Understanding Uncertainty in Groundwater Modeling to Assess Impacts to Groundwater from a CCR Fill

AUTHOR: Shane McDonald, PG, Senior Technical Leader, Hydrogeology and Modeling

Organization: HDR, 1515 Market St., Philadelphia PA 19102

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ABSTRACT:
In the best of all worlds, groundwater models are powerful tools to assess hydraulic and geochemical conditions in the subsurface at CCR storage facilities. Well-formed models can be used to predict the potential for constituents from CCR at the facility to impact subsurface media and be transported by groundwater from one location to another, potentially impacting sensitive receptors, threatening human health and the environment. Once a model is shown to reasonably reproduce measured hydraulic and geochemical conditions through calibration, it can be used to predict the fate and transport of CCR constituents under various conditions, including evaluating proposed corrective measures to mitigate the future movement of the constituents if sensitive receptors are found to be threatened. While the previous statements is a reasonable descriptions of a pragmatic and useful tool, the implementation can often be more complex and what is created becomes a target for technical adversaries to challenge. If the model is not well founded and presented on the best foundation, technical challenges can cause not only the target to fall short, but also cast doubt on other more empirical analyses (by association). Understanding the underpinnings of a well-founded model is critical for defensibility. Technical issues such formulating appropriate geochemical analyses to determine constituent source terms that accurately describe the interactions between recharging water and coal ash, as well as simulating the dynamic hydraulic environment where CCR are frequently stored, are areas where too much generalization can lead to uncertainty. This paper will use case studies to discuss common and inherent uncertainties in groundwater models and methods to mitigate the vulnerability they create.

Introduction

Statistician George E. P. Box – “All models are wrong, some models are useful.”

The CCR Rule has made groundwater assessment a necessary task for power generation facilities who store coal ash. However, data gathering prescribed for the rule-required Detection Monitoring and Assessment Monitoring focus on the CCR facility and do not include gathering information about the larger hydrogeologic system. When Assessment Monitoring leads to Alternative Source Determination and Corrective Measures Assessment, questions can arise that require understanding the whole groundwater system where the facility exists. Groundwater modeling is an effective way...
to put data, analyses, and questions generated by following the CCR Rule into the ‘system’ context. However, when the uncertainty in a groundwater model is not understood or acknowledged, the information generated by the model can lead to misleading conclusions or hidden vulnerabilities.

**The Modeling Process**

When all factors align and ideal circumstances for modeling take place, a groundwater modeling effort will be conducted in iterative phases that build from previous efforts and cycle back through the process developing more and more refined understanding. For example, questions that arise during the fate and transport modeling process may identify the need for additional data that will further refine the flow modeling that took place earlier in the process. As modeling progresses, data gaps are identified and filled and uncertainty is bounded. Under these ideal conditions, the groundwater modeling process for CCR facilities will follow a well-defined pathway, with on-going dialogue between the modelers and those collecting supporting data and evaluating geochemical and hydraulic conditions:

1. **Conceptual Site Model (CSM) Development**
   a. Model Domain - a model domain that wholly encompasses the flow system and hydrodynamic and chemical processes is identified;
   b. Boundary Conditions – water and chemical budgets are developed and constrained by data, sources and sinks within the model (e.g., recharge from precipitation, withdrawal from wells, and discharge to streams) are parameterized, interaction of the model domain with the larger world is described and understood, uncertainty for these processes are characterized;
   c. Hydrostratigraphic Framework – horizontal and vertical distribution and properties of geologic materials within the model domain pertinent to groundwater movement and contaminant fate and transport are identified and parameterized, calibration targets such as groundwater head and stream flows are identified and measured, uncertainty in the parameterization and calibration targets are characterized (note there are methods, such as parameter estimation algorithms, that can stochastically identify the most probable value of specific parameters, but these algorithms require knowledge of a reasonable range of values to start with, which must be understood as part of the CSM);
   d. Temporal Variations in Aquifer Stresses and Source Terms – the timeframes and intensities of boundary conditions, stresses, and sources are sequenced and aligned with the problem, uncertainty in the timing is acknowledged.

