MODELLING UNCERTAINTY AND VARIABILITY IN ENVIRONMENTAL SYSTEMS

Renata ROMANOWICZ and Ray MACDONALD

Lancaster University, Lancaster LA1 4YQ, U.K.
e-mails: R.Romanowicz@lancaster.ac.uk; R.Macdonald@lancaster.ac.uk

Abstract
Scientists from different disciplines now routinely work together on complex, multi-interactive, geochemical and biochemical environmental processes and it has become necessary to define a common language that can be understood by all the relevant scientific community. This in turn will aid the transfer of expertise between scientists from different disciplines. This paper attempts to relate different modelling approaches dealing with uncertainty in environmental processes. The literature review is based on hydrological, geophysical and environmental risk modelling, but the conclusions are relevant to all scientists working on environmental problems, which are almost invariably poorly defined. We argue that modelling of environmental processes should be stochastic rather than deterministic. After listing the basic definitions and possible sources of uncertainty in environmental models, we present the main approaches to the modelling of uncertainties in, and variability of, environmental processes. We propose a general methodology for dealing with uncertainty, using as an example aspects of uncertainty assessment in modelling of rainfall-flow process at a catchment scale.

Key words: uncertainty estimation, environmental processes, risk assessment, Generalised Likelihood Uncertainty Estimation (GLUE), Data-Based Mechanistic Modelling

1. INTRODUCTION
There are two main reasons for building a model (Hjorth, 1994). One is to predict the behaviour of a real system under external conditions different from those observed. The second is to formulate a description of a historical event to get a better understanding of the processes involved. In both cases, predictive properties can be used to
make objective comparisons between different models. Approaches to the modelling will differ depending on the goal, but in both the predictive and descriptive modes, an evaluation of model performance can be made objectively only through comparison of model output variables with observations. The uncertainties present in the description of the model will variably influence the model predictions, depending on how they enter the equations describing the system.

An environmental system is understood here to be a specified set of interconnected, non-linear, dynamic physical processes. An environmental system model is a simplified description of the real processes, usually given in algorithmic form, in the context of the observation equation:

$$y_t = g(u_0, ..., u_t, \xi, \zeta, \theta, t),$$

where $y_t$ denotes the observed model output, $u_t$ is the model input, $\theta$ denotes the vector of model parameters which may or may not correspond to certain physical properties of the processes involved. The errors on the inputs, $\xi$, and the measurement error $\zeta$ are not known, and, in the general case, may be non-Gaussian (and might indeed be required to compensate for model structural error).

Both input and output variables can be measured with some accuracy and are not adjusted in the calibration exercise. In statistics, uncertain input variables are usually treated as the so-called “nuisance” variables, which introduce uncertainty to the model but are not of interest. The parameters are estimated (calibrated) by comparison of the model results with observations, using some specified measure of model performance.

Factors causing uncertainty in the predictions can include:

(a) The input variables are not known for the whole time horizon (only past values are observed), and/or are contaminated with noise.

(b) Measurement errors.

(c) The model describes the physical process in only an approximate way (structural errors).

(d) The goal of the modelling is uncertain.

(e) The parameters of the model are unknown and must be estimated (parameter estimation errors).

(f) Observations of the process output variables have measurement errors and change with time and site, i.e. they are different for each application and different input variables.

The model should describe how input variables are transformed within the model to output – the so-called forward problem. Model parameters are adjusted to ensure that the model output variables are close to the observed physical reality. Due to a lack of complete information on all the variables influencing the environmental system (uncertainty of input variables), its non-linearity and unavoidable simplifications in the description of the real processes, the parameter values calibrated for one set of
conditions will not give the same model performance for different conditions (input variables). The estimation of parameters from available observations of the variables simulated by the model is called an inverse problem.

Several issues follow on from the representation above, for example, how complex the model should be, what methods we should choose to describe the real process, and which methods for solving the problem should be chosen. All these issues are inter-related and depend on both the goal of the modelling and the quality and abundance of the available data. In what follows, we shall describe some existing methods to deal with uncertainty in models of environmental processes.

