

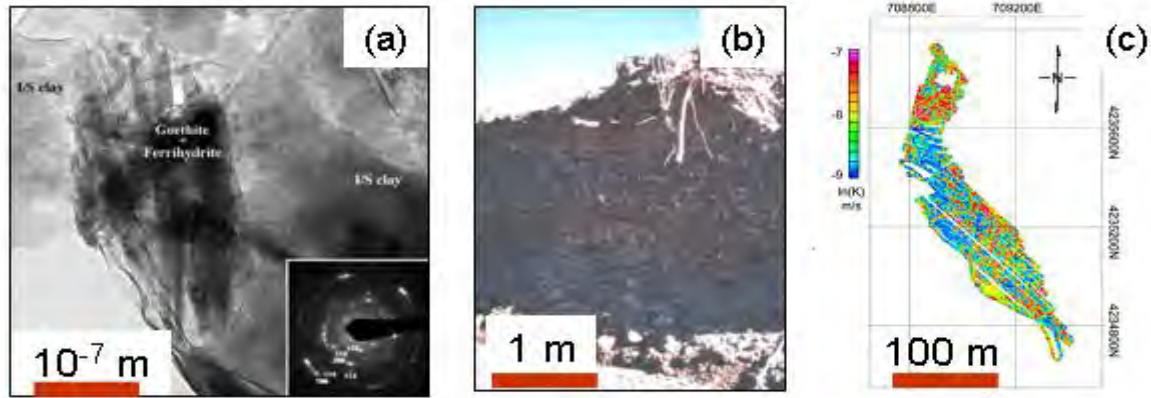
**US Department of Energy, Office of Science**  
**Office of Biological and Environmental Research (BER)**  
**Subsurface Biogeochemical Research (SBR) FY11 Third Quarter**  
**Performance Measure**

This SBR Long Term Measure for 2011 under the Performance Assessment Rating Tool (PART) measure is to “Refine subsurface transport models by developing computational methods to link important processes impacting contaminant transport at smaller scales to the field scale.” The third quarter measure is to “*Provide a report on Computational Methods to Better Understand Parameter Sensitivity and Prediction Uncertainty of Field Scale Reactive Transport Simulations.*” This milestone includes applications to research being performed at the Rifle Integrated Field Research Challenge (IFRC) site, located near Rifle CO and the Naturita Uranium Mill Tailings Remediation Action (UMTRA) program site located near Naturita, CO. The investigations related to both sites consider sensitivity and uncertainty of simulations of complex reactive phenomena observed in field experiments of bioremediation and natural attenuation processes. A major challenge in making these assessments is including site-specific physical and biogeochemical variability into the reactive transport simulations. However, it is infeasible to fully characterize this variability and therefore subsurface reactive environments are open to multiple interpretations. The focus of this project is to embrace these multiple interpretations and incorporate them into the sensitivity and uncertainty modeling framework. Within this framework we seek to understand and reduce prediction uncertainty and to evaluate which new data should be collected to maximize the reduction in prediction uncertainty.

## **1. Introduction**

Over the next 20 years, the U.S. Department of Energy (DOE) is scheduled to make critical waste management decisions on the fate of large contaminant inventories of radionuclides, heavy metals and organic contaminants that reside in complex subsurface environments. A necessary condition for the scientific defensibility of these decisions is an understanding of the processes and properties controlling contaminant behavior. A specific goal of the Subsurface Biogeochemical Research (SBR) program is to “provide sufficient scientific understanding to allow a significant fraction of DOE sites to incorporate coupled biological, chemical, and physical processes into decision making for environmental remediation.” Numerical simulation provides an important framework and organizing principle for achieving this goal through systematic identification, evaluation, and integration of hydrologic and biogeochemical conceptual process models into a quantitative description of subsurface behaviors. The ultimate goal for the development of these modeling analyses, however, is to assess risk and remediation performance for waste management decision-making. This will require an additional and commensurate effort to characterize and quantify uncertainty in the model predictions and assessments. To that end, an important and currently unmet need is to account for the uncertainty due to the inherent complexity of the subsurface and our limited ability to observe processes *in situ*.

The inherent complexity of the subsurface can be attributed to both physical and geochemical heterogeneity of groundwater aquifers. Figure 1 illustrates that sediment at the Naturita site has complex surface coatings consisting of clays and various iron oxides. Each of these minerals can interact with uranium with varying affinity. Similarly, the aquifer sediment has significant physical heterogeneity as illustrated in Figure 1b and 1c. Overall, heterogeneity is readily apparent at spatial scales covering nine orders of magnitude. It is not possible to accurately and thoroughly characterize the importance of this



**Figure 1. Multiscale heterogeneity observed at the Naturita site showing (a) TEM images of surface coatings from aquifer sediment (Davis et al., 2006), (b) aquifer sediments consisting of a heterogeneous mixture of silt, sand, gravel and cobbles (Davis and Curtis, 2003), and (c) the vertically averaged hydraulic conductivity estimated from a site-wide geophysical survey (Brosten et al, 2010).**

heterogeneity at typical field sites. This heterogeneity leads to inherent uncertainty in the description of geochemical and hydrogeological processes in even the most advanced numerical simulators.

A primary objective of this project is to develop integrated computational and statistical approaches to assess multi-scale predictive uncertainty in coupled reactive transport models. To achieve the objective entails the following:

- (1) Identifying sources of uncertainty, including parametric and model uncertainties,
- (2) Characterizing the uncertainty sources and quantifying their propagation through coupled reactive transport models, and
- (3) Assessing predictive uncertainty with consideration of all uncertainty sources.

The Bayesian model averaging method being used in this project to quantify the joint effect of parameter and model uncertainties is described in Section 2. Estimation of uranium reactive transport predictive uncertainties using this method are discussed in Section 3 for models based on column data and in Section 5 for modeling of a tracer experiment at the Naturita site. The potential impact of model conceptualization on the identification and characterization of parametric uncertainties is described in Section 4 for a model based on data from the Rifle Site.

A second key objective of this project is to evaluate which new data should be collected with the aim of reducing model uncertainty. Typically several alternative hypotheses can be proposed to explain deviations between observations and model predictions. Rather than rely on an adhoc analysis or intuition to decide on what new data to collect, numerical simulations can be conducted to quantitatively assess the value of new data for reducing model uncertainty. The use of sensitivity analysis to identify data deficiencies in modeling at the Rifle site is discussed in Section 4. A more formal methodology akin to the groundwater flow modeling of Tiedeman et al. (2003) is described in Section 6. This approach is being evaluated for use in reducing prediction uncertainty in complex reactive transport simulation.

