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THE FUTURE OF DISTRIBUTED MODELS: MODEL CALIBRATION AND UNCERTAINTY PREDICTION

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ABSTRACT

This paper describes a methodology for calibration and uncertainty estimation of distributed models based on generalized likelihood measures. The GLUE procedure works with multiple sets of parameter values and allows that, within the limitations of a given model structure and errors in boundary conditions and field observations, different sets of values may be equally likely as simulators of a catchment. Procedures for incorporating different types of observations into the calibration; Bayesian updating of likelihood values and evaluating the value of additional observations to the calibration process are described. The procedure is computationally intensive but has been implemented on a local parallel processing computer. The methodology is illustrated by an application of the Institute of Hydrology Distributed Model to data from the Gwy experimental catchment at Plynlimon, mid-Wales.

KEY WORDS Distributed models Calibration uncertainty Likelihood

INTRODUCTION

In a critical discussion of the process of physically-based distributed modelling, Beven (1989a) has pointed to the limitations of the current generation of distributed models and argued that a possible way forward must be based on the realistic estimation of predictive uncertainty. Beven (1989b) and Binley and Beven (1991) have outlined a general strategy for model calibration and uncertainty estimation in such complex models. This strategy is explored further in this paper with a proper exposition of the approach, which we call Generalized Likelihood Uncertainty Estimation (GLUE). The GLUE procedure is placed in the context of other calibration and uncertainty estimation techniques, and its use is demonstrated by an application to the Gwy storm runoff data set from the Institute of Hydrology's experimental catchments at Plynlimon, mid-Wales which was previously used by Calver (1988) and Binley *et al.* (1991).

In outlining the basis of the GLUE procedure, Beven (1989b) starts from the premise that prior to the introduction of any quantitative or qualitative information to a modelling exercise, any model/parameter set combination that predicts the variable or variables of interest must be considered equally likely as a simulator of the system. It is further suggested that because all model structures must, to some extent, be in error and that all observations and measurements on which model calibration is based must also be subject to error, then there is no reason to expect that any one set of parameter values will represent a true parameter set (within some particular model structure) to be found by some calibration procedures. Rather, it is suggested that it is only possible to make an assessment of the likelihood or possibility of a particular parameter set being an acceptable simulator of the system. We may then assign a likelihood weight to any model structure/parameter set combination on the basis of the evidence considered. Each likelihood weight may be based on a number of different sources of evidence, that may include qualitative as well as quantitative measures.

Such an approach is, of course, different to most calibration procedures used in hydrology, in which some

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global optimum parameter set is sought, and any assessment of parameter and predictive uncertainty is made with respect to that global optimum. There have been may studies of techniques for facilitating the search for an optimal parameter set which have illustrated the difficulties of finding such an optimal set in the high-dimensional parameter space associated with hydrological models (see, for example, Ibbitt and O'Donnell, 1971; Sorooshian and Dracup, 1980; Sorooshian *et al.*, 1983; Gupta and Sorooshian, 1985; Kuczera, 1983; Hornberger *et al.*, 1985; Kuczera, 1990). Such difficulties arise from the use of threshold parameters, from intercorrelation between parameters, from autocorrelation and heteroscedascity in the residuals and from insensitive parameters. Such effects result in local minima, valleys and plateaux in the parameter response surface and will lead to difficulties in using either automatic search, random search, or trial and error calibration techniques. The problems tend to get worse with an increasing number of parameter values. In the case of physically-based distributed models which inevitably have a large number of parameters and in which one would expect highly intercorrelated parameters from physical principles, such difficulties will be experienced in an extreme form.

Indeed, it can be argued that in hydrological systems, equivalence of parameter sets should be expected. Hydrological terminology recognizes a number of different mechanisms of catchment hydrological response, including Hortonian or infiltration excess overland flow, saturation excess overland flow, subsurface stormflow, and throughflow or interflow. It is also recognized that these mechanisms are not mutually exclusive, but may occur in different parts of a catchment within the same storm, or at a point in the catchment during different storms depending on rainfall intensities and antecedent conditions. Clearly, any model that purports to be a general physically-based model of catchment hydrology must have the capability of predicting storm runoff responses based on all these mechanisms or combinations of them. It might therefore be possible that a particular storm hydrograph or combination of storm hydrographs might be predicted by the model, given a suitable combination of parameter values, by different combinations of the above mechanisms. How then does the hydrologist recognise what might be the 'correct' combination of parameter values, given that the effects of both errors in the model structure and errors in the observed data must also affect how well the model apparently fits the observations. The answer is, of course, that the hydrologist might have reason to prefer some combination of parameter values over others (perhaps (s)he has never seen overland flow in this catchment, although perhaps (s)he may never really have looked), but there may be many sets of parameter values that are really equally likely as simulators of the system under study.

At this point it is common practice to choose the set of parameter values that gives the 'optimal' fit to the observed data and, if the modeller is enlightened (for example Goren and Burges, 1981), to calculate an estimate of the uncertainty bounds around the optimum. This may be a little short sighted in the case of hydrological models. It might, for example, exclude sets of parameters that give a qualitatively more correct simulation of the response mechanism in the catchment, but which has parameters in a completely different part of the parameter space. This is the difficulty of distinguishing between multiple optima in the response surface. It might also exclude parameter sets distant from the current optimum that, while giving more accurate results than the current optimum for a different period of observations.

