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Accounting for model error in risk assessments: Alternatives to adopting a bias towards conservative risk estimates in decision models

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ABSTRACT

Two recently developed approaches to quantification of model (conceptual) error in a single groundwater model, a per-datum calibration methodology and a Bayesian model error analysis, were applied to a problem of ^{90}Sr migration to water wells at Chernobyl, Ukraine. The intent of this composition is to demonstrate their utility to accounting for the uncertainty due to model error in estimating risks (or costs) in decision models. Bayesian model error analysis resulted in a more conservative estimate of the probability of the Pripyat Town well field contamination than did the per-datum calibration approach. This difference in risk estimates is a result of the conceptual differences between the two methods. Per-datum calibration relies primarily on information on model error contained in the measurements of the dependent variables to quantify its effect on model predictions. The Bayesian model error analysis assigns equal importance to prior information on the parameters and measurements of the dependent variable, thus allowing the incorporation of a more informative description of parameter distributions, as well as subjective judgement into a risk analysis. The suitability of either of the two methods, when applied to a specific problem, may be determined based on the nature and quantity of available data.

1. Introduction

Hydrogeological decision models provide a methodology for incorporating the uncertainty in model predictions within a framework used to evaluate different management alternatives [9]. In this approach, management alternatives are compared under conditions of uncertainty using an objective function defined as the net present value of the expected costs and risks taken over a specified time horizon and discounted at the market interest rate. The evaluation of different management alternatives requires the use of a hydrogeologic model to predict the future response of the true hydrogeologic system under a set of naturally occurring or expected stresses. The role of simulation models in the decision process is to provide the technical input to the objective function by predicting the probability (or risk) of failure of each management alternative.

The construction of a decision model is ideally an iterative process. Data collection and modeling should proceed in tandem [9,21]. Early calculations based on simple simulation models are replaced, if required, by more detailed models as additional data become available. When calculating risks, especially during early cycles of the analysis when the data available to assist in constructing the model and to characterize the hydraulic and transport properties of the subsurface environment may be sparse, any model prediction will be subject to large uncertainties due to both parameter error (error produced from uncertainties in the parameter values) and model error (errors in the model structure). In order to deal with the uncertainties inherent in mathematical modeling an inverse approach can be employed. Inverse methods use field data on the dependent variables to assess whether or not model and parameter errors are significant and/or to enhance the accuracy of model predictions. In model calibration, measurements of the dependent variables are used to select a set of parameter values that enable the model to closely match the observed behavior of the physical system it represents. Model selection is used to identify the most likely model among alternative conceptual models in terms of achieving a smaller fitting residual of model output to observations, in conjunction with narrower confidence intervals on the estimated parameters [5,18].

These approaches may result in a successful application of mathematical modeling in decision analyses. However, failure or inconsistency of such applications is not an uncommon phenomenon [15]. The success or failure of mathematical modeling in practical problems is determined by the validity of various assumptions underlying these methods. Perhaps the most significant assumption made in uncertainty analyses and inverse methods is that the model structure is correct (negligible model error). Model selection methodologies may assist in selecting the most likely model structure among competing models or optimizing a model

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structure [24] based on the criteria mentioned earlier. However, selecting the "best" approximating model does not justify the assumption of a correct model structure in most practical applications. Two main reasons can be cited: (1) a small fitting residual, which is probably the most important criterion for model selection, does not necessarily imply that model error is also small [23], and (2) a number of model structures are often possible due to data limitations, measurement error and large parameter uncertainties [1,2,17]. When a complex hydrogeologic system is described by a simplified numerical model, it is more likely that model error dominates other errors [23]. The presence of model error may result in a misleading uncertainty analysis and in parameter estimates that have little value for predictive modeling and risk assessments [16]. Model error may represent the primary cause of failure of a model application [23].

The effect of possible errors in the model structure in the risk calculation is usually taken into account by adopting a bias in assigning probability distributions to a number of model parameters that favors a conservative estimate of the probability of failure, e.g. [6,8,21]. It may also be the case that conservatism is an inherent feature of the structure of the simulation model. However, the degree of conservatism which is typically adopted is often based on common practice or subjective judgement rather than on some theoretical principle. Such conservative assumptions potentially lead to a decision regarding the selection of a design or management alternative that involves unnecessary expenditures. A decision analysis may be more sound and less biased when it includes an evaluation of the effect of model error on the estimation of risks (or costs) in addition to that of parameter error, and an evaluation of the reliability of model predictions [14].

