COMBINED ESTIMATION OF HYDROGEOLOGIC CONCEPTUAL MODEL, PARAMETER, AND SCENARIO UNCERTAINTY

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Abstract: We describe the development and application of a methodology to systematically and quantitatively assess predictive uncertainty in groundwater flow and transport modeling that considers the combined impact of hydrogeologic uncertainties associated with the conceptual-mathematical basis of a model, model parameters, and the scenario to which the model is applied. The methodology is based on an extension of a Maximum Likelihood implementation of Bayesian Model Averaging. Model uncertainty is represented by postulating a discrete set of alternative conceptual models for a site with associated prior model probabilities that reflect a belief about the relative plausibility of each model based on its apparent consistency with available knowledge and data. Posterior model probabilities are computed and parameter uncertainty is estimated by calibrating each model to observed system behavior; prior parameter estimates are optionally included. Scenario uncertainty is represented as a discrete set of alternative future conditions affecting boundary conditions, source/sink terms, or other aspects of the models, with associated prior scenario probabilities. A joint assessment of uncertainty results from combining model predictions computed under each scenario using as weights the posterior model and prior scenario probabilities.

INTRODUCTION

Regulatory and design applications of hydrogeologic models of flow and contaminant transport often involve using the models to make predictions of future system behavior. These predictions are inherently uncertain as a result of incomplete knowledge of the system, variability in system properties, randomness in the system stresses, measurement and sampling errors, and disparity among sampling, simulation, and actual scales of the system. These uncertainties are manifested in a hydrogeologic model as uncertainty in model conceptualization (including the mathematical implementation of that concept), model parameters, and model scenarios. Assessing the impact of parameter uncertainty on model predictions is accepted in policy (EPA 1997; NRC 2003) and is fairly common in practice. Parameter uncertainty analysis proceeds by characterizing the uncertainty in model parameter values and propagating this uncertainty into the predicted quantities produced by the model. It is implicit in this process that the resulting predictive uncertainty is conditional on the structure of the model. It is generally recognized, however, that a hydrogeologic model of a site is invariably an approximation of the actual system. As a consequence, it may be possible to postulate more than one conceptual model for a site that is consistent with site characterization data and observed system behavior. Although the potential importance of conceptual model uncertainty is accepted in theory, practical methods to assess the impact of model uncertainty on prediction have not found their way into widespread practice. A scenario is a description of the future conditions under which a model is applied. Scenario development is most commonly associated with radioactive waste disposal performance assessment (NEA 2001), but the concept applies to any modeling application in which prediction of future system behavior is made. Scenarios are inherently uncertain since they describe conditions in the (uncertain) future.

What evidence is there for the relative importance of conceptual model, parameter, and scenario uncertainties in modeling practice? Published results from hydrogeologic model post-audits were reviewed to attribute the primary modeling errors in these applications to conceptual, parameter, or scenario uncertainties. Six additional modeling applications described in Bredehoeft (2005) were included in this review. Results are shown in Table 1 and demonstrate the importance of conceptual and scenario uncertainties in contributing to model predictive errors. In 9 of the 15 applications, conceptual model errors were most significant. Model scenario errors were the most significant in 4 of the 15 applications. Parameter errors were most significant in only two of the applications. This (limited) review suggests that conceptual model and scenario uncertainties cannot be ignored in hydrogeologic modeling if a realistic estimate of predictive uncertainty is desired. This paper describes a methodology for estimating uncertainty in hydrogeologic modeling that jointly considers conceptual model, parameter, and scenario uncertainties.

Table 1. Attribution of primary errors in hydrogeologic model applications (see Bredehoeft [2005] for underlying references unless otherwise noted).

