strategy may be needed. For both sites, the transport of boron was simulated to determine the maximum extent of potential CCR-related COIs and to evaluate how long it would take to reach compliance with only natural attenuation mechanisms. Boron was chosen as the indicative COI of the maximum extent of CCR effects because boron showed plume-like characteristics, is generally non-reactive, and moves readily with groundwater.

Both models were calibrated to field-measured hydraulic heads, flow rates, and observed COI concentrations until they were able to give reasonable fits to observed data. The calibrated model for Site A had an NRMSE for the flow model of 1.9 percent and an NRMSE for the transport model of 1.7 percent. The calibrated model for Site B had an NRMSE for the flow model of 2.1 percent and an NRMSE for the transport model of 1.6 percent. The calibrated models were then used to run predictive transport models that simulated boron transport and attenuation under anticipated site conditions following closure of each basin by excavation (Figure 7).

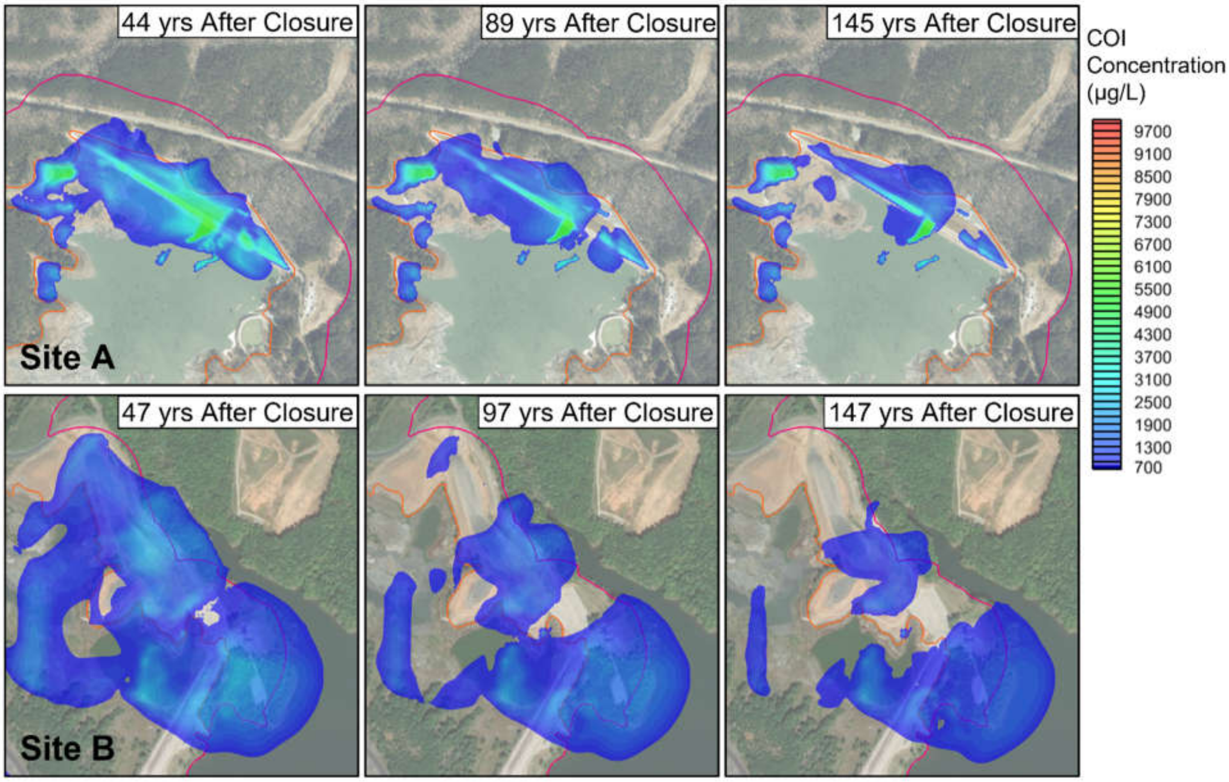

Figure 7. Comparison of predicted future boron plumes at Site A and Site B (boundary for compliance shown in pink)

The calibration and predictive models for Site A indicated that boron never extended beyond the regulatory boundary for the CCR unit prior to or following closure of the unit. Field data also indicated boron had not extended beyond the boundary. Boron is expected to be more mobile than other CCR-related COIs at Site A; therefore, it can be assumed that plumes from other CCR-related COIs would not extend any further than the predicted boron plume. These results indicated that MNA would likely be a viable remediation strategy for the site.