## 2. Bayesian Model Averaging (BMA) Method for Uncertainty Quantification

The method of uncertainty quantification used in this study is the Bayesian model averaging (BMA) method that jointly addresses uncertainties in model structure (conceptual and mathematical), model parameters, and samples of the quantity of interest (Draper 1995; Hoeting et al., 1999). In comparison with other methods of uncertainty quantification used in subsurface environmental modeling, BMA is unique in that it explicitly addresses model uncertainty. Subsurface environmental modeling is commonly based on a single model. Yet subsurface environments are open and complex, rendering them prone to multiple interpretations and mathematical descriptions. This is true regardless of the quantity and quality of available data. Bredehoeft (2003) pointed out that “more often than not, data will fit more than one conceptual model.” Beven (2002) argued that “there may be no way of uniquely defining model structures or parameter sets for a particular application, even when significant quantities of data are available for model ‘calibration’.” Model uncertainty arises when multiple models are acceptable based on available data and information. In subsurface modeling, ignoring model uncertainty and focusing exclusively on optimizing parameters of a single model often leads to overconfidence in the predictive capability of the model, which may not be justified by available data. As pointed out by Neuman (2003), predictions based on a single hydrologic conceptual model are prone to statistical bias and underestimation of uncertainty.

Uncertainty quantification using BMA starts from postulating a set of alternative models,  $M_k$  ( $k = 1, 2, \dots, K$ ), that characterizes model uncertainty. For an individual model, predictive uncertainty of a quantity of interest,  $\Delta$ , (e.g., uranium concentration) is conditional on the particular model chosen and a discrete set of available data,  $\mathbf{D}$ , and is quantified using the posterior probability,  $p(\Delta|\mathbf{D}, M_k)$ . By including model uncertainty, the predictive uncertainty of  $\Delta$  can be estimated as the *joint* posterior distribution

$$p(\Delta|\mathbf{D}) = \sum_{k=1}^K p(\Delta|\mathbf{D}, M_k) p(M_k|\mathbf{D}), \quad (1)$$

which is the average of the probabilities,  $p(\Delta|\mathbf{D}, M_k)$ , weighted by the model posterior probabilities  $p(M_k|\mathbf{D})$ . Evaluating these weights is the most critical step in BMA. This can be done numerically using Bayes’ theorem, but is often computationally expensive. To reduce the computational cost of evaluating model probabilities, Neuman (2003) and Ye et al. (2004) estimated  $p(M_k|\mathbf{D})$  using the Laplace approximation based on the maximum likelihood theory,

$$p(M_k|\mathbf{D}) \approx \frac{\exp(-KIC_k/2) p(M_k)}{\sum_{l=1}^K \exp(-KIC_l/2) p(M_l)} \quad (2)$$

where  $p(M_k)$  is the prior probability of  $M_k$ , which represents the plausibility of the model before collecting data  $\mathbf{D}$ , and  $KIC_k$  is a function of model fit, model complexity, and the information content of the data. Implementing BMA using Equation (2) based on Maximum Likelihood (ML) theory is referred to as MLBMA.

It is common to use the mean and variance to represent a predicted value and its uncertainty, as these are easier to understand and interpret (although less informative) than  $p(\Delta|\mathbf{D})$  in equation (1). For a single

model  $M_k$ , the mean and variance of  $\Delta$  are denoted as  $E(\Delta|\mathbf{D}, M_k)$  and  $Var(\Delta|\mathbf{D}, M_k)$ , with the variance arising from parametric uncertainty. In BMA, the mean and variance of  $\Delta$  include the impact of parametric and model uncertainties and are given by

$$E(\Delta|\mathbf{D}) = \sum_{k=1}^K E(\Delta|\mathbf{D}, M_k) p(M_k|\mathbf{D}), \quad (3)$$

$$Var(\Delta|\mathbf{D}) = \sum_{k=1}^K Var(\Delta|\mathbf{D}, M_k) p(M_k|\mathbf{D}) + \sum_{k=1}^K [E(\Delta|\mathbf{D}, M_k) - E(\Delta|\mathbf{D})]^2 p(M_k|\mathbf{D}). \quad (4)$$

Equation (3) suggests that considering multiple models may yield less biased model predictions than using individual models. It has been proved mathematically in Neuman et al. (2011) that predictive uncertainty considering model uncertainty (Eq. 4) is greater than the predictive uncertainty of individual models measured by  $Var(\Delta|\mathbf{D}, M_k)$ . Equation (4) thus suggests that BMA is able to resolve the problem of underestimating predictive uncertainty when a single model is used.

This project is the first case of applying BMA to groundwater reactive transport modeling, which is significantly more challenging than previous applications of BMA to groundwater flow and transport modeling. As an extension of our previous work (Ye et al., 2004, 2005, 2008), we first developed a general procedure of using BMA to quantify predictive uncertainty in reactive transport modeling. This procedure was implemented numerically to quantify predictive uncertainty of uranium transport in the column experiments of Kohler et al. (1996). Using cross-validation methods, it was demonstrated that model uncertainty dominates parametric uncertainty and that BMA improves the predictive performance of these reactive transport models. The developed procedure is being extended to the field scale using data from the Rifle IFRC and the Naturita UMTRA sites. We also evaluated the importance of reactive transport model nonlinearities in estimating predictive uncertainties and found that global optimization methods may be required to find optimal parameter estimates and that linear and Gaussian approximations may underestimate parameter uncertainties. These and other issues are discussed in further detail below.

### **3. Column Experiments and Surface Complexation Models for Studying Uranium Reactive Transport**

To study reactive transport of uranium, U(VI), in the subsurface environment, Kohler et al. (1996) conducted a series of seven column experiments using well characterized columns containing reagent-grade quartz powder as the surface on which uranium is absorbed. In each experiment, uranium-contaminated groundwater was injected at one end of the column, and uranium concentrations were recorded at the other end. Plots of the breakthrough curves (here measured by the number of pore volumes, PV) are shown in Figure 2. The breakthrough curve is the most commonly used prediction target when simulating uranium transport in the subsurface environment. Although the experimental setup is significantly simpler than field conditions, there is a significant amount of parametric and model uncertainty when simulating the breakthrough curves. The data of Kohler et al. (1996) was thus used to develop a general procedure for using BMA to quantify predictive uncertainty in reactive transport modeling. The model execution time required to simulate the experiments was sufficiently short to allow us to develop advanced algorithms for uncertainty quantification.

Seven alternative surface complexation models (SCMs) listed in Table 1 were used in Kohler et al. (1996) to simulate the column experiments. The simplest SCM (C1) contains only one functional group ( $S_1OH$ ), on which mobile uranyl ( $UO_2^{2+}$ ) absorbs to form the immobile surface complexation  $S_1OUO_2OH$ . A more complicated model (C2) can be formulated with two functional groups,  $S_1OH$  and  $S_2OH$ , and two reactions. Adding one more reaction to C2 leads to a more complicated model C4. Similarly, one may

add one more functional group,  $S_3OH$ , and one more reaction to C4 to form model C5.

Uncertainty in this case is caused by the unknown number of functional groups on the carefully cleaned quartz surface. A total of seven models were developed in Kohler et al. (1996) using up to three functional groups ( $S_jOH$ ,  $j=1,2,3$ ) of different binding affinity and surface site density. The alternative conceptual models have different reaction stoichiometries and different numbers of reactive site types.

For each model, parameter uncertainty arises from the unknown values of surface complexation formation constant ( $K_j$ ) and surface site density  $f_i$ . Adding one more reaction to C2 leads to a more complicated model C4. Similarly, one may add one more functional group,  $S_3OH$ , and one more reaction to C4 to form model C5.