2. APPROACHES TO ENVIRONMENTAL MODELLING UNDER UNCERTAINTY

Work in environmental modelling can be grouped into three major themes: (1) modelling the variability of environmental processes (i.e. natural heterogeneity across time and space), (2) forward modelling – deterministic and stochastic approaches to the description of the physical rules controlling the processes, and (3) inverse modelling – parameter estimation techniques. The main stress here will be on stochastic approaches to modelling. The work cited relates mainly to hydrological modelling, but we are familiar with research on atmospheric, geomorphological and geological modelling. Water, however, plays a linking role between those different environmental areas, and hydrological research fairly represents general trends in recent research in these related disciplines.

Variability modelling

Variability modelling is understood here to be the statistical modelling of spatially- and time-variable environmental processes, in order to achieve a better basis for predictive model assumptions and a fuller understanding of the processes themselves. Variability modelling can thus be seen as the statistical modelling of different environmental variables, e.g. the modelling of a spatially variable conductivity field from observational data. Work on this topic is widely available in the literature. The spatial variability of soil hydraulic properties, for example, has been studied over the last two decades. To list a few examples, Beckett and Webster (1970) reviewed soil variability and its changes with sampling area and sampling depth. In their work on scaling, Simmons et al. (1979) gave an interesting analysis of spatial variability of soil properties. The development of computer power allowed more sophisticated multidimensional analyses of soil properties in the form of random fields (see e.g., Unlu et al., 1989; Rajaram and McLaughlin, 1990; Desbarats and Srivastava, 1991). Work on global climate change and global scale hydrology has included research on meteorology, climatology, ecology and hydrology (Wood, 1991), giving rise to problems of coupling models with different time and spatial scales and different structural resolution (Bloschl and Sivapalan, 1995).
Forward modelling

Forward modelling is a mathematical (algorithmic) description of the physical rules governing the system. A review of the stochastic modelling of groundwater flow and solute transport can be found in Beven and Binley (1995). As exact solutions to non-linear, complex, stochastic environmental processes are not feasible, approximated solutions are used, such as perturbation methods based on the first order approximation of random variables around mean values. The use of spectral methods gives a solution to the problem in the form of a covariance function of output variables under the assumption of the stationarity and linearity of the model structure (Bakr et al., 1978; Mantoglou and Gelhar, 1987; Yeh et al., 1985).

The Monte Carlo approach has found wide application in the analysis of stochastic problems and is based on repeated solutions of the deterministic equations using realisations of input values. There is no need to implement linear approximations and the method is very flexible. It is generally used as the sampling method to ease the large computer and storage requirements of regular grid sampling. Harter and Yeh (1996a, b) described Monte Carlo simulations of a 3-dimensional flow model with an input in the form of a randomly generated conductivity field, whilst Dagan et al. (1996) presented a particle tracking (Lagrangian) approach to flow and transport modelling. The particle tracking methodology can be combined with a numerical 2D flow model, giving a so-called Multiple Interacting Pathways (MIPS type) model (Beven, 1989). Oakley and O’Hagan (2004) developed probabilistic sensitivity analysis of complex models of real world processes based on Bayesian methods. Conditioning of the forward model on output measurements was done by Harter and Yeh (1996b), who gave an interesting analysis of the influence of observations on the results and variance of the predictions, providing insight into the processes involved and the dependence of the modelling on data.

A new approach to environmental modelling incorporates the use of fuzzy logic. A methodology based on fuzzy set theory was applied to a steady state groundwater flow simulation problem by Dou et al. (1995), to incorporate imprecise input parameters. The authors showed that this technique can provide a measure of the dependence of the results on input uncertainties. The biggest advantage of the fuzzy set approach in environmental sciences is its great flexibility in the quantitative representation of often only qualitatively defined, imprecise goals and constraints of the modelling, as well as poorly defined, spatially- and time-variable parameters and input variables.

Inverse modelling – calibration methods

Model calibration techniques have been studied extensively over the last two decades. Reviews of methods are given by Beck (1987) and Sorooshian and Gupta (1995). Recently, a number of papers have been published on groundwater inverse problems and geostatistically based inverse approaches to transmissivity estimation (e.g. Gallardo and Meju, 2003). Solution of the inverse problem of environmental models can be
found through statistical inferences from deterministic models (Garthwaite et al., 2002; Bates et al., 2000), while accounting for the uncertainty of inputs to the model (understood to be both parameters and external inputs to the system), output observations and model structural uncertainty.