There is a particular problem associated with distributed models in this respect. The sheer number of parameter values involved has already been noted. Even when the hydrologist is prepared to accept that a distributed model is predicting the right sort of response mechanism, there may be many different combinations of the grid element parameters that might lead to equivalently accurate predictions. Without detailed internal state observations, it may be difficult to distinguish between these equivalent predictions. It should also be noted that such internal observations will generally be few in number and their value may be limited by the fact that such measurements are normally made at a much smaller scale than the grid element scale predictions (see Beven, 1989 for a discussion of this point). In fact, the preliminary work by Wood *et al.* (1988, 1990) on trying to assess the scale of an appropriate 'representative elementary area' in hydrological storm response would suggest that at the scale of a small catchment, getting the right pattern of parameter values may not, in fact, be crucial. However, taking account of the fact that those parameters may have some distribution function may be important, so that assuming that a catchment can be modelled by an appropriate homogeneous 'effective' set of parameter values will lead to significant errors.

GENERALIZED LIKELIHOOD UNCERTAINTY ESTIMATION (GLUE): AN OVERVIEW

The GLUE procedure recognizes the equivalence or near-equivalence of different sets of parameters in the calibration of distributed models. It is based upon making a large number of runs of a given model with different sets of parameter values, chosen randomly from specified parameter distributions. On a basis of comparing predicted and observed responses, each set of parameter values is assigned a likelihood of being a simulator of the system. That likelihood may be zero when it is considered that the set of parameter values gives a behaviour that is not characteristic of the system, either because of the direct comparison with the available data, or because of conditioning on the basis of some *a priori* knowledge about the system (e.g. overland flow has never been seen in the catchment). Note that any interaction between the parameters is not a problem in this procedure, it will be implicitly reflected in the likelihood values. Different sets of initial and boundary conditions may also be evaluated in this way, indeed, in the general case, different model structures can be considered.

We use the term likelihood here in a very general sense, as a fuzzy, belief, or possibilistic measure of how well the model conforms to the observed behaviour of the system, and not in the restricted sense of maximum likelihood theory which is developed under specific assumptions of zero mean, normally distributed errors (Sorooshian and Dracup, 1980; Sorooshian *et al.*, 1983). Our experience with physically-based distributed hydrological models suggests that the errors associated with even optimal parameter sets are neither zero mean or normally distributed.

In the GLUE procedure, all the simulations with a likelihood measure significantly greater than zero are retained for consideration. Rescaling of the likelihood values such that the sum of all the likelihood values equals 1 yields a distribution function for the parameter sets. It may then be seen that the traditional calibration search for an optimal parameter set is an extreme case of this procedure in which the 'optimal' solution is given a likelihood of 1 and all others are set to zero.

Such likelihood measures may be combined and updated using Bayes theorem (see Box and Tiao, 1973; Lee, 1989). The new likelihoods may then be used as weighting functions to estimate the uncertainty associated with model predictions (see below). As more observed data become available, further updating of the likelihood function may be carried out so that the uncertainty estimates gradually become refined over time.

The requirements of the GLUE procedure are as follows:

1. A formal definition of a likelihood measure or set of likelihood measures. It is worth noting at this stage that a formal definition is required but that the choice of a likelihood measure will be inherently subjective.
2. An appropriate definition of the initial range or distribution of parameter values to be considered for a particular model structure.
3. A procedure for using likelihood weights in uncertainty estimation.
4. A procedure for updating likelihood weights recursively as new data become available.
5. A procedure for evaluating uncertainty such that the value of additional data can be assessed.

These requirements will be addressed in the following sections, together with an example application to modelling the Institute of Hydrology Gwy catchment in Mid-Wales using the Institute of Hydrology Distributed Model (IHDM).

MODELLING THE GWY CATCHMENT

The IHDM represents a catchment as a series of hillslope planes an channel reaches. In the current version of the IHDM (IHDM4) surface flows on each hillslope and stream channel flow are modelled in a one-dimensional sense by a kinematic wave equation solved by a finite difference scheme. Subsurface flow, both saturated and unsaturated is modelled by the two dimensional (vertical slice) Richards equation, incorporating Darcy's Law and mass conservation considerations. It is solved by a Galerkin finite element scheme with allowance for varying slope widths and slope angles to account for slope convexity/concavity and convergence/divergence. Linkages are made between the different flow types: hillslope overland flow can arise from saturation-excess and/or infiltration-excess of the soil material. and saturated zones within the soil