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### Quantification of Parametric and Model Uncertainty Using BMA

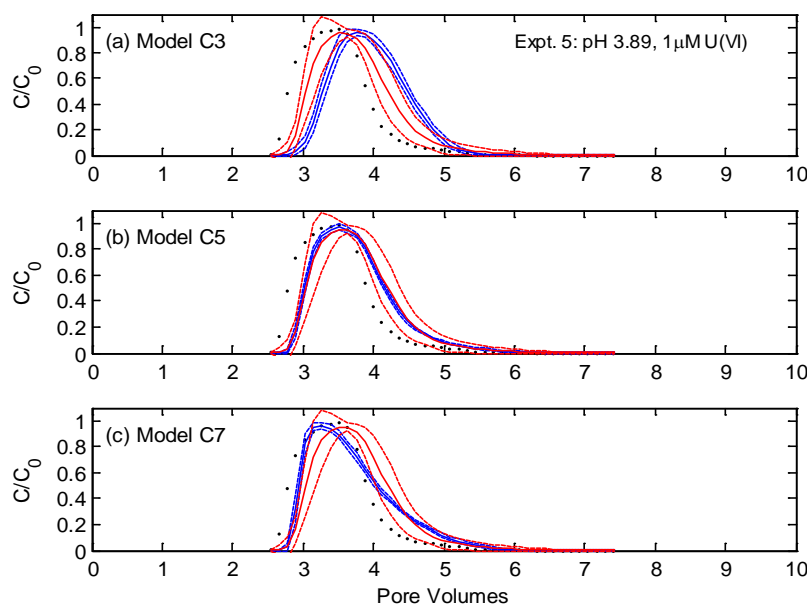
Following Ye et al. (2004, 2005, 2008), MLBMA was used to jointly assess parametric and model uncertainty in uranium reactive transport modeling. The seven SCMs were first calibrated using data from three of the seven column experiments. The calibrated models were subsequently used to predict the remaining four experiments. This cross-validation procedure enabled us to evaluate predictive performance of the individual models and of MLBMA. For the individual models, parameter uncertainty

Table 1. Alternative surface complexation models postulated to describe uranium adsorption on quartz.

Model	Reactions
C1	$S_1OH + UO_2^{+2} + H_2O = S_1OUO_2OH + 2H^+$
C2	$S_1OH + UO_2^{+2} + H_2O = S_1OUO_2OH + 2H^+$ $S_2OH + UO_2^{+2} + H_2O = S_2OUO_2OH + 2H^+$
C3	$S_1OH + UO_2^{+2} + H_2O = S_1OUO_2OH + 2H^+$ $S_2OH + UO_2^{+2} = S_2OUO_2^+ + H^+$
C4	$S_1OH + UO_2^{+2} + H_2O = S_1OUO_2OH + 2H^+$ $S_2OH + UO_2^{+2} + H_2O = S_2OUO_2OH + 2H^+$ $S_2OH + UO_2^{+2} = S_2OUO_2^+ + H^+$
C5	$S_1OH + UO_2^{+2} + H_2O = S_1OUO_2OH + 2H^+$ $S_2OH + UO_2^{+2} + H_2O = S_2OUO_2OH + 2H^+$ $S_2OH + UO_2^{+2} = S_2OUO_2^+ + H^+$ $S_3OH + UO_2^{+2} + H_2O = S_3OUO_2OH + 2H^+$
C6	$S_1OH + UO_2^{+2} + H_2O = S_1OUO_2OH + 2H^+$ $S_2OH + UO_2^{+2} + H_2O = S_2OUO_2OH + 2H^+$

	$S_2OH + UO_2^{+2} = S_2OUO_2^+ + H^+$ $S_3OH + UO_2^{+2} = S_3OUO_2^+ + H^+$
C7	$S_1OH + UO_2^{+2} + H_2O = S_1OUO_2OH + 2H^+$ $S_2OH + UO_2^{+2} + H_2O = S_2OUO_2OH + 2H^+$ $S_3OH + UO_2^{+2} + H_2O = S_3OUO_2OH + 2H^+$

was evaluated for the surface complexation formation constant and surface site density. Model uncertainty was evaluated for the seven models using MLBMA based on equations (3) and (4). Figure 2 plots the observed breakthrough curve of Experiment 5 (not used in the model calibration), mean and 95% confidence interval of the three individual models (C3, C5, and C7), and mean and 95% confidence intervals based on the model averaging. Figure 2 shows that the confidence interval of MLBMA is larger than that of individual models, indicating that model uncertainty is significantly larger than parametric uncertainty. In other words, without considering model uncertainty, predictive uncertainty would be underestimated, which may lead to inappropriate decision-making in environmental remediation and protection.



**Figure 2. Comparison of model predictions of single models (C3, C5, and C7) and model averaging for experiment 5. The black symbols in each figure represent the observed breakthrough curve. Blue lines in each figure represent the mean prediction (solid) and associated 95% confidence intervals (dashed) of each model. Red lines in each figure represent the mean prediction (solid) and associated 95% confidence intervals (dashed) of model averaging.**

Predictive performance of the individual modes and MLBMA is quantified using two statistical measures, predictive logscore and predictive coverage. The former is a measure of the information lost upon eliminating some data (e.g., data of Experiment 5) from model calibration and prediction. The latter is the percent of the cross-validation data falling within the 95% prediction interval. A smaller logscore and larger predictive coverage indicate a better predictive performance. These two measures of model performance evaluated for Experiment 5 are summarized in Table 2 for the individual models and MLBMA. The table indicates that MLBMA predictions are superior to those of the individual models.

## Special Challenges in Uncertainty Quantification for Reactive Transport Modeling

Since reactive transport models are highly nonlinear, there are several special challenges in quantifying their predictive uncertainty. One challenge is in finding optimal model parameters corresponding to the closest match between model simulations and corresponding observations. While local optimization methods are the most popular in current reactive transport modeling, we found that global optimization methods are indispensable to find the optimal model parameters. Another challenge lies in characterizing

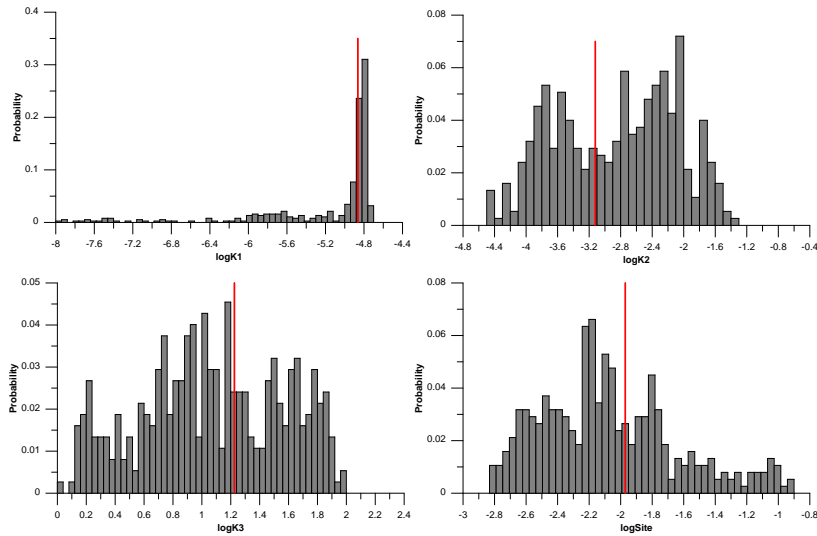
Table 2. Predictive logscore and predictive coverage of single models (C1 – C7) and MLBMA for simulations of experiment 5. Smaller predictive logscore and larger predictive coverage indicate better predictive performance.