In one class of statistical inference techniques, parametric or non-parametric approaches may be taken. In the parametric approach, after assuming the most appropriate distribution for the randomly sampled variables, we focus on obtaining the best estimates of mean, variance and possibly further moments of the distribution. In the non-parametric approach, the focus is put on obtaining a good estimate of the entire distribution of these variables. The first approach is more powerful, the second more flexible (Scott, 1992). The parametric methods consist of two steps: (a) specification of the parametric density family and (b) estimation of its parameters. As a result, there is a danger of misspecification, when an inadequate family of distributions is taken, leading to a bias that cannot be removed using large samples alone. Non-parametric methods are less efficient but they eliminate the need for model specification. In order to compare different estimators of unknown density function and to find the best, some error criteria are assumed. These may be Minimum Square Error (MSE), Minimum Integrated Square Error (MISE), $L_\infty$ norm, as well as $L_1$ norm, or even $L_p$ norm (Scott, 1992).

The difference between parametric and non-parametric estimators may be difficult to specify. In general, in nonparametric estimation, assumptions about the distribution of the observed data are less rigid. A smoother is a tool for non-parametric regression (Hastie and Tibshirani, 1990). In a single predictor case it is called scatter-plot smoothing. There are two important decisions to be made in scatter-plot smoothing: (a) how to average the response values in each neighbourhood (data range) and (b) how much neighbourhood to incorporate. Large neighbourhoods would produce low variance, but potentially large bias, small neighbourhoods the converse. This exemplifies the trade-off between bias and variance, controlled by a smoothing parameter, which in the case of scatter-plot smoothing is the width of the bin.

The second class of statistical inference techniques involves a division of the problems into Maximum Likelihood and Bayesian approaches. The classical Maximum Likelihood approach is related to parametric methods (Garthwaite et al., 2002), but may also be used in non-parametric estimation as an empirical likelihood (Owen, 2001). The Bayesian approach also applies likelihood function but treats the likelihood function parameters as random variables with some assumed prior distribution. The prior distribution of the parameters is based on expert opinion and/or past data or on some uninformative, flat, prior distribution. The Bayesian approach allows detailed studies to be targeted at the most informative areas and variables and also allows us to update information on certain variables as more observations become available. The choice of the distribution of errors required in parametric likelihood function or Bayesian approaches is equivalent to the choice of the goodness-of-fit criteria in non
-parametric estimation (Owen, 2001). The Bayesian estimator of the state variables in a linear, stochastic, dynamic system is the famous Kalman Filter (KF: Kalman, 1960); while the Bayesian estimator of the parameters in a linear-in-the-parameters regression model is the classic recursive least squares estimation algorithm (Young, 1984).

When dealing specifically with inverse problems in environmental modelling, it is rarely possible to assume that the distribution of parameters or the distribution of the modelling errors are known, or are Gaussian. Moreover, the inverse problem is very often ill-defined, i.e. it does not have a unique solution. The fact that there may be no solution to calibration problems has led to the introduction into hydrology of the concept of equifinality of models (structures and parameter sets) (Beven and Binley, 1992; Beven, 1993). Their Generalised Likelihood Uncertainty Estimation (GLUE) technique uses a likelihood measure to evaluate the acceptability of the parameter sets. Detailed descriptions of the GLUE technique can be found in Beven and Binley (1992) and Romanowicz et al. (1994), whilst Beven (2005) discusses the philosophical aspects of this approach. Related approaches were taken by Hornberger and Spear (1981), Fedra (1980), Tarantola (1987), and Dilks et al. (1992). A Multiple Interacting Pathways, i.e., MIPS type model (Beven, 1989), in combination with GLUE (Generalised Likelihood Monte Carlo) methodology, was applied by Buckley et al. (1994) to modelling groundwater contamination.