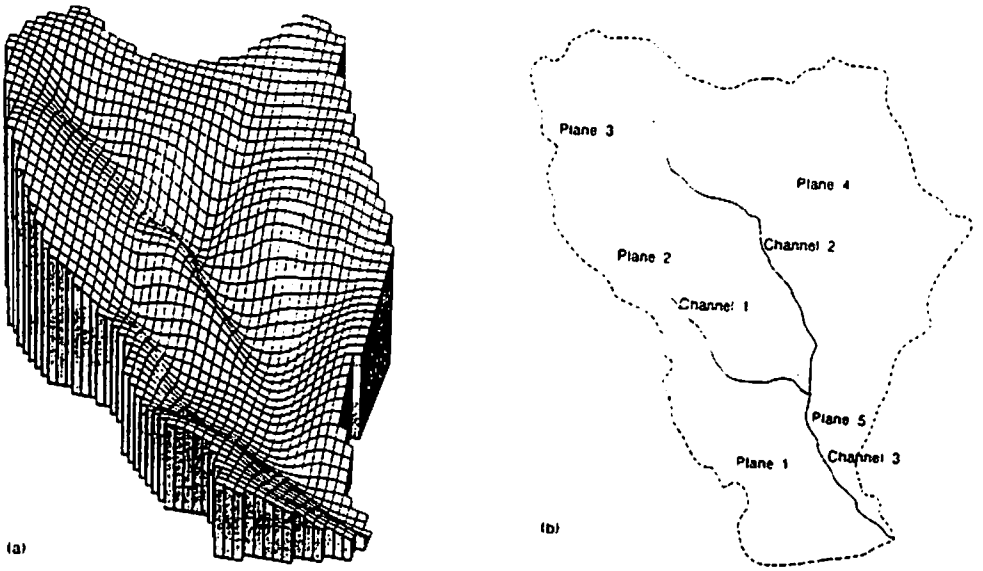


Figure 1. The Institute of Hydrology Gwy Experimental Catchment, Plynlimon, mid-Wales. (a) Catchment topograpny. (b) Discretization into hillslope and channel elements for use in the Institute of Hydrology Distributed Model

of the lower hillslopes provide lateral flow contributions to the stream system. Further details of the IHDM, including descriptions of the pre-programs for determination of effective precipitation, can be found in Beven *et al.* (1987).

The Gwy catchment at the head of the River Wye in central Wales has a drainage area of 3·9 km^2 (Figure 1a). It is an upland area of impermeable bedrock, predominantly shallow soils and grassland vegetation where streamflow is derived from throughflow, natural soil pipe flow and some overland flow. In using the IHDM on the Gwy catchment, the drainage area was divided into five sections of hillslope and three channel reaches (Figure 1b). Ten events were selected for study (see Table I). Five events were treated as calibration events (storms 1 to 5), the remaining events (storms 6 to 10) were retained for a validation exercise. The calibration sequence includes four winter events with a recurrence interval of between 1 and 10 years. The other calibration storm (storm 4 in Table I) was a very large runoff event of 5 August 1973 which was of a magnitude that caused some geomorphological changes to hillslopes and channels (Newson, 1980). Its return

Table I. Storm characteristics for the Gwy catchment

Storm no.	Date	Total Rainfall (mm)	Maximum intensity (mm h^{-1})	Peak flow (m^3 s^{-1})
1	17-19 Nov 81	80·51	9·17	8·0
2	27-29 Jan 83	111·44	8·60	6·1
3	11-13 Feb 76	107·25	10·43	8·5
4	5-7 Aug 73	121·77	25·66	16·8*
5	17-19 Nov 78	124·18	8·74	7·6
6	8-10 Dec 83	98·23	8·72	7·2
7	5-7 Oct 80	94·78	13·34	10·5
8	13-15 Jan 81	74·91	11·56	8·3
9	19-22 Apr 78	75·60	5·86	3·70
10	20-22 Jul 81	55·30	5·54	2·21

*Estimated

Table II. IHDM parameter distributions

Parameter	Description	Minimum	Maximum
K_s	Saturated hydraulic conductivity (m h^{-1})	0·02	2·00
θ_s	Saturated moisture content (m^3 m^{-3})	0·15	0·60
ψ_{in}	Initial soil moisture potential (m)	−0·40	−0·05
f	Overland flow roughness coefficient ($m^{0.5}$ h^{-1})	50·00	1000.00

period has been estimated at 50–100 years. This event has been included in the series to study the effect of a 'non-uniform' sequence of observed events in the GLUE procedure. The validation sequence consists of three winter events, which have very similar characteristics to the four winter events in the calibration sequence, plus two less intensive non-winter events (storms 9 and 10).

Although the IHDM , in theory, requires a large number of parameter values we have employed the model in a more practical and typical fashion by recognising uncertainty from only a few parameters (in this case four) to which the IHDM is considered to the most sensitive. The parameters, which are listed in Table II, were considered to be effective values as spatial variability was not treated. The other parameters of the IHDM were fixed on the basis of field estimates.

DEFINITION OF THE LIKELIHOOD FUNCTION

As with any calibration procedure, the GLUE methodology requires the definition of some measure of goodness-of-fit, in this case the likelihood measure, in comparing observations and predictions of the model. The likelihood measure must have some specific characteristics. It should be zero for all simulations that are considered to exhibit behaviour dissimilar to the system under study, and it should increase monotonically as the similarity in behaviour increases. These are not restrictive requirements, and could be satisfied by adapting many of the goodness-of-fit indices used in the past. Some example likelihood measures are:

a) A model efficiency or coefficient of determination defined by

$$\mathscr{L}_e = (1 - \sigma_e^2/\sigma_o^2);\ \sigma_e^2 < \sigma_o^2 \qquad (1)$$

which is zero when the variance of the residuals (σ_e^2) is equal to the variance of the observations (σ_o^2), and one when the residuals are everywhere zero;

b) The likelihood function used by Binley and Beven (1991) which is also based on the sum of squares of the residuals as

$$\mathscr{L}_\ell = (\sigma_e^2)^{-N} \qquad (2)$$

where N is a parameter chosen by the user. Note that when $N = 0$, every simulation will have equal likelihood and when $N \to \infty$ the single best simulation will have a rescaled likelihood of 1 while all others will have a likelihood of zero.