	C1	C2	C3	C4	C5	C6	C7	MLBMA
<i>Predictive logscore</i>	2825	76	194	103	172	174	104	31
<i>Predictive coverage</i>	27	46	37	32	39	29	37	68

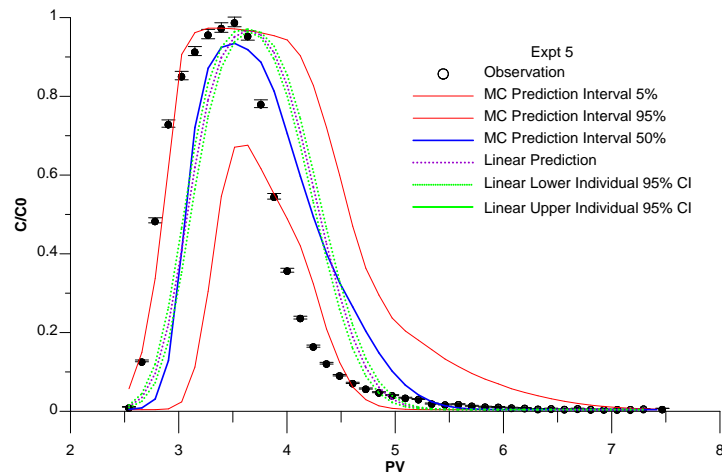
parameter uncertainty. In conventional methods used in subsurface environmental modeling, it is typically assumed that model parameters follow a normal (or lognormal) distribution with a single mode. This assumption is valid for linear models, but not for the highly nonlinear reactive transport models. By running 120,000 realizations in a brutal-force Monte Carlo (MC) simulation, parameter distributions were found to be non-Gaussian with multiple modes, as shown in Figure 3. If the Gaussian distribution is assumed in this situation, the estimated predictive uncertainty will be smaller, as demonstrated in Figure 4. This may lead to incorrect decision-making for subsurface environmental remediation and protection.

Three algorithms were evaluated to investigate which is the most computationally efficient in characterizing the multimodal parameter distributions. They were the Delayed Rejection Adaptive Metropolis algorithm (DRAM) (Haario et al., 2006), Differential Evolution Adaptive Metropolis algorithm (DREAM) (Vrugt et al., 2007, Vrugt et al., 2009) and Shuffled Complex Evolution Metropolis algorithm (SCEM-UA) (Vrugt et al. 2003). DREAM was found to be most computationally efficient, as 20,000 DREAM simulations yielded similar parameter distributions obtained using 120,000 naïve MCMC simulations. With 20,000 realizations, DRAM was not able to locate the multiple modes and SCEM-UA could not find the same modes of the naïve MC simulations.

Given the findings described above for model C4, it is considered necessary to extend the methods of



**Figure 3. Histograms of four model parameters of model C4 obtained from 120,000 naïve MC simulations. The parameter distributions are non-Gaussian with multiple modes. Red lines indicate globally optimal model parameters.**



**Figure 4. Prediction intervals for Experiment 5 obtained from MC (red) without the assumption of Gaussian parameter distribution and linear approximation (green) with the Gaussian assumption. The prediction interval (a measure of predictive uncertainty) is smaller when the Gaussian assumption is used and the multiple modes are ignored.**

global optimization and quantifying parametric uncertainty to the other six models. This will provide more accurate estimation of parametric uncertainty. It is also critical to extend it to the model averaging analysis for better evaluation of model uncertainty. This is ongoing work.

The detailed modeling studies of the highly idealized quartz-packed columns reveal significant ambiguity in the development and description of surface complexation models to describe uranium adsorption. The cause of this conceptual uncertainty most likely results from the incomplete knowledge of the quartz surface which may be heterogeneous as well as the lack of a detailed understanding of the distribution of bonding mechanisms at the surface. In groundwater aquifers, however, many other factors can contribute to the uncertainty of the reactive transport processes as described below.



## 4. Conceptual Models for Reactive Transport of Uranium in Aquifers

A conceptual model for reactive transport in groundwater describes a scientific understanding of the interacting processes and properties controlling movement and transformation of system components, including contaminants, for a specific aquifer system (Tsang, 1991; Davis et al., 2004b; Steefel et al., 2005). A conceptual model consists of three main parts: the hydrogeochemical structure, which describes the distribution of physical and biogeochemical properties that characterize the site (e.g., hydraulic conductivity, anisotropy, porosity, dispersivity, microbial populations, sorption site density, bioavailable Fe(III) minerals, organic carbon); the physical and biogeochemical processes that govern the occurrence and movement of water, chemical constituents, and biological entities; and the boundary and initial conditions, which determine the inputs to and outputs from the site. A conceptual model serves as the basis for mathematical and numerical models used to interpret or predict site behavior and should be expected to evolve as additional data and information about the site become available.

Figure 5 illustrates a generic conceptual model for the reactive transport of uranium in groundwater. Simulations based on such a conceptualization must integrate an understanding of processes across spatial scales (field, grid, and pore scale) and require decisions on the dimensionality of the simulation, a description of the spatial and temporal variations of the boundary conditions and distributed stresses such as recharge, and a description of the spatially variable properties such as hydraulic conductivity, porosity, and storativity. U(VI) transport is affected by a diverse set of geochemical processes including speciation (Bernhard et al., 1996; Bernhard et al., 2001), precipitation-dissolution and other U phases (Duff et al., 2002; Kelly et al, 2003), adsorption (Waite et al., 1994; Duff and Amerhein, 1996), intraparticle diffusion (Liu et al., 2006), and microbiologically-mediated reduction of U(VI) to the relatively immobile U(IV) (Lovley et al, 1991; Suzuki et al., 2004). Uranium can also be impacted by variations in pH, alkalinity, and indirectly by ion exchange and mineral reactions involving calcium.