However, the calibration and predictive models for Site B indicate that the boron plume had extended beyond the regulatory boundary and is predicted to remain beyond the boundary for extended periods in the future (100+ years). The persistent plume beyond the regulatory boundary is due to several factors but the most significant one is that once boron enters the groundwater system below the major discharge feature in the area (a large reservoir) it enters a stagnant area with very low hydraulic gradients where it persists for extended periods of time because boron is non-reactive and doesn't decay in the environment. Based on the results from the predictive model, MNA may not be an appropriate remediation strategy for Site B and a more active approach (*i.e.*, groundwater extraction) may be required to meet regulatory goals.

MODEL APPLICATIONS – REDUCTION OF SATURATED CCR MATERIAL

One concern that comes up when looking at closure options for CCR units is saturated CCR material remaining in place after closure and providing a mechanism for COIs to continue to enter the environment. When looking at different closure options, this is one of the critical aspects that must be considered. Flow modeling is a particularly useful tool to evaluate whether saturated CCR material is expected to remain in place for a given closure strategy and if so, are there methods for eliminating or reducing the volume of saturated CCR material.

Flow modeling was conducted for several sites in the southeastern United States to predict the volume of saturated CCR material that would remain in place for a cap-in-place closure option. These models were then used to evaluate potential strategies for reducing the volume of saturated CCR material under this closure method.

The site discussed in this example contains two CCR units that were constructed in two dammed perennial stream valleys in the southeast. The closure option evaluated in these models was one in which the CCR material would be left in place and a low permeability cap would be installed across both units. Prior to developing these predictive closure models, a calibration model was developed that was calibrated to hydraulic head data and flow rate data collected up to the point of model creation. This calibrated model gave a good fit to the observation data and had a NRMSE of 2.4 percent.

This calibrated model was modified to represent the conditions expected at the site after cap-in-place closure was completed. A steady-state predictive model was run to predict the long-term water levels at the site under cap-in-place conditions. These water levels were used to estimate where saturated CCR material would remain and what the volume of saturated CCR material would be (Figure 8). The model predicted that saturated CCR material would remain in an area surrounding the original stream channels within the CCR units. The total volume of saturated CCR material was estimated at 1.6 million cubic yards (~1.2 million cubic meters).

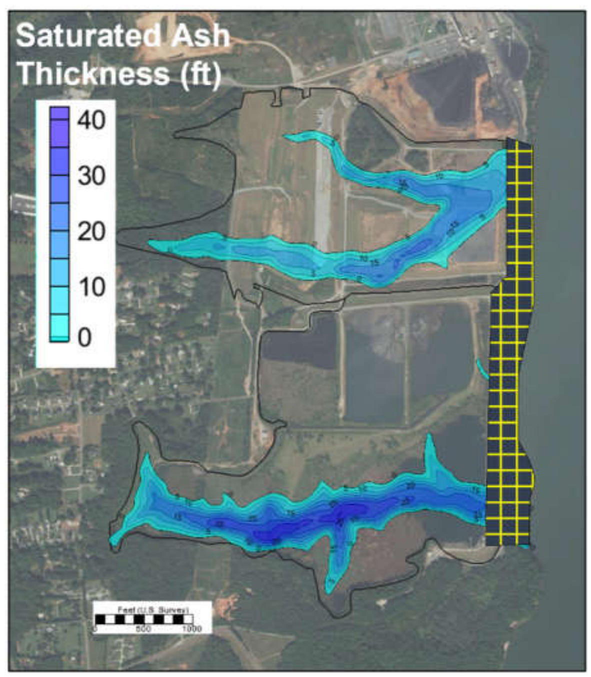

Figure 8. Estimated saturated CCR material within the CCR units under cap-in-place conditions

The second part of this modeling effort was to evaluate potential strategies for reducing the total volume of saturated

CCR material. Several strategies were evaluated, but the three that are discussed here are extraction wells below CCR material in the capped CCR units, extraction wells along the periphery of the CCR units, and a French drain system along the periphery of the CCR units.