Prototype	Comments	Error
Phoenix	Assumed past groundwater pumping would continue in future	Scenario/Conceptual
Cross Bar Ranch Wellfield	Assumed a 75-day, no-recharge scenario would represent long-term maximum drawdown	Scenario/Conceptual (Stewart and Langevin, 1999)
Arkansas Valley	Needed a longer period of calibration	Scenario/Parameter
Coachella Valley	Recharge events unanticipated	Scenario
INEL	Dispersivities poorly estimated	Parameter
Blue River	Storativity poorly estimated	Parameter/Conceptual
Houston	Including subsidence in model improved predictions	Conceptual
HYDROCOIN	Boundary condition modeled poorly	Conceptual
Ontario Uranium Tailings	Inadequate chemical reaction model	Conceptual
Los Alamos	Flow through unsaturated zone not understood	Conceptual
Los Angeles	Flow vectors 90° off in model	Conceptual
Summitville	Seeps on mountain unaccounted for	Conceptual
Santa Barbara	Fault zone flow unaccounted for	Conceptual
WIPP	Assumed salt had no mobile interstitial brine	Conceptual
Fractured Rock Waste Disposal	Preferential flow in unsaturated zone unaccounted for	Conceptual

A BRIEF REVIEW OF BAYESIAN MODEL AVERAGING

A practical method for evaluating prediction uncertainty in hydrogeologic modeling with consideration of model and parameter uncertainty is Maximum Likelihood Bayesian Model Averaging (MLBMA) (Neuman, 2003; Ye et al. 2004). This method is a maximum likelihood implementation of Bayesian Model Averaging (BMA) (Draper, 1995; Hoeting et al., 1999). In BMA, the posterior distribution of a predicted quantity, Δ, given a set of data, $\boldsymbol{D}$, is

$$p\left(\Delta|\boldsymbol{D}\right)=\sum_{k=1}^{K} p\left(\Delta|M_k,\boldsymbol{D}\right)p\left(M_k|\boldsymbol{D}\right) \tag{1}$$

where $\boldsymbol{\mathcal{M}}=(M_1,...,M_K)$ is a discrete set of postulated alternative models representing the relevant conceptual model uncertainties, $p\left(\Delta|M_k,\boldsymbol{D}\right)$ is the posterior distribution of Δ for model M_k, and $p\left(M_k|\boldsymbol{D}\right)$ is the posterior model probability for model M_k. Parameter uncertainty enters (1) as the random contribution to

$$p\left(\Delta|M_k,\boldsymbol{D}\right)=\int p\left(\Delta|M_k,\boldsymbol{D},\boldsymbol{\theta}_k\right)p(\boldsymbol{\theta}_k|M_k,\boldsymbol{D})d\boldsymbol{\theta}_k \tag{2}$$

where $\boldsymbol{\theta}_k$ is the vector of parameters associated with model M_k and $p\left(\boldsymbol{\theta}_k|M_k,\boldsymbol{D}\right)$ is the posterior probability density of $\boldsymbol{\theta}_k$ given M_k and $\boldsymbol{D}$. Given $p\left(\boldsymbol{\theta}_k|M_k,\boldsymbol{D}\right)$, (2) could be solved using, for example, Monte Carlo simulation.

Posterior model probability is given by Bayes' theorem,

$$p\left(M_k|\boldsymbol{D}\right)=\frac{p\left(\boldsymbol{D}|M_k\right)p\left(M_k\right)}{p\left(\boldsymbol{D}\right)}=\frac{p\left(\boldsymbol{D}|M_k\right)p\left(M_k\right)}{\sum_{l=1}^{K}p\left(\boldsymbol{D}|M_l\right)p\left(M_l\right)} \tag{3}$$

where $p\left(\boldsymbol{D}|M_k\right)$ is the likelihood of model M_k and $p\left(M_k\right)$ is the prior probability of model M_k. The model likelihood can be expressed as

$$p\left(\boldsymbol{D}|M_k\right)=\int p\left(\boldsymbol{D}|\boldsymbol{\theta}_k,M_k\right)p\left(\boldsymbol{\theta}_k|M_k\right)d\boldsymbol{\theta}_k \tag{4}$$

where $p\left(\boldsymbol{\theta}_k|M_k\right)$ is the prior probability density of $\boldsymbol{\theta}_k$ under model M_k, and $p\left(\boldsymbol{D}|\boldsymbol{\theta}_k,M_k\right)$ is the joint likelihood of model M_k and its parameters $\boldsymbol{\theta}_k$. MLBMA (Neuman 2003) uses a maximum likelihood approximation to solve (4) and a result due to Kashyap (1982) for (3).