In most reactive transport models of uranium behavior, processes are included based on an understanding of site-specific conditions. It can be difficult to distinguish among various processes that have similar controls on U(VI) mobility; thus, conceptualizing the process models, the property distributions, and the interactions between them is inherently uncertain. Uranium sorption models, for example, can span a

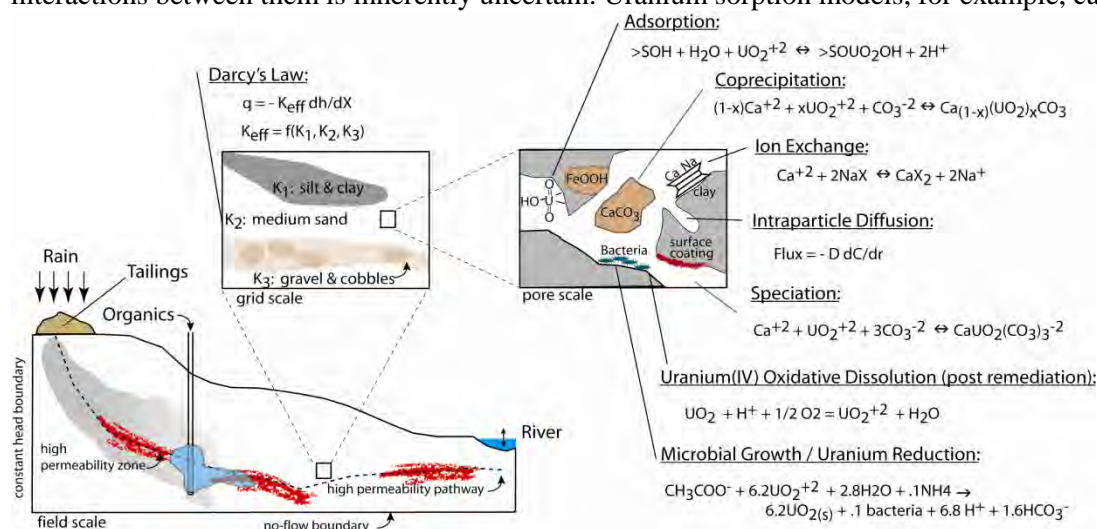


Figure 5. Generic conceptual model for the reactive

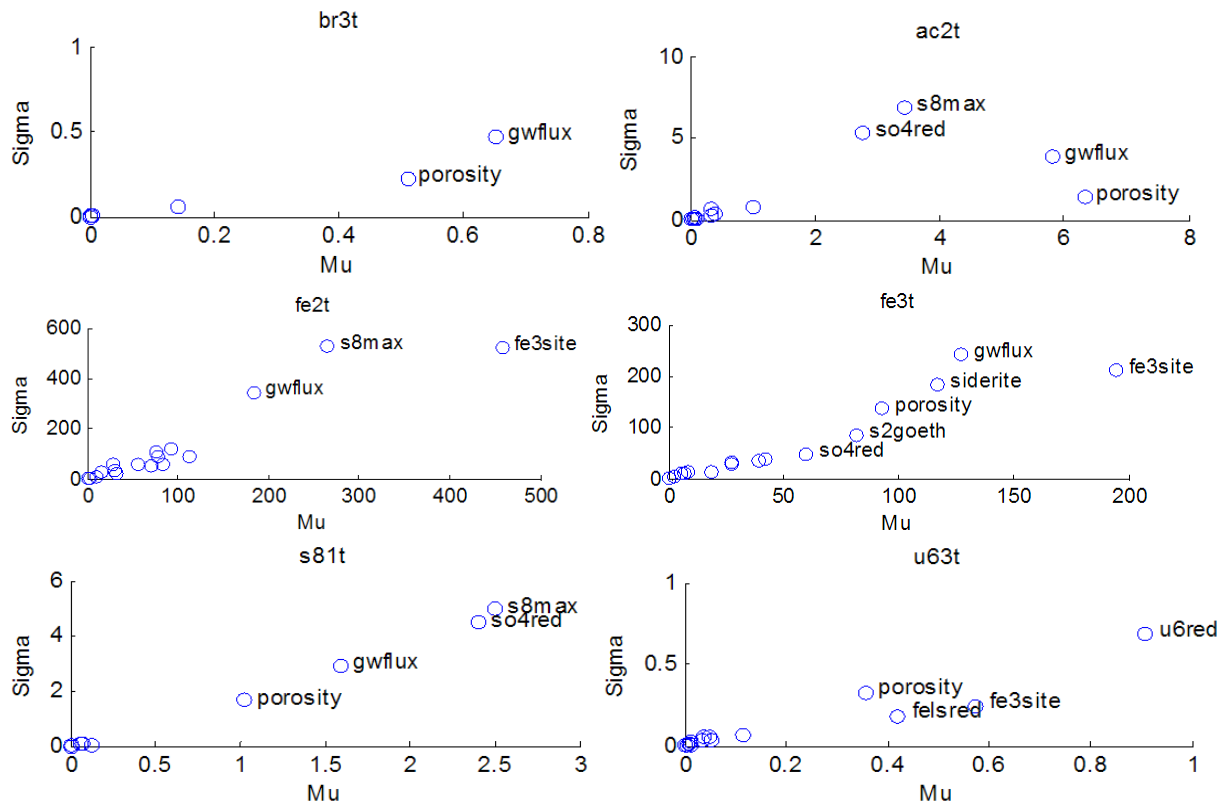
large range of mechanistic detail with respect to the treatment of the coulombic interactions at the mineral-water interface. Similarly, alternative process models exist for many of the principal microbially-mediated processes: reaction rate laws, bioavailable iron pools (e.g., poorly-crystalline iron oxide versus phyllosilicate iron), uranium bioreduction (e.g., iron reducers versus sulfate reducers), bioreducibility of

specific uranium species (e.g., uranyl ion versus calcium-uranyl-carbonate complexes) and long-term uranium immobilization (e.g., biosorption versus abiotic uranium reduction). Finally, these processes dynamically interact within an evolving biogeochemical system (e.g., pH increase during sulfate reduction results in additional desorption of uranium which undergoes altered speciation, because calcite is precipitating during the drop in redox potential, ultimately affecting the uranium bioreduction rate). A site-specific reactive transport model can best support management decisions when the model is as simple as possible while still reflecting the important site complexities that have the greatest impact on inputs to management decisions. Important uncertainties, both parametric and conceptual, need to be identified, evaluated, and reduced either through model refinement or the collection of additional data. Sensitivity and uncertainty analyses are the tools used to address these issues.

Sensitivity and uncertainty analyses are being conducted using a three-dimensional, variably saturated flow and multicomponent biogeochemical reactive transport model of a uranium bioremediation field experiment to generate synthetic data (Yabusaki et al., 2011). The model was based on the 2008 Big Rusty Field Experiment at the Rifle IFRC site, which used acetate biostimulation of indigenous metal reducing bacteria to catalyze the conversion of aqueous uranium in the +6 oxidation state to immobile solid-associated uranium in the +4 oxidation state. The model represents the experimental conditions of 110 days of pulsed bromide and acetate amendment, seasonal water table variation, and spatially-variable physical (hydraulic conductivity, porosity) and geochemical (reactive surface area) material properties. Equilibrium and kinetic reactions were used to address iron- and sulfate-reducing microorganisms (FeRB and SRB), four terminal electron acceptor processes (TEAPs) (i.e., phyllosilicate Fe(III), poorly crystalline Fe(III), U(VI), and sulfate), 102 biogeochemical species (including surface complexes and exchanged cations), and seven minerals (FeOOH, Fe<sub>3</sub>O<sub>4</sub>, FeS, S, calcite, siderite, and uraninite). Sorbed U(VI) and Fe(II) were assumed to be in equilibrium with their aqueous counterparts through the respective surface complexation models. Major ions (e.g., Ca, Mg, Na, K) were included in the initial and boundary conditions because of the importance of calcium and carbonate chemistry in aqueous uranium complexation, mineral precipitation, and pH. Synthetic field observations were simulated biogeochemical concentrations in three rows of four wells, 2.5, 5.0, and 8.5 m from the injection wells, with 2-m lateral spacing for wells in the same row.