c) Scaled maximum absolute residual

$$\mathscr{L}_m = \max[|e(t)|];\ t = 1, \ldots, T \qquad (3)$$

where $e(t)$ is the residual between observed and predicted variables at time t. This type of measure has been used, for example, by Keesman and van Straten (1989, 1990) and van Straten and Keesman (1991) in modelling lake eutrophication, with the additional requirement that residual lies within measurement error bounds (else $\mathscr{L}_m = 0$). This will generally require, however, that the observed data must be smoothed to remove outliers; otherwise no parameter sets may give an acceptable simulation under this likelihood

definition. They found that it was necessary to make the 'measurement error bounds' unduly wide to obtain a reasonable number of parameter sets that would satisfy this latter criterion at *all* time steps, an interesting reflection on the quality of the theory that underlies our mechanistic models of environmental systems. Other likelihood measures based on the absolute values of the residuals are also possible such as the sum of the absolute values

$$\mathscr{L}_a = \sum^{T} |e(t)| \tag{4}$$

LIKELIHOOD FUNCTIONS FOR MULTIPLE OBSERVATIONS

Most studies of calibration procedures in hydrology have examined goodness-of-fit measures based on observed and predicted discharges (Sorooshian and Dracup, 1980; Hornberger *et al.*, 1985). In the present context we may also be interested in comparing predictions of internal state variables. Some way of combining information from different measures of behaviour is therefore required. In this respect, the approach suggested here has something in common with the conditional simulation used in groundwater modelling (e.g. Delhomme, 1979) in which uncertainty in the model predictions is estimated by Monte Carlo simulation conditioned on parameter distributions for the grid elements of the model. Those distributions are calculated by the kriging of measured values, such that the parameter variances are low close to measurement points and increase with distance away from the measurement points. This may be considered as a special case of the procedure proposed here in which the likelihood values are defined *a priori* on the basis of locally Gaussian distributions defined by the kriged variances.

For the general case of multiple sites or types of observation contributing to an overall likelihood weight for each simulation, some way of combining the individual measures of goodness of fit is required. There are also a number of different ways of doing this. An obvious choice is to use a weighted sum of the individual measures, for example the likelihood function in Equation 2 becomes:

$$\mathscr{L}_{lm} = \left\{ \sum_{j=1}^{m} \frac{(W_j)}{\sigma_{ej}^2} \right\}^N \tag{5}$$

where: m is the number of observed responses,
W_j is the weight for observation j such that $\sum W_j = 1$,
σ_{ej}^2 is the error variance of the jth observed variable,
but this has the effect of averaging out the effect of poor performance on one or more measures. This may be made a dimensionless measure if the weights are chosen to be equal to the variance of the observations.

An alternative automatic weighting procedure for multiple goodness-of-fit criteria has been suggested by van Straten (1983) as the pseudomaximum likelihood measure

$$S_{pml} = \prod_{j=1}^{m} \sigma_{ej}^2 \tag{6}$$

for which an appropriate likelihood measure might be

$$\mathscr{L}_{pml} = 1/S_{pml}$$

A different function adopted by Klepper *et al.* (1991) is based on the maximum of the series of model-observation errors, weighted according to their 'usefulness', for each realization. A weighted product of individual error criterion could also be considered, or if the likelihoods are treated as fuzzy measures of the set of acceptable simulators of the system, a number of generalized fuzzy set operations could be conisidered. Given the m fuzzy or likelihood measures $\mathscr{L}_a, \mathscr{L}_b, \ldots \mathscr{L}_m$ associated with each realization, we seek to

combine those measures in some way. Two possible ways are:
Set union

$$\mathscr{L}_a \cup \mathscr{L}_b \cup \cdots \mathscr{L}_m = \max[\mathscr{L}_a, \mathscr{L}_b, \ldots \mathscr{L}_m]$$

Set intersection

$$\mathscr{L}_a \cap \mathscr{L}_b \cap \cdots \mathscr{L}_m = \min[\mathscr{L}_a, \mathscr{L}_b, \ldots \mathscr{L}_m]$$

More complex union and intersection operators are described by Klir and Folger (1988).

Again it should be emphasized that there is a considerable subjective element involved in the choice of the likelihood function, which should reflect not only the observations available but also the purposes for which the model is required. For example, some studies might place great weight on the accuracy with which the model can predict peak discharges, while others would place much more emphasis on correctly reproducing the occurrence of saturated conditions at a given level in the soil. The important point is that an explicit definition of the likelihood function used must be made for each study. It should also be stressed that the likelihood measure is associated with a *set* of model parameter values and, as such, different simulations with very similar values of any single parameter might be associated with a wide range of likelihood values. We will illustrate this point in the application presented below.

UNCERTAINTY AND MODEL STRUCTURAL ERROR

There are many sources of error in any modelling study: error due to poorly defined boundary conditions and input data; error associated with measurements used in model calibration; and error due to deficiencies in model structure. The likelihood weights of the GLUE procedure will reflect all sources of error in the modelling process and allow the uncertainties associated with those errors to be carried forward into the predictions.