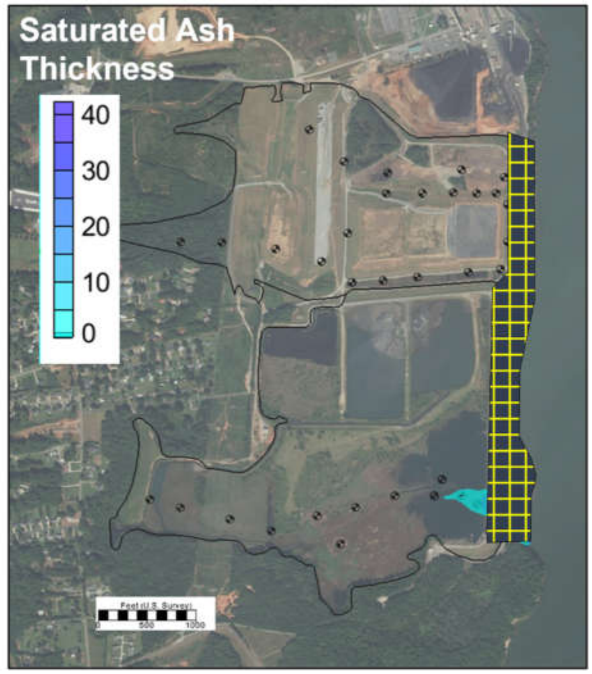

Figure 9. Estimated saturated CCR material with extraction wells below CCR material under cap-in-place conditions

For the extraction wells below CCR material scenario, 34 extraction wells along or near the axis of the original stream channels were simulated. These wells were simulated using the MODFLOW "Drain" package with drain elevations set to approximately the top of bedrock below the CCR units. Drain conductance values for the wells were calculated considering radial flow to a well following the Anderson and Woessner approach.[1] This drain conductance value is equivalent to the resistance to flow into an extraction well. This approach assumes that the head in the wells is maintained at approximately the top of bedrock which can range from several tens of feet to over a hundred feet (ten plus meters to 30-40 plus meters) within the CCR units. The simulations predicted that with this approach the overall saturated CCR material volume could be reduced by over 99 percent and would only leave approximately 10,000 cubic yards (~8,000 cubic meters) of saturated material in place (Figure 9).

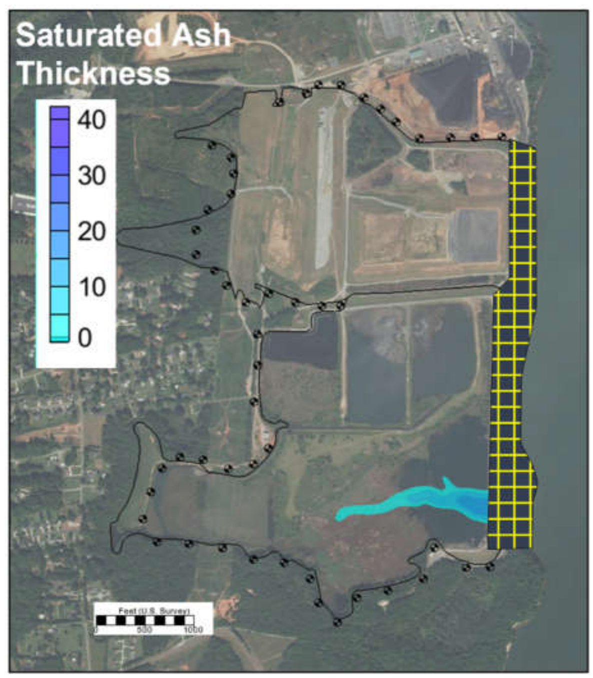

Figure 10. Estimated saturated CCR material with extraction wells around the periphery of CCR units under cap-in-place conditions

The second scenario, extraction wells outside of the CCR units, was simulated with 50 extraction wells located around the periphery of the capped CCR units and installed to bedrock. These wells were modeled using the same drain method as above, and water levels in these wells were also maintained at approximately the top of bedrock. These simulations predicted that this dewatering method would be less effective than wells within the footprint of the CCR units but still could reduce saturated CCR material volumes by up to 96 percent with an estimated 60,000 cubic yards (~46,000 cubic meters) of saturated CCR material (Figure 10).