2. **Groundwater Flow Modeling**
   a. Model Set Up – the basic model is set up following the CSM, discretization of the model domain is chosen that best describes the system and focuses the model detail to areas of interest, parameters are assigned to the various water sources and sinks as well as to hydrostratigraphic
materials simulated in the model (see the note on parameter estimation above);

b. Calibration – model output is compared to measured conditions to assess how well the model simulates those conditions, parameters are adjusted within data constraints until the optimal reproduction of observed conditions is met (again, this may be accomplished using parameter estimation algorithms), the closeness of fit to the model is given in terms of uncertainty (e.g., root mean squared error);

c. Sensitivity Analyses – modeled parameters are tested by systematic adjustment to see which parameters cause the greatest effects on the model results (again, this can be an automated process using parameter estimation algorithms), the most sensitive parameters are identified and data to constrain the sensitive parameters is sought to assess if the model is biased by uncertainty in the sensitive parameters;

d. Predictive Simulations/Particle Tracking – the model which is shown to reasonably simulate the known conditions is used to predict either historical groundwater movement or the movement of the groundwater when hypothetical stresses are applied to the system. This is useful to show that water arriving at a certain location originated at another specific location or the reverse, water originating at a certain location will arrive at a specific location.

3. Fate and Transport Modeling

a. Model Set Up – the basic fate and transport model is set up following the CSM and using the flow model as the engine for advective transport; sources and sinks as well as geochemical parameters controlling constituent interactions with hydrostratigraphic materials are input into the model;

b. Calibration – model output is compared to measured conditions to assess how well the model simulates those conditions (usually in terms of concentration curves at specific monitoring locations over time), parameters are adjusted within data constraints until the optimal reproduction of observed conditions is met, the closeness of fit to the model is given in terms of uncertainty (e.g., coefficient of determination);

c. Sensitivity Analyses – modeled parameters are tested by systematic adjustment to see which parameters cause the greatest effects on the model results, the most sensitive parameters are identified and data to constrain the sensitive parameters is sought to assess if the model is biased by uncertainty in the sensitive parameters;

d. Predictive Simulations – the model which is shown to reasonably simulate the known conditions is used to predict either historical contaminant fate and transport, the fate and transport of currently identified constituents into the future, or the fate and transport of constituents when hypothetical stresses are applied to the system. Fate and transport modeling can be used to show how conditions came to be as they are and what may happen in the future under a variety of conditions.
When this process is followed effectively a tool is developed that can be used for multiple purposes. The main use of a well calibrated model being to answer the “what if we do this?” types of questions prior to expending resources in the field. While the cost of modeling is likely more than simple empirical data evaluations, the tool developed is always much less costly than actual implementation of measures in the field and done effectively can reduce the cost of those measures resulting in an overall cost savings. However, the ideal circumstances for creating groundwater models rarely occur and, in addition to an accelerated, deadline driven schedule that does not allow for iteration, one or more of the following likely interferes with the ideal modeling process:

1. Conceptual Site Model
   a. Model domain – is prescribed and data within the domain is limited to the immediate focus area, other areas will need to be based on generalizations;
   b. Boundary Conditions – there is little existing boundary condition data, there might be some surface water or groundwater information from the USGS, but usually this is remote from the area of interest or was discontinued due to budgetary concerns in 1992 and your modelling starts in 1994…
   c. Hydrostratigraphic Framework – data on the hydrostratigraphic framework was collected for a different purpose and does not fully characterize the model domain so boring logs lack pertinent detail and pumping tests were too short to estimate the hydraulic parameters needed by the model; chemical analyses of groundwater samples was for different purposes and does not include all the parameters needed for the model;
   d. Temporal Variations in Aquifer Stresses and Source Terms – very little information is available to describe historic conditions so it is hard to extrapolate time-variable conditions beyond the present.