It would normally be expected that the residuals between the observations and predictions for any particular simulation might have structure. In general, those residuals will be biased and autocorrelated with heteroscedastic variance (for example Sorooshian and Dracup, 1980). In what follows, we will take no further account of the structure of the residuals since the effects of such structure are retained implicitly in the likelihood weight associated with the parameter set producing that residual sequence.

The result of applying the GLUE procedure is a range of likelihood weight predictions that may be compared with observed behaviour. We may find, as will be demonstrated below, that the observations with which model predictions are to be compared may still fall outside the calculated uncertainty limits. If it is accepted that a sufficiently wide range of parameter values (or even model structures) has been examined, and the deviation of the observations is greater than would be expected from measurement error, then this would suggest that the model structure(s) being used, or the imposed boundary conditions, should be rejected as being inadequate to describe the system under study.

When this is found to be the case, a model can be redeemed by redefining the likelihood function used to produce wider uncertainty limits (e.g. by reducing the power N in Equation 2). The importance of an explicit definition of the likelihood function is then readily apparent as the calculated uncertainty limits will depend upon the definition used. The modeller can, in consequence, manipulate the estimated uncertainty of his predictions by changing the likelihood function used. At first sight, this would appear to be unreasonable but we would hope that more careful thought would show that this is not the case, provided that the likelihood definition used is explicit. After all, if the uncertainty limits are drawn too narrowly, then a comparison with observations will suggest that the model structure is invalid. If, on the other hand they are drawn too widely, then it might be concluded that the model has little predictive capability. What we are aiming at is an estimate of uncertainty that is consistent with the limitations of the model(s) and data used and that allows a direct quantitative comparison between different model structures. Hopefully, with time and improved

understanding of both system and appropriate model structures, more demanding likelihood measures can be used and the uncertainty limits will accordingly be drawn more tightly.

It is perhaps worth noting that more traditional techniques of uncertainty estimation in linear statistics are also dependent upon the definition of likelihood used, although the assumptions of the theory (normally distributed, uncorrelated, zero mean, constant variance residuals at the most restrictive) are commonly violated.

PRIOR PARAMETER DISTRIBUTIONS

Given the definition of an appropriate likelihood measure, the next stage in the GLUE procedure is the definition of appropriate initial or prior parameter distributions. There may again be a considerable degree of subjectivity involved at this point. The prior parameter distributions must be broad enough to ensure that the model behaviours will span the range of observations. This may not always be easy to assess *a priori*, even given some physical insight or reasoning. For example, in physically-based distributed models it will be necessary to specify hydraulic conductivities for different soil types and soil horizons for each grid element in the model. Given some information on soil texture or particle size distributions, the estimation procedures reported by Clapp and Hornberger (1978) or Rawls and Brakensiek (1989) would appear attractive. In those studies, the mean and standard error of estimation of hydraulic conductivity values can be estimated for different soil types based on the very large data sets accumulated by the USDA. Some care is in order, however. The measured hydraulic conductivities used in those studies were carried out on small soil samples and must be most representative of the soil matrix. The model requires hydraulic conductivity estimates at the grid element scale, where both mean and variance might be very different (see discussion in Beven, 1989a, b). It is therefore probably safest to start with unduly wide ranges of possible parameter values, since the Bayesian likelihood weighting procedure will refine the range of acceptable parameter sets as more data is added.

From a Bayesian point of view, we may express the problem of defining these initial parameter distributions in terms of a set of assumptions reflecting our prior knowledge of the parameter values or, more normally perhaps, a set of assumptions that is consistent with our lack of prior knowledge about what might be appropriate values. The prior distributions will consequently often be defined purely subjectively, with the only requirement of the current procedure being that the resulting distributions should be 'proper' in the sense that the assumed probability density function should integrate to unity. This will normally require that the modeller must decide on an appropriate prior range of the parameters to be considered together with the form of the distribution function within that range. In the case of little prior knowledge, a uniform distribution function over a chosen (wide) range will be appropriate to define a suitable 'reference' or standard prior distribution. The suitability of the chosen range may be evaluated by comparison of the predicted responses within that range.

The assumption of a locally uniform prior distribution reflecting limited knowledge about appropriate values of the parameters is a convenient one, but has been the subject of considerable discussion in the literature of Bayesian statistics (see for example Box and Tiao, 1973). An important objection, that is relevant to hydrological modelling, is that a uniform distribution associated with a parameter, θ, may not be uniform in transformations of θ, i.e. the effect of θ within the model. Ideally, we would chose a prior distribution consistent with the effectiveness of changes in a model parameter on changes in model response. For example, it might be more appropriate to chose a uniform distribution of log-transformed hydraulic conductivity. This is, of course, consistent with a modeller's prior knowledge of the sensitivity of a particular model to different parameter values in different circumstances.

In practice, the assumption of a uniform reference prior, is unlikely to prove critical, because as soon as information is added in terms of comparisons between observed and predicted responses then, if this information has value, the distribution of calculated likelihood values should dominate the uniform prior distribution when uncertainty estimates are recalculated. Estimates of the prior parameter distributions for the Gwy catchment have been based on the previous experience of modelling this catchment reported in Binley *et al.* (1991). Uniform distributions have been chosen with a range wide enough to encompass the

expected modes of response of the catchment (see Table II). Again it is emphasized here that the procedures are applied to parameter sets, rather than values of individual parameter values, so that any interactions between parameters are taken into account implicitly in the procedure.