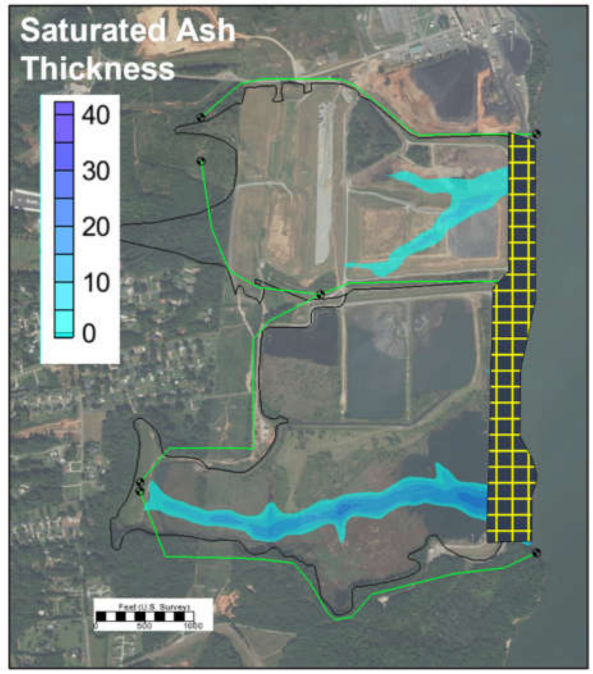

Figure 11. Estimated saturated CCR material with French drains around the periphery of CCR units under cap-in-place conditions

The final example presented here is a system of French drains located along the periphery of the two CCR units. These drains were simulated as linear drain features with drain elevations along the French drains that were based on engineered designs that would allow them to gravity drain to discharge locations along the reservoir to the east. The conductance of these drains was based on the conductance used for modeled streams in the area. This is the only passive system evaluated that would not require active pumping. Simulations predicted that, though less effective than active pumping systems, these French drains could reduce the overall volume of saturated CCR material by almost 80 percent with an estimated saturated CCR material volume of approximately 300,000 cubic yards (~230,000 cubic meters) (Figure 11).

Through groundwater flow modeling it could be demonstrated that dewatering methods could be effective at reducing the volume of saturated CCR material.

MODEL APPLICATIONS – UNDERDRAIN DESIGN

The final example of applications for flow and transport models discussed in this paper is the use of modeling to assist in the design of an underdrain system for a proposed CCR landfill. The landfill is being constructed to dispose CCR material being removed from unlined CCR units. This modeling effort involved modeling a number of scenarios and determining if an underdrain system would be effective at decreasing the time to meet the necessary groundwater separation requirements for landfill construction.

The first part of the modeling effort was to develop a transient calibration model. The transient calibration model used historical and recently collected water-level data from 109 observation wells and piezometers from across the site and was calibrated to groundwater level trends over the past several years. This calibration model accounted for the major site changes that have occurred over that time that may affect local groundwater elevations. During calibration, it was found that the hydraulic parameters that were most important to the calibration and to matching the observed trends were the hydraulic conductivity and specific yield of the shallow aquifer. Calibration resulted in a total NRMSE of 4.5 percent.

After model calibration, predictive simulations were developed that represented conditions prior to and after installation of the proposed landfill underdrain system and the landfill itself. The predictive simulations were run for several years after the proposed landfill construction date to evaluate the long-term performance of the proposed underdrains. These predictive models included a baseline model (without the proposed underdrain) and several iterations of models with various underdrain designs.

The baseline model predicted that without the underdrain system, anticipated site activities alone would result in the necessary separation within approximately 8 months (Figure 12). The primary activities responsible for the predicted groundwater level decrease to below the proposed landfill were the excavation and dewatering of nearby CCR material.