The majority of the existing approaches that quantitatively account for structural model uncertainties are based on the identification of several alternative model structures and their use to jointly render optimum predictions and to assess the uncertainty of those predictions, e.g. [1,2,7,17,27]. A brief description of these approaches can be found in [17,27]. All these methods may provide a more sound alternative than the adoption of a conservative bias in risk and decision analyses. However, there is no established literature on ways to construct a set of probable alternative hydrologic model structures [17]. The set of predictions produced by any given choice of alternative structural models is conditional on the choice of models and the data used to support them. Therefore, these predictions do not represent all possibilities but only a limited range of such possibilities, associated with these models and data [17]. In an operational risk estimation setting, the ability to evaluate model and parameter errors using a single model would be advantageous due to its simplicity. In the field of groundwater hydrology, there has been little research on quantification of the combined effect of model structure and parameter uncertainty. Two methods recently developed by Gaganis and Smith [10,11] reflect an attempt to evaluate model error, simultaneous with parameter error, based on a single model structure. The approaches may represent attractive alternatives to deal with model error in risk estimation and decision analysis.

The first method [11], so called per-datum calibration, uses a per-datum formulation to the inverse problem to include all information on errors in the parameter estimates. The effect of model error on the inverse problem and model predictions is then evaluated through an analysis of the spread of the per-datum parameter estimates in the parameter space. The second approach [10] uses Bayesian principles and insight gained in updating the prior probability distributions of the parameters, to assess model correctness and the expected magnitude of model error given the existing parameter uncertainty. The magnitude of model error estimated by both these methods can be used to calculate confidence intervals that describe the uncertainty in estimated risks that is associated with both parameter and model error. Such a risk analysis offers a better description of the uncertainties involved in the decision process, and need not rely on conservatism to account for unknown structural errors. Furthermore, it also provides a theoretical base for selecting the degree of conservatism that should be adopted in relation to the existing uncertainty in the parameter values and the given simulation model structure. Note that the reliability of the model predictions is not guaranteed by the application of either method; the reliability of the predictions depends, as with any other method, on the quantity and quality of the data that is available.

The main objectives of this paper are (1) to explore the utility of per-datum calibration and Bayesian model error analysis in risk assessments using a real world problem, and (2) to investigate the conceptual and philosophical differences between the two approaches in relation to the reliability of their results when applied to a specific problem. The next section of this paper provides a brief conceptual and mathematical description of the above methods. It is followed by their application to the problem of ^{90}Sr migration to water wells near the Chernobyl reactor site in assessing the uncertainty in model predictions associated with both model error and parameter error within the framework of a decision model for evaluating the necessity of remedial actions. The paper concludes with an assessment of the performance, data requirements, strengths and limitations of both methods.

2. Methodology

2.1. Per-datum model calibration

As was shown in [10] the influence of errors in the model structure (model error) on model predictions is not random in a probabilistic sense but systematic. Furthermore, the effect of model error on model predictions varies in space and time according to the spatial and temporal variation of model sensitivity to the existing structural errors, and it is different for the flow and solute transport components of a groundwater model.

To capture the statistical, as well as the spatial and temporal characteristics of model error, Gaganis and Smith [11] adopted a strategy of containing in the parameter estimates all the information about errors that exists in the data, by driving the residual of a calibration process to zero. The combined effect of parameter error e_{o} and model error e_{m} was then evaluated in the parameter space. For achieving a zero fitting residual, the inverse problem was solved at each data point $d_{(\text{v,l,t})}$, where v specifies the dependent variable (hydraulic head or solute concentration), l specifies the location and t the time of each available measurement. A unique set of maximum likelihood per-datum (for each data point) parameter vectors $\hat{\theta}^*_{(\text{v,l,t})} = \hat{\theta}^*_{(\text{v,l,t})}(e_{\text{o}(\text{v,l,t})}, e_{m(\text{v,l,t})})$ were obtained by using the following two criteria:

$$\Phi(\theta_{(\text{v,l,t})}) = G[d_{(\text{v,l,t})} - f(\theta)_{(\text{v,l,t})}] - \ln p_\theta(\theta) \approx 0 \tag{1}$$

$$\min(\text{with respect to } \hat{\theta}_{(\text{v,l,t})})[\Theta p(\hat{\theta}_{(\text{v,l,t})})] \tag{2}$$

where $\Phi(\theta_{(\text{v,l,t})})$ is the per-datum objective function and G is a performance criterion that measures the deviation of model response $f(\theta)$ from the observed dependent variable d. The quantity $p_\theta(\theta)$ is the prior probability density of the parameter vector θ. The second term on the right hand side of Eq. (1) enforces the constraints imposed by prior information on the parameters by assigning an infinite penalty on estimates lying outside the feasible parameter range Θ (prior parameter space). Since the per-datum formulation Eq. (1) to the inverse problem is always algebraically underdetermined, it does not have a unique minimum. Criterion Eq. (2) solves the problem of non-uniqueness of Eq. (1) by providing the means for selecting a unique $\hat{\theta}^*_{(\text{v,l,t})}$ from all possible solutions $\hat{\theta}_{(\text{v,l,t})}$ at each data