UNCERTAINTY ESTIMATION

The likelihood value associated with a set of parameter values may be treated as a fuzzy measure that reflects the degree of belief of the modeller in that set of parameter values (within its particular model structure) as a simulator of the system. That degree of belief is derived from and may be carried over to the predicted variables arising from that set of parameter values. Treating the distribution of likelihood values as a probabilistic weighting function for the predicted variables, therefore allows an assessment of the uncertainty associated with the predictions (conditioned on the definition of the likelihood function, input data and model structure used). For example at any particular time step, the discharges predicted by each sample model run may be ranked in order of magnitude and, using the likelihood weights associated with each run, a distribution function of the predicted discharges may be calculated. Some examples are shown in Figure 2. From this distribution various summary values can be calculated, such as the weighted mean predicted discharge, the centroid and modal values, the weighted variance and selected quantiles.

Figure 3 shows the results of multiple IHDM simulations of the Gwy catchment hydrograph for storm 1 given a known rainfall record, using parameter sets selected from the specified uniform prior distributions. Each simulation can be associated with a likelihood value based on how well it corresponds to the observed discharge. The likelihood function used here is that defined by Equation 2 above, as used by Binley and

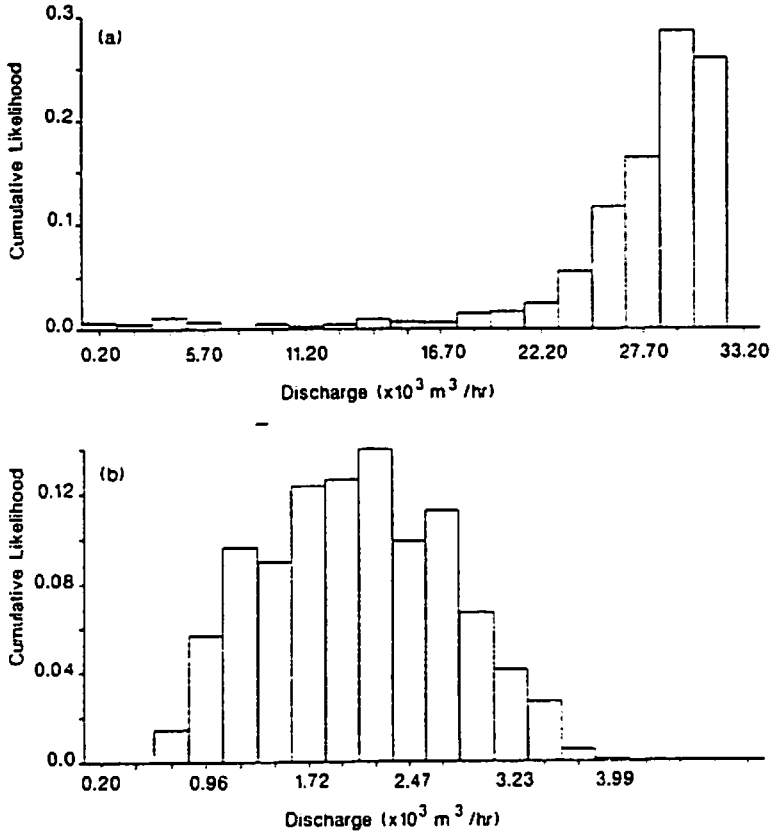


Figure 2. Distribution function of predicted discharges for storm 3 based on a priori likelihood distribution. (a) Distribution at peak mean flow (b) Distribution at end of event

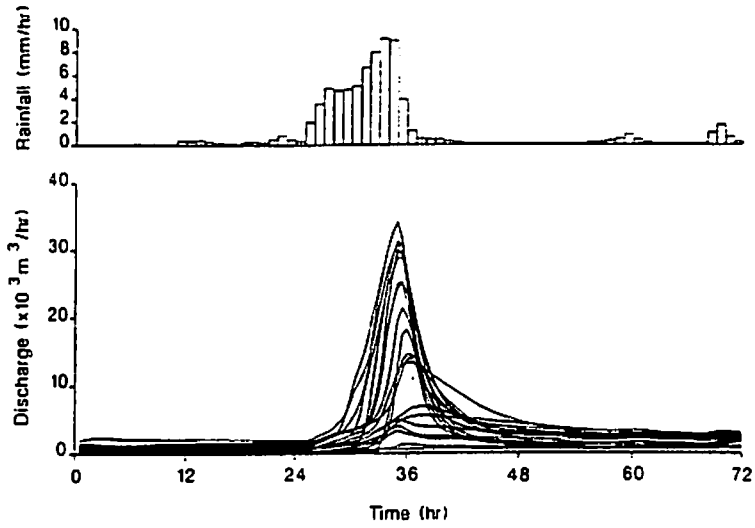


Figure 3. A subset of 20 simulations for storm 1

Beven (1991). The cumulative likelihoods are scaled to 1, so that at any time step the discharges associated with the individual model runs can be expressed as a cumulative distribution function.

Two points are worth noting about this procedure. The first is that, although the distribution of predicted discharges appears approximately Gaussian at some time steps and other time steps in the same simulation period it may be highly skewed (Binley *et al.*, 1991). Thus in general the normal calculation of uncertainty limits as a function of the variance of the predicted values will not be generally applicable. In this study we have chosen to use the estimates of the 5th and 95th percentiles of the cumulative likelihood distribution as the uncertainty limits of the predictions, and the centroid as a measure of the modal behaviour. Figure 4 shows the predicted 90 per cent uncertainty limits defined in this way for storm 1.