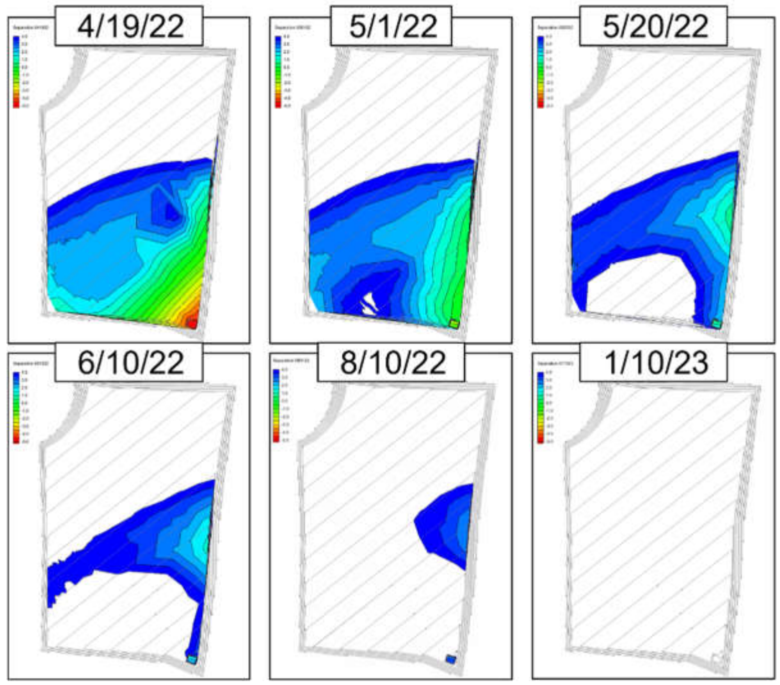

Figure 12. Groundwater separation below proposed landfill without an underdrain (No color represents separation is achieved)

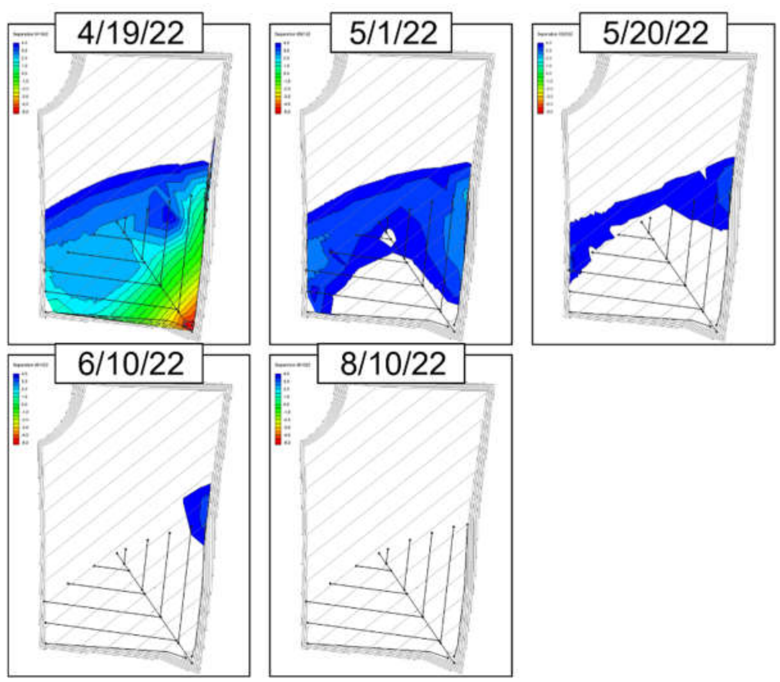

Figure 13. Groundwater separation below proposed landfill with the initial underdrain design (Linear underdrain segments shown as black lines, no color represents separation is achieved)

The second predictive model was a model that had all the same conditions as the baseline model but with the inclusion of the initial proposed underdrain design provided to the modeling team by engineers working on the landfill construction. This design incorporated a number of linear drain features that extended from the southeastern portion of the proposed landfill area (where groundwater was predicted to be the highest compared to the bottom of the landfill) to the north, northwest, and west (Figure 13). Results from the simulation assuming this design predicted that it would be able to achieve the necessary separation in approximately 4 months and could potentially reduce the time to separation by 50 percent (Figure 13).

Time to constructability, which was contingent on groundwater separation, was critical for this project. Therefore, additional simulations were run to determine if modifications to the underdrain design could achieve separation sooner than the initial design. These simulations indicated that with an extension of the two underdrain segments along the eastern side of the landfill, in the area where separation was predicted to be achieved last, the underdrain potentially could reduce the time to separation by an additional 2 months or a 75 percent reduction compared to the baseline case (Figure 14).