A key assumption in past studies (Fang et al., 2009; Yabusaki et al., 2007) was that a comprehensive reaction network could be developed largely through one-dimensional modeling. Parameter sensitivity was evaluated for a one-dimensional reactive transport model abstracted from the three-dimensional model described above. A sensitivity analysis method (Morris, 1992) was used to evaluate which model parameters have a significant impact on the key biogeochemical concentrations (and by extension, those that have minimal impact). Twenty parameters (groundwater flux, porosity, dispersivity, and 17 reaction parameters) were evaluated using 84 forward model simulations that explored the full range of likely parameter values.

Sensitivities were calculated for bromide, acetate, Fe(II), sulfate, and U(VI) concentrations at each of the three well row locations. Results for bromide in Row 3 and acetate in Row 2 at a simulation time of 70 days after the start of injection are shown in Figure 6. Mu is the average sensitivity of the simulated concentration to a given parameter; those parameters exerting the greatest influence over the specific simulated concentration are labeled in each plot of Figure 6. Sigma is the variation in the sensitivity; a large Sigma indicates that the simulated concentration is a nonlinear function of the parameter value or a function of the parameter and one or more other (undetermined) parameters. Note that Mu and Sigma are dimensional quantities and thus not directly comparable across different chemical components unless normalized. As shown in Figure 6, bromide is largely sensitive only to groundwater flux and porosity (and to a lesser extent dispersivity). Along with these two parameters, acetate concentration is sensitive to its rate of oxidation during bioreduction of sulfate (so4red) and to the maximum limit placed on acetate consumption via sulfate reduction (s8max). While the relative importance of parameters to a given simulated concentration varied across time and across monitoring well rows, the group of significant parameters was generally consistent. This was not always the case, however, as shown in Figure 6 for the Fe(II) sensitivities in Rows 2 and 3. Although Fe(II) concentration was most sensitive in both rows to the initial number of surface complexation sites (fe3site), the remaining set of influential parameters differed significantly, with the Row 3 Fe(II) concentrations being sensitive to the siderite precipitation rate and the rate of sulfide-promoted goethite dissolution (s2goeth). Sensitivities of sulfate and U(VI) concentrations are also shown in Figure 6 and for U(VI) included the acetate oxidation rate for U(VI) bioreduction (u6red) and the rate of layer silicate Fe(III) bioreduction (felsred). Other parameters with significant sensitivities at certain simulation times included stability constants of surface complexation reactions and



**Figure 6. Sensitivity results for bromide in Row 3 (top left), acetate in Row 2 (top right), Fe(II) in Row 2 (middle left) and Row 3 (middle right), sulfate in Row 2 (bottom left), and U(VI) in Row 3 (bottom right) at a simulation time of 70 days.**

the FeS precipitation rate [Fe(II) sensitivity], the decay rate for SRB (sulfate sensitivity), and cation exchange parameters [U(VI) sensitivity] .

The sensitivity analysis identified the parameters with the greatest impact on key biogeochemical concentrations; these parameters have the greatest potential to contribute to model predictive uncertainty and are likely to be the most important to include in a calibration. The relatively large Sigma values shown in Figure 6 indicate that model nonlinearities and/or parameter interactions are typical (consistent with results from the surface complexation modeling discussed above) and may need to be accounted for in a calibration. Relative to the average observed concentration, Fe(II) sensitivities are significantly larger than the sensitivities of the other chemical components examined, and they increase the most over the simulation time. This result and the large number of parameters influencing the Fe(II) concentrations (see Figure 6) reflect the complexity of the model's representation of processes affecting Fe(II) in this system. Under these conditions it may be difficult to correctly attribute observed Fe(II) behavior to modeled processes.

Parameters of the 1-D reactive transport model were estimated using UCODE (Poeter et al., 2005). For each sampling time, synthetic field observations generated from the 3-D model described above were averaged along each row of monitoring wells to provide calibration values that were commensurate with the simulated concentrations of the 1-D model. In general, the 1-D model is driven by the same initial and boundary conditions, and uses the same reaction network, as the 3-D model. The calibration was thus used to evaluate the effect of the 1-D abstraction on parameter estimation and predictive uncertainty.

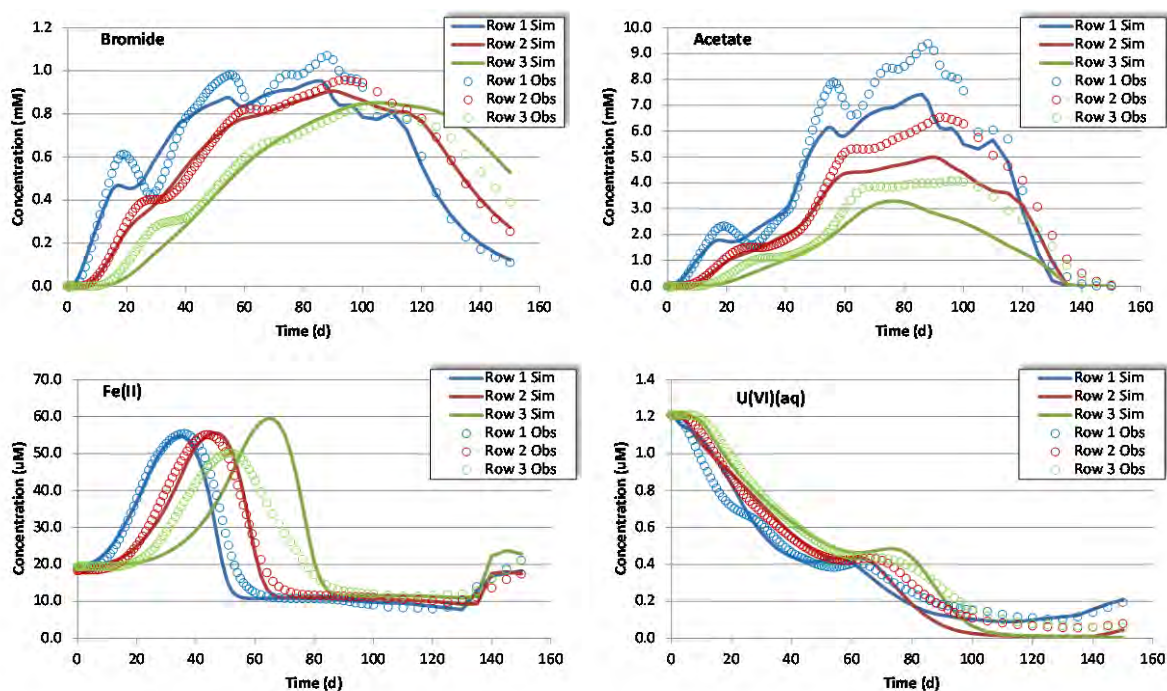
As in previous studies, we began by calibrating the groundwater flux, porosity, and longitudinal dispersivity using only the bromide injection and observation data. A reasonable fit to the observations was achieved as shown in Figure 7 (top left). However, this fit was obtained with parameter values significantly different than used in the 3-D model to generate the synthetic observations: porosity 50 percent larger and dispersivity almost four times larger. Holding the three parameters at their calibrated values, reaction parameters were subsequently estimated using acetate, Fe(II), sulfate, and U(VI) observations from the 3-D model. In many cases the calibrated values of reaction parameters were significantly different than used in the 3-D model: Fe(III) bioreduction rate an order of magnitude smaller, FeS precipitation rate eight times larger, U(VI) bioreduction rate doubled, and SRB decay rate increased by a factor of four. Comparisons between the observations and concentrations simulated by the calibrated 1-D model are shown in Figure 7; for the most part, the 1-D model is able to provide a reasonable fit. In particular, the 1-D model provided a good fit to the U(VI) observations. However, significant errors are also apparent, particularly in the acetate peaks and the Fe(II) concentrations in Row 3.