2. Groundwater Flow Model
   a. Development – is initially done quickly from literature-based assumptions and generalizations, the uncertainty of the assumptions could be large, but is unquantified;
   b. Calibration – modeling results are compared to groundwater levels from the site only (this may be a limited data set due to multiple studies, each with a separate location survey), no stream flow measurements are available near the site, so groundwater discharge is unconstrained, there may be a pumping test done by a driller to estimate the yield of a well, but was of limited duration and does not have observation well data, so comparison to known aquifer stresses is hard to accomplish.
   c. Sensitivity Analyses – while it might be a great idea to determine which parameters are sensitive and whether those parameters are causing bias or can be constrained more tightly, there is little time in the accelerated schedule to accomplish this, so sensitivity analyses are done in arrears once the predictive model is completed (and the report in the hands of the regulator). Sensitivity analyses might be used as a tool to bound potential outcomes of predictive scenarios.
d. Predictive Simulations/Particle Tracking – Even though there is high uncertainty in the model, it may still be informative to conduct predictive simulations but uncertainty will be high. Running analyses at high and low parameter values might bound the predictive simulations to within “reasonable” outcomes, but sometimes this is a wide range with significantly different implications at the upper and lower bounds.

3. Fate and Transport

a. There may be little data to support anything other than advective transport modeling; it is unlikely the parameters like organic carbon content of the aquifer material have been measured and site specific organic partitioning coefficient values for constituents to be modeled are not knowable. The concentrations of constituents measured for the CCR determination and assessment monitoring are from immediately adjacent to a 40-year-old CCR storage facility, meaning the plume has long been stable in this area and the variation seen in the data is due to seasonal variability and cannot be used to quantify constituent arrival for calibration.

b. As with groundwater flow modeling, predictive modeling will still be done without true understanding of the underlying uncertainty, sensitivity analyses may be used to determine outcomes at high and low parameter values.

One common misconception that routinely arises when initiating modeling is that due to the existence of prior studies and/or monitoring data new data is not needed to provide defensible predictive data. The data from prior studies were typically collected for specific purposes, e.g., regulatory requirements, and may not establish an appropriate CSM or provide data of sufficient quality to develop defensible model output. However, it is usually expected before the modeling process starts that the available data is sufficient to perform modeling and provide defensible predictive results and that neither additional time nor budget is required to collect data. While to the modeler this is not ideal, it is hard to justify additional studies to a program manager who has already spent a significant amount of money on groundwater studies and is under a deadline and living within a restrictive budget. But the impact of using insufficient data and/or data of poor quality can be significant to the remedial decision making and/or regulatory compliance process.

**Uncertainty in the underlying data**

Heraclitus, a Greek philosopher born in 544 B.C. said, “*No man ever steps in the same river twice, for it’s not the same river and he’s not the same man.*”

While this discussion is about uncertainty in groundwater models, the source of much of the uncertainty is the data used to construct the model. How well we understand the underlying data is fundamental to characterizing the model’s uncertainty. We are making “statistical” generalizations of reality. Because we must generalize, knowing the breadth and depth of the conditions is important and having sufficient data is the key to that understanding. There needs to be enough data on each pertinent parameter to determine means, standard deviations, and confidence intervals. This need is best exemplified by steady state calibration of the flow model to groundwater elevations.
(typically the first standard of groundwater model calibration). Many models are calibrated to a water levels measured on a specific date, which begs the question “did that day represent the most common conditions?” The steady state model is intended to represent the central tendency of the flow system, so rather than calibration to a specific day, models should be calibrated to geometric mean water levels measured across the known conditions. Enough water levels need to be measured over wide-ranging conditions to determine the central tendency. Knowing this range gives the truest measure of computed to observed (i.e., within x standard deviations). Figure 1 shows the range of water levels used in a model calibration for individual wells. These measurements were taken when the wells were sampled for the CCR program. They show that there is a range of conditions when measured. Note from the median that MW-11 is the up-gradient well, but at times other wells have had water levels near the maximum in MW-11. What would be the conclusion if the model was created from a day when one of the other wells was higher? The model needs to at least simulate water levels that fall into the range, and the closer it is to the geometric mean the better! The model calibration is based on how well the model reproduces the observed data, so how well do you know the data?