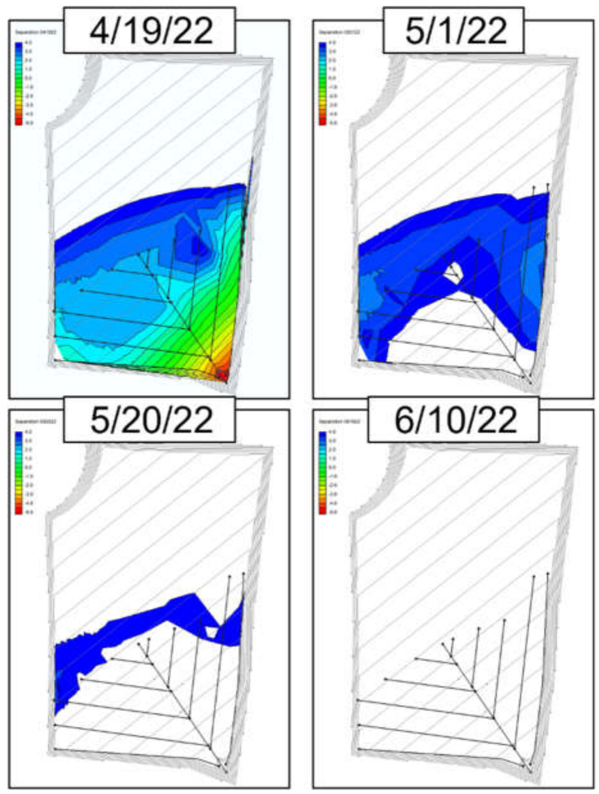

Figure 14. Groundwater separation below proposed landfill with the final underdrain design (Linear underdrain segments shown as black lines, no color represents separation is achieved)

Because of the inherent uncertainty in the future site conditions and construction activities and the estimated model parameters, sensitivity analyses were run to evaluate how changes in the construction timeline and model parameters most likely to affect the performance of the underdrain may affect the predicted times to reach separation (Table 1). The sensitivity analyses indicated that the specific yield (or volume of water in aquifer storage in the shallow aquifer) was the most impactful parameter determining when separation would be achieved. Doubling the specific yield from 10 percent (the calibrated value) to 20 percent resulted in an increased time to separation of approximately 9 months for the baseline model and an increased time to separation of approximately 3 months for the final underdrain design model (Table 1). The analysis also indicated that the conductance of the drain (how much resistance to flow from the aquifer into the underdrain) would have a notable effect on the performance of the underdrain. Reducing the conductance by an order of magnitude resulted in an increase in the time to reach separation of approximately 3 months.

Modeled Scenario	Sensitivity Analysis Parameter	Predicted Date when Vertical Separation Achieved	Modeled Date when NSLF Recharge Ceases	Predicted Time when Drain Operation Ends	Predicted Duration of Drain Operation (months)
Model with No Construction Drain	*Base case*	1/20/2023	N/A	N/A	N/A
	Backfill K = 0.1 ft/d	4/21/2023	N/A	N/A	N/A
	Specific Yield = 0.01	6/1/2022	N/A	N/A	N/A
	Specific Yield = 0.2	10/18/2023	N/A	N/A	N/A
Construction Drain Model	*Base case*	6/10/2022	10/14/2022	May 2025	38
	Conductance = 0.1 ft^2/d	9/1/2022	1/5/2023	Jun 2025	38
	Backfill K = 0.1 ft/d	7/10/2022	11/13/2022	May 2025	38
	Specific Yield = 0.01	4/25/2022	8/29/2022	Feb 2023	10
	Specific Yield = 0.2	9/1/2022	1/5/2023	Aug 2027	65

Table 1. Sensitivity analysis results for the baseline model and final construction drain model

Using modeling, it was possible to demonstrate to stakeholders and regulators that ongoing site activities would result in continuously decreasing water-level trends in the region of the landfill. The models also demonstrated that with an underdrain system the time to reach separation could be drastically reduced and help keep the project on track, which is critical for ongoing closure activities at the site. Furthermore, recent water-level measurements at the site confirm these findings and have shown an increase in the rate of water-level decline with installation of the underdrain and currently look to be on track to reach separation in a timeframe consistent with the model predictions.