Secondly, from time step to time step the position of any particular simulation run within the distribution will vary. A run that overpredicts at one time step may well underpredict at another time step. This should be

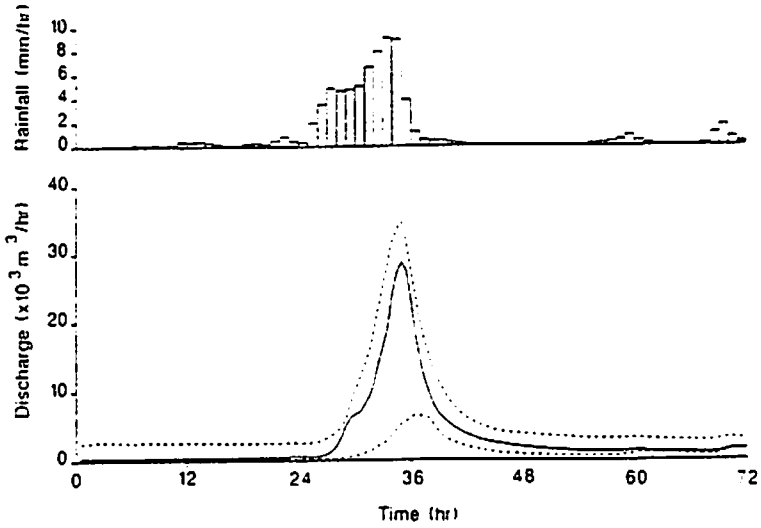


Figure 4. Predictive uncertainty for storm 1 based on posterior parameter distribution. Solid line indicates observed flow, dashed line indicates 5 and 95 per cent simulation limits

expected from the interaction between the individual parameters and the dynamics of the model, but implies that the uncertainty limits cannot be related directly to a variance of estimation for individual parameter values. Remember, each likelihood value is associated with a *set* of parameter values.

We have specifically chosen to avoid the use of single simulation runs to represent, for example, the 'best fit' to the observed data. We wish to avoid the idea that there is one set of parameter values that can, with any given model structure, represent a catchment area when it is known that the model structure must be in error.

UPDATING OF LIKELIHOOD WEIGHTS

The modeller will frequently be in a position of having a continuing input of new observation periods, or different types of observations that can be utilized to update the likelihood values and estimated uncertainties. There may be different ways of utilizing such data to refine the model of a particular catchment. In the past, this has usually been done on a purely ad hoc basis. One advantage of the GLUE procedure suggested here is that this procedure must be formalized while still accepting that different types of observation might be given different weight in the modelling procedure.

Recalculation of the distribution function associated with the parameter sets is carried out easily using Bayes equation in the form (Fisher, 1922):

$$\mathscr{L}_A(\Theta|y) = \mathscr{L}_y(\Theta|y)\mathscr{L}_o(\Theta) \tag{8}$$

where $\mathscr{L}_o(\Theta)$ is the prior likelihood distribution of the parameter sets,

$\mathscr{L}_y(\Theta|y)$ is the calculated likelihood function of the parameter sets given the set of new observations, y, and

$\mathscr{L}_A(\Theta y)$ is the posterior likelihood distribution of the parameter sets.

Bayes equation in this form presupposes that the likelihood distribution has a cumulative value of unity. It is particularly easy to apply in the case of the Monte Carlo procedure used here, since each sample parameter set is associated with its own prior likelihood, and its own likelihood function value so that Equation 8 can be applied on a sample by sample basis. The definition of the distributions will, of course, remain subject to the sampling limitations of the Monte Carlo procedure.

The updating of the resulting uncertainty limits is demonstrated for the Gwy catchment in Figure 5. Figures 5b and c show the resulting uncertainty limits on the predicted discharges as calculated using the prior and posterior likelihood distributions. This shows that there is a slight reduction in uncertainty associated with taking account of the new observations. The calculated posterior likelihood distribution may be used to project the uncertainty associated with the predictions forward, and becomes the prior distribution in Equation 8 when new observations are available to calculate a new set of values of the chosen likelihood function. Thus, in a well-posed model with accurate observations we should expect that the posterior likelihoods should become increasingly constrained as additional observations are considered. Whether this will also be true of hydrological models and hydrological observations remains to be seen. Figure 6 shows the prior and posterior uncertainty limits calculated for the high magnitude event storm 4. In this case it can be seen that the limits widen. This suggests that the event dependency of the IHDM's apparently physically-based parameters will limit the possibility of finding an 'optimum' parameter set.