To apply BMA, one formally requires that the prior model probabilities sum up to one,

$$\sum_{k=1}^{K}p\left(M_k\right)=1\,. \tag{5}$$

This implies that all possible models of relevance are included in $\boldsymbol{\mathcal{M}}$ (i.e., the set is collectively exhaustive), and that all models in $\boldsymbol{\mathcal{M}}$ differ from each other sufficiently to be considered mutually exclusive (i.e., the joint probability of any two models is zero). In practice, it may be impossible to demonstrate that the set of models is collectively exhaustive. In this case, model uncertainty may be underestimated and model probability must be interpreted as relative to the other models in $\mathcal{M}$, a condition implied by the fact that all probabilities computed using BMA are conditional on $\mathcal{M}$. For additional comments on the interpretation of model probabilities, see Ye et al. (2004) and Meyer et al. (2004).

INCORPORATION OF SCENARIO UNCERTAINTY

In the MLBMA method, existing observations of system behavior (i.e., $\boldsymbol{D}$) are used to provide model probabilities and to determine parameter values and their estimation errors (uncertainty). The period of time covered by the observations in $\boldsymbol{D}$ is referred to as the calibration or history-matching period. Each model in $\mathcal{M}$ is calibrated in the history-matching period using the dataset $\boldsymbol{D}$. The calibrated models are then used to simulate the system behavior in the predictive period with each model's result weighted by its posterior model probability. Parameters and model probabilities are referred to as posterior in the sense that they are conditioned on $\boldsymbol{D}$. Scenarios characterize conditions during the period of prediction: that is, outside the time period represented by $\boldsymbol{D}$. As a result, these predictions cannot be conditioned on data since there are, by definition, no observations of system behavior during the prediction period. This modeling framework is illustrated in Figure 1; a single model is shown in this figure with scenario uncertainty represented discretely as three alternative scenarios.

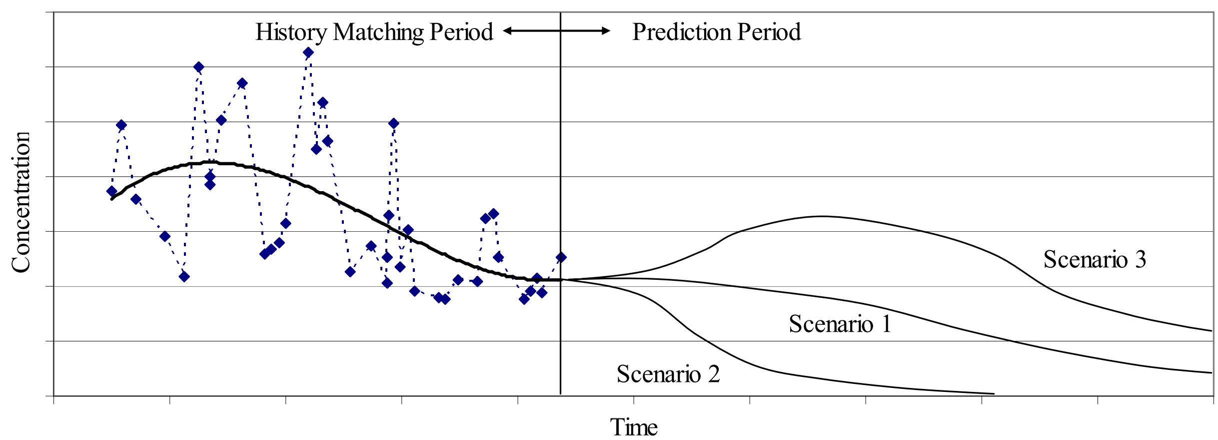

Figure 1. Framework for predictive modeling with scenario uncertainty.