Parameters of the 1-D reactive transport model were estimated using UCODE (Poeter et al., 2005). For each sampling time, synthetic field observations generated from the 3-D model described above were averaged along each row of monitoring wells to provide calibration values that were commensurate with the simulated concentrations of the 1-D model. In general, the 1-D model is driven by the same initial and boundary conditions, and uses the same reaction network, as the 3-D model. The calibration was thus used to evaluate the effect of the 1-D abstraction on parameter estimation and predictive uncertainty.

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A detailed examination of the 3-D model showed significant spatial variability in bromide concentrations in response to the non-uniformity of the groundwater flux. As a result, the discrete monitoring locations may not adequately sample the domain, for example, by failing to sample preferential pathways carrying the bulk of the transport. Using row-averaged concentration estimates (or data from fully-screened wells) as calibration targets potentially introduces additional error into the observation data via the averaging process. In this synthetic example, these sampling issues contributed to systematic errors in the 1-D model parameters and outputs. This occurred despite using the same reaction network for 1-D modeling as used in the data-generating 3-D model. Similar sampling limitations will typically arise in modeling of natural subsurface systems.



**Figure 7. Row-averaged observed concentrations from the 3-D model compared to simulated results from the 1-D calibrated model: (top left) Bromide, (top right) Acetate, (bottom left) Fe(II), and (bottom right) U(VI).**

Linear parameter uncertainty estimates derived from the calibrations were quite small, with many of the 3-D model parameter values lying well outside the estimated parameter intervals. Based on these results and the evident errors shown in Figure 7, predictive uncertainty of the 1-D model appears to be significantly underestimated by linear parameter uncertainty estimates. That the calibration still did a relatively good job of matching the data (and may be predictive under some scenarios) is deceptive -- the model is addressing a different reality. Accurate predictive understanding requires a better representation of model uncertainty, which is the subject of ongoing work.

## 5. Application of BMA to Uranium Transport in Small-Scale Tracer Tests

Tracer tests were conducted at the Naturita UMTRA site to demonstrate that induced changes in U(VI) concentrations caused by variable alkalinity concentrations could be simulated using a reactive transport model the used a surface complexation model to simulate adsorption. The tracer tests were conducted in a contaminated region of the shallow alluvial aquifer shown in Figure 8. The tracer tests were conducted by pumping 550 liters of groundwater containing  $4\mu\text{M}$  U(VI) into tanks, adjusting the alkalinity with  $\text{NaHCO}_3$  or  $\text{H}_2\text{SO}_4$  and then adjusting the pH by varying the partial pressure of  $\text{CO}_2$ . Finally a Br tracer was added as its potassium salt (Curtis and Davis, 2006). The solution was injected into three upgradient wells and samples were collected at nine multilevel wells shown in Figure 8. Four complete Br breakthrough curves recorded at wells A3, M2, N2 and O1 were used in the uncertainty analysis described below.

The key components of the conceptual model for reactive transport of U(VI) for these tracer test include (1) a representation of U(VI) adsorption reactions, (2) a description of the rate of adsorption and desorption and (3) a description of the key major ions. Alternative model formulations are being investigated in modeling studies of two small-scale tracer tests that were conducted at the Naturita site

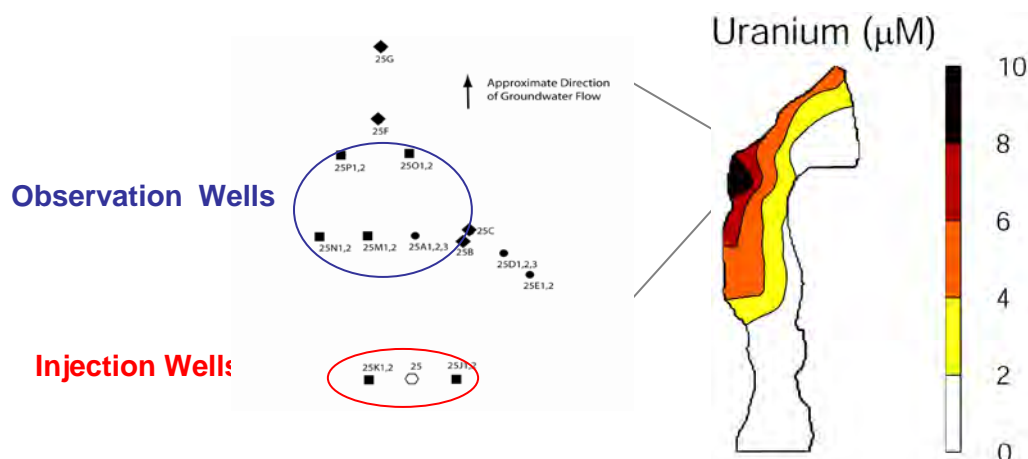


Figure 8. Tracer test site at the Naturita, CO UMTRA site (Curtis and Davis, 2006)

Figure 9 shows the concentration histories observed at a sampling well located 1.8m downgradient of the injection zone. A nonreactive transport model fit the Br data very well. Similarly, an the major cations were well described by an ion exchange model which was calibrated to observed Ca, Mg and Na concentrations. Accurately modeling major ion concentrations is particularly important for the case of Ca because aqueous Ca-U(VI)- $\text{CO}_3$  complexes typically dominate the aqueous speciation in carbonate rich waters such as those at Naturita. A mobile-immobile zone model was used in the simulations although for the results shown in Figure 9 the impact of the immobile zone is minimal; observations at other wells did show significant tailing thus requiring the mobile-immobile zone model.

The primary focus of the A review of the literature shows that a number of different reaction stoichiometries have been used to simulate U(VI) adsorption by natural sediments. Table 2 includes a summary of the reactions previously studied in addition to a few that were added to fill out the obvious patterns in reaction stoichiometry.