GLUE assumes that, in the case of large over-parameterised models, there is no inverse solution and, hence, that the estimation of a unique set of parameters optimising the goodness-of-fit criteria given the observations is not possible. In its formal description (Romanowicz et al., 1994), the method is shown to be analogous to Bayesian analysis and it uses Monte Carlo sampling of the parameter values in order to avoid dimensionality problems. The technique is based on the estimation of the weights associated with different parameter sets, based on arbitrarily chosen goodness-of-fit criteria and the derivation of a posterior probability function, which is subsequently used to derive the predictive probability of the output variables. The choice of a goodness-of-fit criterion, as used in the original GLUE method, may be interpreted as the choice of a distribution of errors between simulated and observed variables (Romanowicz et al., 1996; Romanowicz and Beven, 2005). As this approach requires multiple model simulations, it is restricted to comparatively simple models. However, it has successfully been applied to both lumped and distributed models. One of us (RR) took an active part in the development of the methodology and its application to rainfall-flow modelling (Romanowicz et al., 1993; 1994), and the modelling of the probability of flood inundation (Romanowicz and Beven, 1998; 2003; Romanowicz et al., 1996). It has also been applied to air pollution modelling (Romanowicz et al., 2000) and modelling of the transfer of pollutants in marine biota (Romanowicz and Young, 2003).

Another approach to coping with uncertainty in environmental processes is Data Based Mechanistic (DBM) modelling, introduced by Young (1998). It consists of
building models derived directly from the data. The main steps are (a) the derivation of a stochastic dynamic relationship between the input and output variables using time series analysis tools and, in particular, Stochastic Transfer Function (STF) methods, with possible non-linearities introduced by means of the non-linear transformation of input variables, and (b) a meaningful physical interpretation of the model. This methodology can also be applied to the analysis and simplification of large deterministic models (e.g., Young et al., 1996). The time series analysis tools mentioned above are available in the form of the CAPTAIN (Computer Aided Procedures for Time series Analysis and the Identification of Noisy systems) Toolbox, developed at Lancaster University for use within the multi-platform, Matlab™ software system.

In contrast to the GLUE technique, the STF-based approach chooses, from among linear STF model structures, only those that have an inverse solution, i.e. the model parameters can be estimated uniquely. Moreover, this technique estimates the covariance structure of the parameters together with the estimation errors, using Gaussian assumptions. Due to the variability of environmental systems and difficulties in the transposition of point measurements to meaningful average estimates, the method will normally yield different estimated parameter values when calibrated over different sets of observations. However, in cases where the data sets have adequately interrogated the internal variability, the parameter values will not be significantly different statistically.

3. PROPOSED APPROACH TO MODELLING UNCERTAINTY AND VARIABILITY IN ENVIRONMENTAL SYSTEMS

The methodology proposed here follows the parametric regression methods, with maximum likelihood function chosen for the best-fit criterion. The choice of non-parametric estimation procedures would avoid the problem of choosing an inadequate distribution for the statistical error model, required for the formulation of the likelihood function. However, non-parametric models involve the process of parameterisation using some chosen kernels, which in turn introduces further uncertainty into the model structure. Following Tarantola (1987), we propose to use the exponential distribution family to describe the error model. As shown by Bates et al. (2000), the choice of error model does not preclude the use of non-parametric kernel estimation methods for the derivation of the posterior distributions of the input and output variables. Within the parametric approach to statistical inference, we choose the Bayesian approach in which the parameters of the likelihood function are treated as random variables (Box and Tiao, 1973; Scott, 1992).

It is proposed that uncertainty and variability modelling are combined into the following hierarchical structural approach:

(1) Detailed analysis of the process, the available data, their uncertainties and the goal of the modelling. Analysis of the spatial and time variability of environmental processes and interactions between different environmental variables.
(2) Choice and development of the model structure or the class to which it should belong (e.g., linear or distributed), corresponding to the goal of the modelling and available measurements of the model input and output variables. Analysis of the degree of model complexity needed to capture the dominant behaviour of the process, conditioned by the available observations (e.g., using time series analysis).

(3) Analysis of the different sources of uncertainties and available observations of the model variables, choice of the prior distributions for the input variables and parameters.

(4) Sensitivity analysis of the problem, choice of the initial parameter ranges. Monte Carlo simulation of the model for the random values of parameters and input variables randomly generated according to the chosen priors.

(5) Inverse modelling. Conditioning of the results by available observations and derivation of the posterior distribution of predictions using a chosen Monte Carlo sampling technique and Bayesian updating. Combination of a priori, experimental and theoretical information to assess the uncertainty of the predictions. Visualisation of the resulting uncertainty of the predictions.