For calibration, the models must reflect the system conditions of the history matching period and must be capable of producing the quantities in $\boldsymbol{D}$ (typically head and concentration measurements). For prediction, the models must reflect the future scenario(s) and must be able to produce the quantities required to evaluate site safety/performance. This will, in general, require that changes be made to the models between the history-matching and prediction periods. For example, a climate change scenario may require modification of the upper boundary condition representing precipitation or recharge. It is assumed here that all the models in $\mathcal{M}$ retained for prediction (i.e., those models with non-negligible posterior model probabilities) were constructed such that they can be easily modified to simulate any scenario considered.

<u>Bayesian Model Averaging Conditioned on a Specific Scenario</u>: Formally, scenario uncertainty can be quantitatively assessed jointly with model and parameter uncertainties following the methodology described by Draper (1995) and applied in a nuclear waste disposal context (albeit without the inclusion of model uncertainty) by Draper et al. (1999). Consider an uncertain scenario in which the uncertainty is modeled discretely as a set of alternative scenarios, $\boldsymbol{S} = (S_1,...,S_I)$. For a given scenario, S_i, the posterior distribution of a predicted quantity can thus be interpreted as conditional on that scenario and equation (1) becomes

$$p\left(\Delta\middle|\mathbf{D},S_i\right)=\sum_{k=1}^{K}p\left(\Delta\middle|M_k,\mathbf{D},S_i\right)p\left(M_k\middle|\mathbf{D},S_i\right). \tag{6}$$

Posterior model probability conditional on a given scenario can be expressed similarly by modifying equation (3).

$$p\left(M_k\middle|\mathbf{D},S_i\right)=\frac{p\left(\mathbf{D}\middle|M_k,S_i\right)p\left(M_k\mid S_i\right)}{p\left(\mathbf{D}\mid S_i\right)}=\frac{p\left(\mathbf{D}\middle|M_k\right)p\left(M_k\mid S_i\right)}{\sum_{l=1}^{K}p\left(\boldsymbol{D}\middle|M_l\right)p\left(M_l\mid S_i\right)} \tag{7}$$

The simplifications made in the rightmost equality of equation (7) are based on the assumption that the dataset, ***D***, is independent of the scenario. That is, the occurrence of any particular scenario in the future does not affect the probability of observing the data , ***D***, in the past. As a result, the model likelihoods, $p\left(\boldsymbol{D}\middle|M_k\right)$, are not a function of the scenario and do not need to be recomputed under each scenario. In contrast, prior model probability, $p\left(M_k\middle|S_i\right)$, is potentially a function of the scenarios. That is, the occurrence of specific future hydrologic conditions may have an impact on the relative plausibility of the various models. Thus posterior model probability is a function of the scenario only through the possible dependence of prior model probabilities on the scenario. As in equation (5), prior model probabilities under a given scenario must sum to one.

$$\sum_{k=1}^{K}p\left(M_k\mid S_i\right)=1\,. \tag{8}$$

Posterior mean and variance of Δ can be written as

$$E\left(\Delta\middle|\mathbf{D},S_i\right)=\sum_{k=1}^{K}E\left(\Delta\middle|M_k,\mathbf{D},S_i\right)p\left(M_k\middle|\mathbf{D},S_i\right) \tag{9}$$

$$\begin{aligned}&Var\left(\Delta\middle|\mathbf{D},S_i\right)=\\&\sum_{k=1}^{K}Var\left(\Delta\middle|M_k,\mathbf{D},S_i\right)p\left(M_k\middle|\mathbf{D},S_i\right)+\sum_{k=1}^{K}\left[E\left(\Delta\middle|M_k,\mathbf{D},S_i\right)-E\left(\Delta\middle|\mathbf{D},S_i\right)\right]^2p\left(M_k\middle|\mathbf{D},S_i\right)\end{aligned} \tag{10}$$

where the two terms on the right hand side of (10) represent within-model and between-model variance for a given scenario.