Table 3: Uranium adsorption reactions tested in model calibration studies

1	$>S_i(OH)_2 + UO_2^{+2}$	$= >S_iO_2H_2UO_2^{+2}$
2	$>S_i(OH)_2 + UO_2^{+2}$	$= >S_iO_2HUO_2^+ + H^+$
3	$>S_i(OH)_2 + UO_2^{+2}$	$= >S_iO_2UO_2 + 2H^+$
4	$>S_i(OH)_2 + UO_2^{+2} + CO_3^{-2} + H^+$	$= >S_iO_2H_2UO_2HCO_3^+$
5	$>S_i(OH)_2 + UO_2^{+2} + CO_3^{-2}$	$= >S_i(OH)_2UO_2CO_3$
6	$>S_i(OH)_2 + UO_2^{+2} + CO_3^{-2}$	$= >S_iO_2HUO_2CO_3^- + H^+$
7	$>S_i(OH)_2 + UO_2^{+2} + CO_3^{-2}$	$= >S_iO_2UO_2CO_3^{-2} + 2H^+$
8	$>S_i(OH)_2 + UO_2^{+2} + 2CO_3^{-2} + H^+$	$= >S_iO_2H_3UO_2(CO_3)_2^-$
9	$>S_i(OH)_2 + UO_2^{+2} + 2CO_3^{-2}$	$= >S_i(OH)_2UO_2(CO_3)_2^{-2}$
10	$>S_i(OH)_2 + UO_2^{+2} + 2CO_3^{-2}$	$= >S_iO_2HUO_2(CO_3)_2^{-3} + H^+$
11	$>S_i(OH)_2 + UO_2^{+2} + 2CO_3^{-2}$	$= >S_iO_2UO_2(CO_3)_2^{-4} + 2H^+$

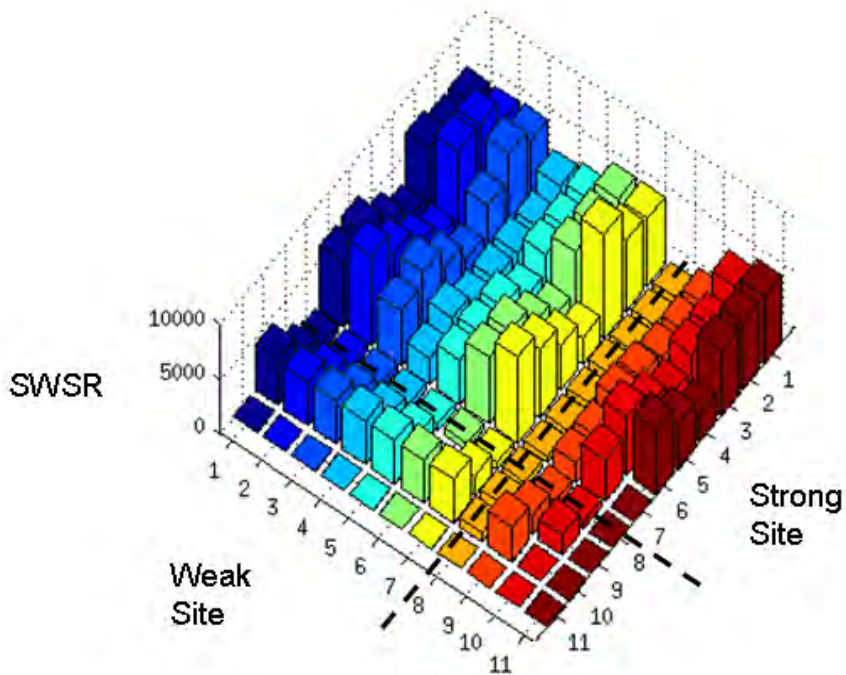


Figure 9. Summary of model calibration studies shown as the sum of weighted squared residuals (SWSR) for the 121 possible models developed from the 11 surface complexation reactions in Table 3. Some of the results for reaction 11 were deleted for clarity. Models indicated by the dashed lines were considered in the BMA analyses.

All 11 reactions in Table 1 were included in a reactive transport model having both a strong and a weak site. Each reaction was used to simulate adsorption on the weak site and the strong site so that a total of 121 models were tested. Each postulated model was calibrated to the observed data at well M2 using the global optimization solver in MATAB. The results of this global calibration were then used as the initial starting point for a UCODE calibration run which was performed to calculate a broad set of model statistics including KIC which was used for model averaging. The results from the model calibration are shown in Figure 11 along with prediction results at well N2 which is about 1m from well M2.

Figure 11. Results of calibrating alternative adsorption models to observations of U(VI) transport at well M2 (left figure) and comparison of model predictions with observations at well N2 (right figure). Both figures show observed data, individual model simulations for the alternative adsorption models and the model averaged prediction.

## **6. Data-Worth Analysis for Uncertainty Reduction**

To effectively manage subsurface contamination at many DOE sites, site managers face a daunting challenge: helping to insure that contaminants in the subsurface do not pose unacceptable future risks to humans and the environment. To quantify and manage these risks one must understand their relationships to existing pollution and alternative pollution remediation schemes. Such understanding requires the collection of suitable data to help characterize the subsurface and monitor its response to existing and future management options such as exploitation, pollution prevention, and/or remediation. It also requires incorporating such data in suitable models of subsurface flow and contaminant transport.

As noted by Back (2007), three strategies have traditionally been used to determine the magnitude of a data collection effort: minimizing cost for a specific level of accuracy or precision, minimizing uncertainty for a given budget, or responding to regulatory demands on data quantity and quality. Various combinations of these strategies have also been described such as a fitness-for-purpose approach. Many today prefer a fourth approach based on value-of-information or data-worth analysis. The decision to collect additional data, or the design of a data collection program, is based on cost-effectiveness. A program is considered cost-effective if the expected benefit from the new information exceeds the cost. A major benefit of new data is its potential to help improve one's understanding of the system, in large part through a reduction in model predictive uncertainty. This benefit, however, is worth the cost only if it has the potential to impact decisions concerning management of the environmental system.

A major limitation of many existing approaches of data-worth analysis is that they rely on a single conceptual-mathematical model of subsurface environmental makeup and processes therein. This project investigated the potential of conducting environmental data-worth analysis with consideration of model uncertainty to explore how different sets of conditioning data impact the predictive uncertainty of multiple models. We developed a multimodel approach to optimum value-of-information or data-worth analyses based on model averaging within a Bayesian framework (Neuman et al., 2011). This method is expected to bring new insights into various applications of groundwater modeling and facilitate on-going and planned site remediation and monitoring network design by optimizing limited resources for collecting the most valuable data.



A proof-of-concept study was conducted (Ye et al., 2011; Lu et al., 2011) to answer the following question: given data **D** from *X* boreholes, *Y* locations of potential data collection, but only money for *Z* additional boreholes, at which of the *Y* borehole locations should one drill/test for maximum uncertainty reduction? The proof-of-concept study demonstrated the robustness of the proposed method for selecting the borehole locations. The method is believed to have potential for more complicated problems of groundwater reactive transport modeling. A similar data-worth analysis for uranium reactive transport modeling based on a small-scale tracer experiment conducted at the Naturita Site (Curtis and Davis, 2006) is being undertaken. The goal is to select locations of monitoring wells in a cost effective manner for maximum reduction of predictive uncertainty. This appears to be the first study of monitoring network design for reactive transport modeling with respect to uncertainty reduction. Experience gained from this study will be extended to the plume scale at the Naturita site.

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