MODEL UNCERTAINTY

As noted above, uncertainty is inherent when making predictions about the future and this applies to all predictive tools including flow and transport modeling. When conducting and relying on flow and transport model results, it is critical that one understands and addresses these potential uncertainties. There are several considerations, methods, and tools that can assist when addressing and quantifying uncertainty.

The first key aspect to developing a good flow and transport model is the data being used to construct and calibrate the model. A model cannot make good predictions if the data used to construct and calibrate it is erroneous or nonexistent. Therefore, the first step to developing a good model is to ensure that the data being used is correct and free of error (or the potential error has been minimized to the best of one's ability). There are several processes that can assist in this, but generally good quality assurance and quality check processes should be in place. Secondly, consideration should be given to data outliers. Often a data outlier, such as an anomalous water-level reading, may be due to some form of data collection or processing error or may be the result of site conditions that are anomalous compared to typical site conditions. If outliers are identified, they should be addressed and the cause should be identified (if possible). These data may need to be discarded so that they do not artificially affect model predictions in a way that is not consistent with the general behavior observed at the site.

The second key component to reducing model uncertainty is model calibration. The purpose of model calibration is to improve a model's ability to make predictions. By improving the model's ability to predict known data (as discussed in a previous section), it can make better predictions about things unknown. Good model calibration is key to developing a model that one can have confidence in for making future predictions.

Another key aspect of model uncertainty is the assumptions that are built into a model, and most flow and transport models require that assumptions be made to generate the model. What these assumptions are can vary and can be anything from assumptions about unknown/unmeasured hydraulic parameters to assumptions about future site activities or changes to the hydrogeologic system being modeled. In general, when making assumptions about model parameters (hydraulic conductivity, storage parameters, porosity, etc.), good judgment is key; if site data are not available then surrogate data may be used if it is available from literature or from other similar sites. Assumptions about future site activities or conditions are inherently necessary for predictive modeling. Therefore, it should be recognized that as actual field conditions vary from the assumptions used to construct a predictive model then the predictions become increasingly unreliable and updates to the simulations may be necessary.

Sensitivity analyses are useful tools for addressing some of the uncertainties inherent to flow and transport modeling. In general, sensitivity analyses are conducted by varying various parameters or assumptions in a model and evaluating how those changes affect the model results. These analyses can provide valuable information and help bound the model predictions within reasonable limits. In the example discussed in the previous section, the sensitivity analysis indicated that the specific yield of the shallow aquifer was one of the critical parameters controlling when separation occurred and how long the underdrain operated before going dry. By bounding the specific yield within the reasonable minimum and maximum values for the type of aquifer being modeled (1 percent to 20 percent) the models could provide a reasonable range of dates for both separation and the time for the underdrain to go dry. Another important aspect of sensitivity analyses is they provide a quantitative tool to evaluate which parameters, conditions, model assumptions, etc. are most important to predicting the behavior of a system and which are not. This provides a method for determining which aspects of a system should be focused on during investigative work and which are less critical.

The underlying physics controlling the calculations in flow and transport models are based on the theory of mass/volume balance. Therefore, one key step when determining if a model is "good" is checking the mass balance. If a model has a poor mass balance, then it should be viewed with skepticism and effort should be put into determining the cause of the poor mass balance and correcting it.

A final note on model uncertainty is that all models should pass the colloquial "sniff test." This means that model results should be viewed critically; if they are not reasonable based on professional judgment or based on known information or field conditions, then the model results should be questioned. For example, if a simulation indicates areas of flooding in areas where no flooding is observed or where it would not be anticipated, additional work should go into understanding why that behavior is being predicted and addressing it.

Though there is inherent uncertainty in flow and transport modeling, this uncertainty can be minimized if approached in a thoughtful and rigorous manner.

CONCLUSIONS

The complexity of CCR sites and variability between sites create special challenges when selecting ways to characterize, evaluate, and manage them. Numerical flow and transport modeling provides a powerful tool to address these challenges and can make predictions to assist throughout the life of a project from initial investigation to site closure, remediation, and monitoring. The predictive capabilities of models can provide useful information that can be used for all aspects of a project from environmental concerns to issues encountered during construction activities and engineering designs.

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