Scenario Averaging: Averaging equation (6) over all scenarios using scenario probabilities $p\left(S_i\right)=p\left(S_i\middle|\mathbf{D}\right)$ as weights gives

$$p\left(\Delta\middle|\mathbf{D}\right)=\sum_{i=1}^{I}p\left(\Delta\middle|\mathbf{D},S_i\right)p\left(S_i\right)=\sum_{i=1}^{I}\sum_{k=1}^{K}p\left(\Delta\middle|M_k,\mathbf{D},S_i\right)p\left(M_k\middle|\mathbf{D},S_i\right)p\left(S_i\right) \tag{11}$$

where $p\left(\Delta|\mathbf{D}\right)$ is implicitly conditioned on all scenarios and model structures. Probabilities $p\left(\Delta|S_i,M_k,\mathbf{D}\right)$ and $p\left(M_k|S_i,\mathbf{D}\right)$ can be obtained by Monte Carlo simulation and (7), respectively. For the averaging in (11) we require that the scenarios given in $\boldsymbol{S} = (S_1,...,S_I)$ are mutually exclusive and collectively exhaustive. That is,

$$\sum_{i=1}^{I} p\left(S_i\right) = 1. \qquad (12)$$

The posterior mean of Δ, including the effects of scenario uncertainty, is

$$E\left(\Delta|\mathbf{D}\right) = \sum_{i=1}^{I} E\left(\Delta|\mathbf{D},S_i\right) p\left(S_i\right) = \sum_{i=1}^{I}\sum_{k=1}^{K} E\left(\Delta|M_k,\mathbf{D},S_i\right) p\left(M_k|\mathbf{D},S_i\right) p\left(S_i\right) \qquad (13)$$

where $E\left(\Delta|\mathbf{D},S_i\right)$ is evaluated by (9). The posterior variance of Δ can be written as

$$Var\left(\Delta|\mathbf{D}\right) = \sum_{i=1}^{I} Var\left(\Delta|\mathbf{D},S_i\right) p\left(S_i\right) + \sum_{i=1}^{I}\left[E\left(\Delta|\mathbf{D},S_i\right) - E\left(\Delta|\mathbf{D}\right)\right]^2 p\left(S_i\right) \qquad (14)$$

where $E\left(\Delta|\mathbf{D},S_i\right)$ and $Var\left(\Delta|\mathbf{D},S_i\right)$ can be estimated by equations (9) and (10). The first term on the right hand side of (14) is the variance within scenarios; the second term is the variance between scenarios.

By substituting equation (10) into (14), the posterior variance can be rewritten in the manner of Draper (1995) as

$$\begin{aligned} Var\left(\Delta|\mathbf{D}\right) = &\sum_{i=1}^{I}\sum_{k=1}^{K} Var\left(\Delta|M_k,\mathbf{D},S_i\right) p\left(M_k|\mathbf{D},S_i\right) p\left(S_i \mid \mathbf{D}\right) \\ &+ \sum_{i=1}^{I}\sum_{k=1}^{K}\left[E\left(\Delta|M_k,\mathbf{D},S_i\right) - E\left(\Delta|\mathbf{D},S_i\right)\right]^2 p\left(M_k|\mathbf{D},S_i\right) p\left(S_i \mid \mathbf{D}\right) \\ &+ \sum_{i=1}^{I}\left[E\left(\Delta|\mathbf{D},S_i\right) - E\left(\Delta|\mathbf{D}\right)\right]^2 p\left(S_i \mid \mathbf{D}\right). \end{aligned} \qquad (15)$$

This three terms in this expression are (1) the variance within models and scenarios, (2) the variance between models within scenarios, and (3) the variance between scenarios.

The equations provided above can be applied to estimate the individual and collective contribution to model predictive uncertainty of parameter, conceptual model, and scenario uncertainties. Parameter and conceptual model uncertainty are considered using maximum likelihood Bayesian model averaging (MLBMA) in the history-matching period (the period for which system state data exist). To incorporate scenario uncertainty, the MLBMA results are repeatedly applied in the predictive period under a set of alternative scenarios. Because the scenarios describe future conditions, the scenario probabilities represent prior estimates and cannot be updated using the (past) system state data. Incorporation of scenario uncertainty using the method described here thus does not require any additional calibration (beyond that conducted in the MLBMA analysis), but does require additional probabilistic calculations. For example, solution of equation (11) could be accomplished using a Monte Carlo simulation of each model within each scenario. This is straightforward, albeit computationally expensive for large or complex numerical models.