(6) Analysis of the influence of measurement and structural errors on the uncertainty of model predictions. Analysis of confidence bands of model predictions: repeating steps (2) to (5) for different model structures, depending on the availability of the observations and the goal of the modelling; use of external objectives to redefine model parameters, such as short term or long term forecasting and modification of the likelihood function to encompass them; introduction of hyper-parameters.

(7) Model validation on an independent data set. Analysis of the results and the formulation of recommendations for any additional measurements required. Answers provided to the following questions: what to measure and when?, which data are the most influential on the uncertainty limits? and how complex should the model be for the available observations? This analysis can be incorporated into the model structure as the monitoring network design (e.g., James and Gorelick, 1994).

In what follows, a discussion will be given of some of the topics listed above. An assessment of the time and spatial variability of environmental processes (point 1) can be made by applying a statistical data analysis. The procedure for selecting the statistical model most appropriate to describe the spatial structure of the medium is iterative (Jury et al., 1987). It should consist of: (a) assuming a hypothesis for the model structure; (b) estimation of the model parameters; (c) a test of model validity; (d) if the test for validity fails, the error must be diagnosed and steps (a)–(c) repeated. Jury et al. (1987) warned that disregarding the spatial structure of measurements leads to biased estimates of the moments of the assumed probability density function (pdf).

The model choice (point 2), analysis of uncertainties in the observations and choice of priors for parameters and input variables (point 3) and sensitivity analysis (point 4) should be regarded as interdependent procedures, because sensitivity analysis gives an indication of the model performance and changes required. We should look at
the problem of modelling on the basis of the available data – starting from the data and not the model at hand. Firstly, the dependencies between the measured process variables should be analysed statistically, using the results of the previous step. This analysis, together with a knowledge of the physics of the process and the goal of the modelling, should be the basis for the choice of model – physical or black-box – with dynamic relationships dictated by the data (the so-called Data Based Mechanistic (DBM) approach; Young, 1998; 2003). Where there are too few measurements, i.e. we cannot infer anything about the possible form of the relationships, we have to base the choice of model on scientific (possibly!) speculation, look for analogies in different environmental processes, or prepare laboratory tests which would allow us to say something about which variables should be measured. Where the model has already been chosen, based on criteria not controlled by the researcher, it is important to determine which dependencies between measured variables are resolved by the model. This might indicate which measurements should be used for parameter estimation. Sensitivity analysis of the selected measure of model performance may indicate the possible parameter ranges and indicate which parameters are the most influential.

Parameter estimation techniques are referred to in point 5. Bayesian estimation methods have found wide applicability in environmental modelling (Bates et al., 2000; Poole and Raftery, 2000). Closely related Markov Chain Monte Carlo (Campbell and Bates, 2001) and Importance Sampling (Bates et al., 2000) approaches have also been used in environmental model estimation. The search for parameter values with the minimum error between the simulated and observed variables is usually called the calibration of the model. Formally, the problem can be formulated as an inverse problem (Tarantola, 1987). The calibration technique proposed here is the GLUE methodology (Beven and Binley, 1992), which reformulates the problem of parameter calibration into the estimation of posterior probabilities of model responses and uses a Monte Carlo search through parameter space. The methodology is based on the Bayes formula (Box and Tiao, 1973). Errors between observed and modelled variables, together with the assumed prior distributions of parameters, are used to build the posterior likelihood, which reflects model performance and allows, for example, an evaluation of predictions of the probability of flooding (Romanowicz et al., 1996). In this way it is possible to incorporate observations from different time periods and/or sites using Bayesian updating. The most crucial step in this procedure is the choice of an adequate model for errors, which would reflect their statistical features and allow their transformation into independent errors required by the Bayes formula for the updating. For independent errors, evaluation of the posterior probability density function consists of \(N\) multiplications of the conditional probability function for each observation of the error \(\varepsilon_t\) given previous data. From this distribution, one can evaluate the confidence limits of the modelled variables at the observation sites. Also a less formal approach, incorporating non-additive model errors, can be applied, as in Romanowicz and Beven (2005).
4. UNCERTAINTY ESTIMATION OF RAINFALL-RUNOFF MODEL PREDICTIONS