Figure 1 - Box and whisker plots of water levels in CCR monitoring wells

Three main areas where understanding of groundwater movement is limited by the quality and quantity of data are Subsurface Conditions, Surface Water Interactions, and Groundwater Uses. While this is not an exhaustive list, these three areas have fundamental impacts on the modeling.

Subsurface Conditions - The distribution of materials in the subsurface is generally characterized by borings done at wide spacing and relies on us to interpret what occurs between the borings. The presence zones where faster groundwater movement occurs may or may not be distributed at scales that would be identified by the borings. For example, lenses of gravel left in the channel of a meandering stream can create sinuous
conduits through floodplain deposits that are hard to identify or connect between the rare borings that penetrate them. There are multiple camps in the hydrogeologic community that advocate methods to address these “hard-to-know” conditions. One relies on geostatistical analyses which estimates the probability of transitioning from one type of material to another based on the sequence of materials observed in borings. This is done in software called Transition Probability Geostatistical Software, or T-PROGS. Figure 2 is an example of the output of a T-PROG analysis of a coastal plain aquifer, clear (or black) spaces represent low-permeability clays and silts while colored masses indicate transmissive sands and gravels with red being the most conductive. Other hydrogeologists feel that leaving the interpretation to a statistical algorithm does not maximize our understanding of how the material got there in the first place. However, mapping fine-detailed stratigraphy based on sedimentology principles can be time consuming and potentially costly (but the outcome may best represent what is actually there).

![Figure 2 – T-PROG output showing probable flow paths in the subsurface of a coastal plain deposit.](image)

One important factor for both of these schools that can be determined in the field is a sense of spatial variability. This is accomplished with co-located borings. If borings adjacent to each other have similar stratigraphic sequences, the variability in the subsurface occurs at a larger scale that can be generalized. If they are significantly different, then the scale is smaller and details become more important. Ultimately these conditions need to be discretized and represented in a model; they must be generalized to be simulated.

The subsurface heterogeneity affects more than just flow path and hydraulic conductivity. This variability also impacts dispersion and constituent interaction with the matrix material, important factors in constituent fate and transport. Additional levels of complexity are added when groundwater flow and constituent fate and transport occur in either fractured rock or karst environments.

**Surface Water Interactions** - Most CCR facilities were constructed near surface water such as lakes and rivers. Also, groundwater, in general, flows from recharge areas
toward discharge at surface water bodies. In some cases, streams and lakes lose water to the subsurface, creating groundwater recharge. In places where flooding occurs, sometimes flow can be to the stream and sometimes to the aquifer depending on the height of the streams stage. Understanding how well the groundwater model reproduces the surface water-groundwater interaction can give a strong sense of the overall performance of the model (water in must equal water out). However, stream flows (particularly dry period stream flows) are almost never measured as part of groundwater studies. The solution to this is to design and implement stream flow monitoring that captures low-flow periods and can be used in model calibration!

Groundwater Users – One of the main underlying purposes of a groundwater model is to understand if water supplies that are being used are at risk of being impacted by constituents from the CCR storage facility. However, uses of groundwater inherently impact the groundwater system proportional to the amount of water withdrawn and must be considered as part of the stresses simulated by the model. Where uncertainty enters into the modeling is when the amount of water withdrawn by a large user is not known. This is often true with irrigation wells. CCR facilities in rural areas often neighbor crop lands that are irrigated by groundwater. Determining how much water is used on any given field in any given year is not a straightforward task (when did irrigation start? how much water is withdrawn on average during a season? is any of the water returned to the subsurface?). There are methods for estimating the quantity of water necessary to irrigate a certain crop type in a given climate (evapotranspiration setting), but these are not direct measures of actual water withdrawal and rely on some assumptions that are not easily bounded. Another approach is to simulate the wells operating at some portion of their tested and reported yield for an assumed growing season (they are often easily identified). Again this uses assumptions that are not bounded. Often, the only option is to simulate worst-case scenarios where the wells pump at their capacity for the duration of the growing season. A complicating factor is that over the lifetime of a CCR storage facility, the number and location of water supply wells (irrigation or other users) can change and the records are not always available to show how they changed. Historic aquifer stress that went out of service can be unknowable sources of uncertainty.