<u>Specifying Scenarios and Their Probabilities</u>: To complete the analysis described here requires specifying a set of alternative scenarios and their probabilities. As discussed above the alternative scenarios must be mutually exclusive and collectively exhaustive. As with the set of model alternatives, it is likely impossible to prove that a set of scenarios is collectively exhaustive. A relatively small set of scenarios may adequately represent the primary sources of uncertainty in future hydrologic conditions, particularly if the scenarios can be expressed at a fairly conceptual (high) level. An example is a climate change scenario, which may have several impacts on the models. By specifying the scenario at a conceptual level we avoid having to consider each of the individual impacts separately. Because we require that the set of alternative scenarios is collectively exhaustive, scenario probabilities should be interpreted as relative probabilities (i.e., relative to the other scenarios in the set).

Alternative scenarios are often likely to be characterized as discrete events. Climate change, floods, and introduction of irrigated agriculture are all examples of discrete events affecting the hydrologic conditions at a site. Such events are often not mutually exclusive (e.g., the occurrence of irrigated agriculture does not preclude the occurrence of climate change). By defining scenarios as possible combinations of alternative events, the scenarios can be made mutually exclusive. An example for three events is shown in Table 2. A "1" in the table signifies the occurrence of the event in a scenario and a "0" indicates the absence of that event. Scenario 1 in Table 2 has none of the events occurring and might be referred to as a reference scenario, perhaps characterized by the continuation of current hydrologic conditions into the future. For n events, this procedure will result in 2^n scenarios; some of these scenarios may be discarded because of an insignificant probability or because they are not of regulatory concern.

As discussed previously, scenario probability represents a subjective evaluation of the probability of occurrence. This evaluation can be based on relevant and available information, including expert judgment. If the scenarios are enumerated from a set of events such as in Table 2, the scenario probabilities can be determined from estimates of the marginal (given in Table 2 by the values of p) and conditional probabilities of the events. If the events are independent, the scenario probabilities can be easily computed from the marginal probabilities of the events, as illustrated in Table 2. Note that the marginal probabilities for the events characterizing the scenarios may sum to more than 1.0, but the scenario probabilities must total 1.0.

CONCLUSIONS

Ye et al. (2004) demonstrated the benefit of the MLBMA approach to jointly assess conceptual model and parameter uncertainties using an application to geostatistical modeling of air permeability at a fractured rock site. An application of MLBMA including the assessment of scenario uncertainty is currently underway using groundwater flow and uranium transport data at the 300 Area of the U.S. Department of Energy Hanford Site in Washington State.

Table 2. Formulation of mutually exclusive scenarios from three scenario-characterizing events.

<table>
<tr><td colspan="2" rowspan="2"></td><td colspan="3">Events Characterizing Scenarios</td><td colspan="2" rowspan="2"></td></tr>
<tr><td>Climate Change (p=0.3)</td><td>Flood (p=0.2)</td><td>Irrigated Agriculture (p=0.6)</td></tr>
<tr><td rowspan="8">Scenarios</td><td>1</td><td>0</td><td>0</td><td>0</td><td>0.224</td><td rowspan="8">Scenario Probability</td></tr>
<tr><td>2</td><td>1</td><td>0</td><td>0</td><td>0.096</td></tr>
<tr><td>3</td><td>0</td><td>1</td><td>0</td><td>0.056</td></tr>
<tr><td>4</td><td>1</td><td>1</td><td>0</td><td>0.024</td></tr>
<tr><td>5</td><td>0</td><td>0</td><td>1</td><td>0.336</td></tr>
<tr><td>6</td><td>1</td><td>0</td><td>1</td><td>0.144</td></tr>
<tr><td>7</td><td>0</td><td>1</td><td>1</td><td>0.084</td></tr>
<tr><td>8</td><td>1</td><td>1</td><td>1</td><td>0.036</td></tr>
</table>

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