The proposed methodology is now illustrated using the rainfall-runoff process. The aim of the modelling is the estimation of the uncertainty of predictions of the mechanistic rainfall-runoff model TOPMODEL (Beven and Kirkby, 1979) applied to the Hodder catchment, U.K. This catchment has 261 km$^2$ and is situated in North West England. The available data are hourly flows and rainfall observations for the year 1990 and a digital elevation map with 50 m$^2$ grid. The choice of TOPMODEL is justified by its simple structure (it uses only 4 parameters in the version applied here) and its mechanistic interpretation. TOPMODEL bases its calculations of the spatial patterns of hydrological response on the pattern of a topographic index for the catchment derived from a Digital Terrain Model (DTM). We have chosen the SIMULINK version of TOPMODEL, described in Romanowicz (1997), because of its clear, modular structure. The saturated zone model is assumed to be non-linear with the outflow $Q_b(t)$ calculated as an exponential function of a catchment average soil moisture deficit $S_3$ as

$$\frac{dS_3}{dt} = Q_0(t) - Q_r(t), \quad Q_b(t) = Q_0 \exp\left(-\frac{S_3(t)}{m}\right),$$

where $Q_0 = SK\theta \exp(-\lambda)$ is the flow when $S_3(t) = 0$, and $Q_r(t)$ denotes the recharge to the saturated zone. $SK\theta$ is a soil transmissivity parameter, $m$ is a parameter controlling the rate of decline in transmissivity with increasing soil moisture deficit and $\lambda$ is the mean value of the topographic index distribution in the catchment (Beven and Kirkby, 1979). Other parameters control the maximum storage available in the root zone ($LRZ$) and the rate of recharge to the saturated zone ($KS$).

Referring to the methodology presented in the previous paragraph, the analysis of the goal of the modelling and the choice of the model structure complete the first two steps. The third step consists of the analysis of uncertainties of input and output observations (i.e., rainfall and flow) and the model structure and its parameters. We assume here that rainfall and flow observation uncertainty is included in the choice of the error model structure and parameter uncertainty is taken care of in the choice of the parameter ranges in the Monte Carlo (MC) simulations. The influence of the model structure uncertainty may be accounted for via a random sample from different model structures (e.g., TOPMODEL with and without dynamic contributing areas). In this paper we restrict the analysis to parameter and observation uncertainty.

The MC sensitivity analysis (the 4th step of the methodology) was performed using the full version of TOPMODEL and January 1991 rainfall-flow data. Following an initial sensitivity analysis the parameter ranges were chosen to ensure that the range of the simulations covers the observations. 3000 simulations were then performed varying the four TOPMODEL parameters according to the prior distributions shown in Table 1.
Table 1
Parameter distributions applied in MC analysis of TOPMODEL; sensitivity analysis stage

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Distribution</th>
<th>Min.</th>
<th>Max.</th>
<th>Mean</th>
<th>Std</th>
</tr>
</thead>
<tbody>
<tr>
<td>SKO</td>
<td>uniform</td>
<td>10 000</td>
<td>40 000</td>
<td>25 000</td>
<td>8 600</td>
</tr>
<tr>
<td>m</td>
<td>uniform</td>
<td>0.001</td>
<td>0.03</td>
<td>0.0157</td>
<td>0.008</td>
</tr>
<tr>
<td>LRZ</td>
<td>uniform</td>
<td>$1 \times 10^{-4}$</td>
<td>0.04</td>
<td>0.02</td>
<td>0.012</td>
</tr>
<tr>
<td>KS</td>
<td>log-uniform</td>
<td>$1 \times 10^{-7}$</td>
<td>0.1</td>
<td>0.007</td>
<td>0.017</td>
</tr>
</tbody>
</table>

The 5th step of the methodology is the inverse problem modelling, i.e. estimation of uncertainty of TOPMODEL predictions. In the GLUE approach the predictive probability of flow takes the form:

$$P(\hat{y}_i < y | z) = \sum_{\{\theta_i \in \Omega\}} f(\theta_i | z),$$

where $f(\cdot)$ denotes the likelihood weight of parameter sets $\Omega = \{\theta_1, \ldots, \theta_n\}$, where $n$ is the number of MC samples, conditioned on the available observations $z$.