A second source of potential uncertainty from irrigation is that it can affect the chemistry of the groundwater. There are several processes that can cause water that is recharged in irrigated areas to have new chemistries that will change geochemical conditions in the groundwater. These processes include evaporation concentrating minerals in the water and leaching of minerals from soils that did not previously receive the amount of water or water chemistry now being applied. Again, data on these effects may be difficult to come by and the impact on the modeling may require more research than is afforded by the schedule and budget. If irrigation is prevalent in the area being modeled, these are factors that should be quantified if possible.

Uncertainty in the model itself

14th Century friar William of Ockham – “That which is done with fewer is done in vain with more.”
Flow modeling and fate and transport modeling are essentially series of equations that are solved by iterative solutions. Limitations on the model occur on many levels and must be acknowledged when relating the model results to the real world. Most of these, as discussed above, come in the form of generalization. With more and more computing power and new approach to discretization (e.g., MODFLOW Unstructured Grid or FeFlow finite element approach) higher resolution models are possible while maintaining a system-wide model domain. However, given the uncertainty in the data discussed above, often the level of detail may not be supported by the data. A long-standing adage for modeling has always been “work from the simple toward the complex”. As details are added always recheck the ability to reproduce observed conditions. Keeping an understanding of the sources of uncertainty and recalling it when the results are interpreted is imperative to making the “wrong” model useful.

There are a couple of common errors that occur during model development that can have large ramifications on the outcome of the model (again not an exhaustive list). These include choosing an appropriate model domain and knowing where to end the model and interpret the outcome.

Choosing the wrong model domain can have several impacts on the outcome of the model. Choose too small a domain and important potential receptors may be outside the domain, boundary conditions may affect simulations and water budgets may be hard to justify. Choose too large a model domain and you may increase data needs for the model (will increase areas that are generalized) and you can add computational baggage slowing model runs. To the extent possible, choosing model domains that are natural (e.g., watersheds that correspond to recharge areas) is the best option. Doing so must assure that questions about potential receptors can be answered.

Determining the point of compliance can be a source of discussion among various involved parties and if chosen poorly can result in uncertainty in the model outcome. Understanding how geochemical processes may be affected by interactions at the boundary (i.e., surface water) may take on modeling efforts of its own and can have a whole new set of uncertainties. Sediment and surface water interface, ecologically speaking, is where the rubber and the road. If the model ends at the end of the aquifer before groundwater enters the sediment bed, then how do you assess if benthic organisms are at risk for transported constituents? A related issue on the point of compliance is: if your facility is on one side of a major (Ohio, Missouri, Mississippi-sized) river, can a supply well across the river (outside your domain) really draw impacted water under the river? How would you know or be able to demonstrate that is or is not the case?

Conclusions and discussion points

Several factors around groundwater modeling cause uncertainty and present challenges. These include uncertainty inherent in the foundational data used to create the model and in the model development process itself. Understanding the sources of the uncertainty and how it affects the modeling results is necessary to put model results into context and make the model useful to the decision making process.

Both flow models and fate and transport models require constraining data to be defensible. It is important to understand the variability in the constraining data to assure
the model is creating the best representation of reality. Generalizations are a necessary part of modeling and the outcomes need to be considered in the frame of the generalization. Although data is king, the model is usually based on studies that were done prior to modeling for different purposes. Acknowledging data gaps and blind spots can only strengthen the model (as opposed to ignoring the same).

Ultimately the modeling will be used in technical discussions with regulators, to evaluate corrective action, and if all else fails, to support litigation, so it needs to be well-founded and the uncertainty understood before it is put out as a target. Both mechanistic and probabilistic approaches can be used to gain information about the system being evaluated and the underlying uncertainty, so perhaps the best way to deal with uncertainty is to put it at the front of the planning and discussion to assure it is considered throughout the modeling process.