We look for the weights which account for both prediction and parameter/structure related errors. We assume the following form of likelihood measure for the $i$-th parameter set $\theta_i$, $i = 1, \ldots, n$:

$$f(\theta_i | z) \sim \exp \left( -\frac{\sum_{t=1}^{T} (y_{t,\text{sim}}(\theta_i) - z_{t,\text{obs}})^2}{\sigma^2} \right).$$

In the formal approach, with an explicit error model (Romanowicz et al., 1994), comes the variance of the prediction error based on observations. The optimal value of this variance may be derived from the likelihood function (Box and Tiao, 1973).

The 6th step of the methodology consists in analysis of the influence of the error model structure on the uncertainty of the predictions. In this study we treat $\sigma$ as a scaling parameter reflecting our lack of knowledge of the true information content of the residuals in constraining the uncertainty in the model predictions. One possible form for this scaling is to take the sum of the variances of the errors between observed and simulated flows over all the behavioural models and all time steps as an estimate, such that:

$$\sigma^2 = \sum_{t=1}^{T} \text{var}(y_{t,\text{sim}}(\Omega) - z_{t,\text{obs}}).$$

This will increase the dispersion of the resulting posterior parameter distribution (relative to the formal case) to account for the predictive model uncertainty without making additional assumptions about the model error structure. Choice of the scaling pa-
parameter is illustrated in Fig. 1. On the upper panel there are shown likelihood weights (4) for the recession parameter $m$, obtained using the sum of variances for the first two months of the model predictions in the calibration stage (January to February 1991) as a variance parameter (5). The lower panel shows the same likelihood weights obtained with $\sigma$ equal to the maximum error variance from this time period (i.e., $\sigma_1 > \sigma_2$). We can see that depending on the choice of this scaling parameter, the uncertainty bands of the predictions will change. The choice of this scaling parameter requires applying additional criteria, such as the minimization of the error variance for the validation period or minimization of the sum of errors between the observations and both lower and upper confidence bands.

Fig. 1. Likelihood weights for the recession parameter $m$; upper panel: scaling parameter $\sigma$ equal to the sum of the error variance; lower panel: scaling parameter $\sigma$ equal to the maximum error variance.

The flow predictions corresponding to the scaling parameter equal to the sum of the variance errors with uncertainty bands are shown in Fig. 2. In this study we also analyzed the application of the logarithmic error structure. For the Hodder catchment this led to very large over-predictions of peak flow values. However this transformation might be useful for other catchments (see Romanowicz et al., 1994; and Romanowicz and Beven, 2005).

The 7th step of the methodology consists of the validation of the results using the data set from November to December, 1991. The model was run for this period using the same parameter samples as for the calibration period. The resulting simulations were weighted by the posterior distribution of parameters obtained from the calibration period. The predictions for the validation period together with 0.95 confidence
Fig. 2. Calibration stage, January-February 1991. The estimates of flow are shown by the continuous line, with shaded areas corresponding to 0.95 confidence bands; observations are marked by dots.

Fig. 3. Validation stage, October-November 1990. The estimates of flow are shown by the continuous line, with shaded areas corresponding to 0.95 confidence bands; observations are marked by dots.
bands are shown in Fig. 3. Both calibration and validation predictions show over-prediction of low flows in certain periods, while in the other periods low flow predictions are accurate. One reason for this strange behaviour of the model may lie in water abstractions from the Stocks Reservoir, situated above the gauging station in the catchment, or the use of only one rainfall gauging station, which might be not representative for all the rainfall events. The further recommendations of step 7 of the methodology consist in the re-analysis of the results using the other validation periods. Hence, the posterior distribution from the first event can be used as the prior distribution for the second event, with scaling variance chosen in such a way as to minimise the variance of the predictions while also minimizing the bias, ensuring that the observations for both time periods lie within the 0.95 confidence bands.

5. SUMMARY

The authors believe that “complexity out of simplicity” (Young et al., 1996), or in another formulation, a top-down approach to the modelling of environmental processes (Young, 2003), is the way to gain a better understanding of the processes and to derive the uncertainty in the model predictions. The formulation of the problem should take into account the goal of the modelling, the available data and the existence of a solution. Among the different approaches, Bayesian estimation gives the widest perspective. The question remains as to how the description of the process should be chosen to ensure that the goal of the modelling is fulfilled. This statement includes the assumption that the goal of the modelling is clearly specified, which is often not the case. The iterative approach seems to be the most appropriate, consisting of iterative redefining of the goal and model, depending on the available observations.

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