RESAMPLING OF PARAMETER DISTRIBUTIONS

Initial experience in using the GLUE procedures has revealed that the effect of using the Bayesian updating procedures described above is to gradually reduce the number of parameter sets that have posterior likelihood values significantly greater than zero. This will gradually therefore reduce the sample size defining the appropriate distributions. This is effectively saying that the area of the parameter space that contains parameter sets that are acceptable simulators of the catchment becomes increasingly constrained as more data is taken into account. This would be expected (if a model has any value at all) and in a traditional model calibration context would indicate that there is a convergence on an optimal set of parameter values. This is

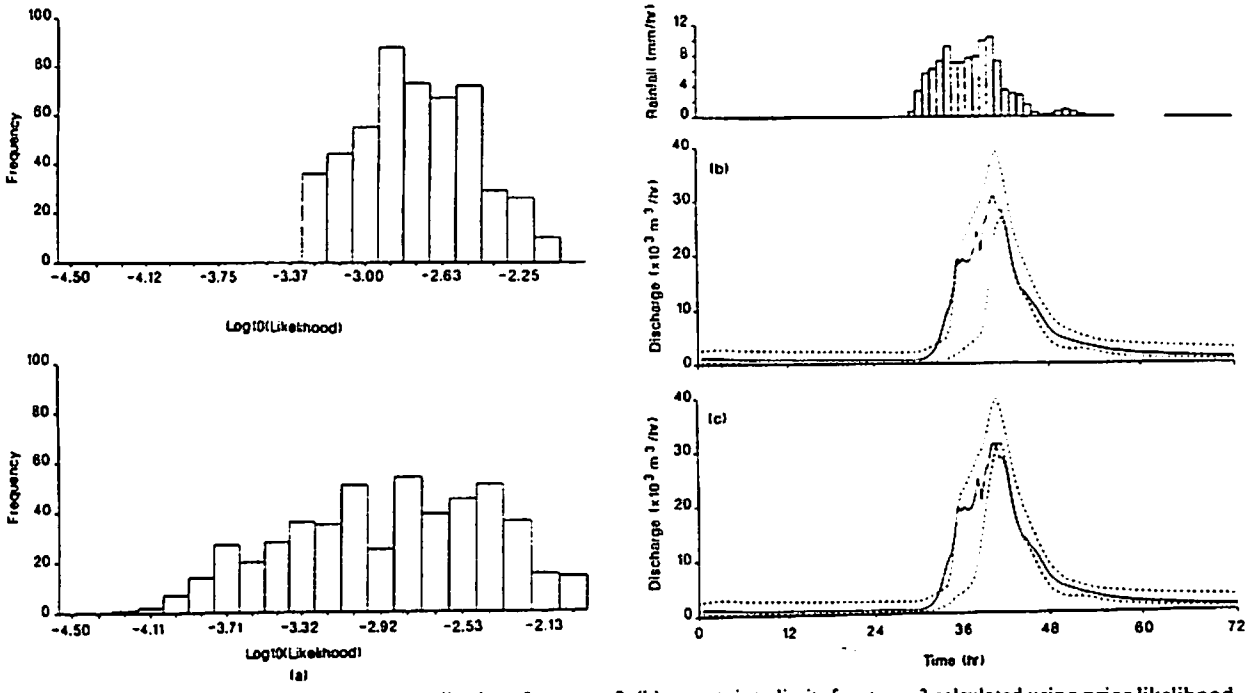


Figure 5. (a) prior and posterior likelihood distributions for storm 3. (b) uncertainty limits for storm 3 calculated using prior likelihood distribution. (c) uncertainty limits for storm 3 calculated using posterior likelihood distribution after conditioning based on observed discharges in storm 3

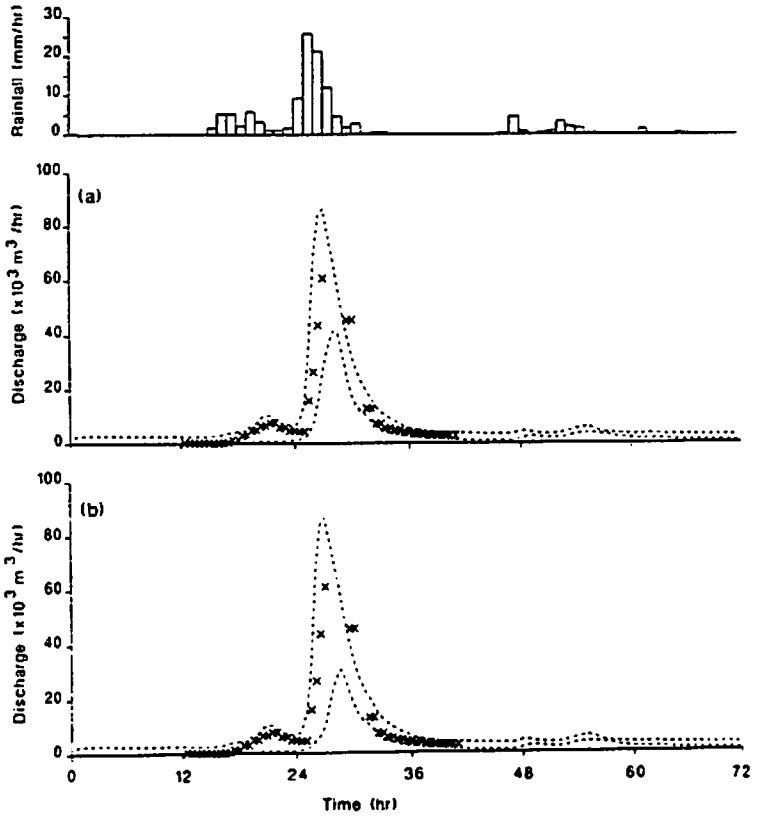


Figure 6. (a) Uncertainty limits for storm 4 calculated using prior likelihood distribution; (b) Uncertainty limits for storm 4 calculated using posterior likelihood distribution after conditioning based on observed discharges in storm 4

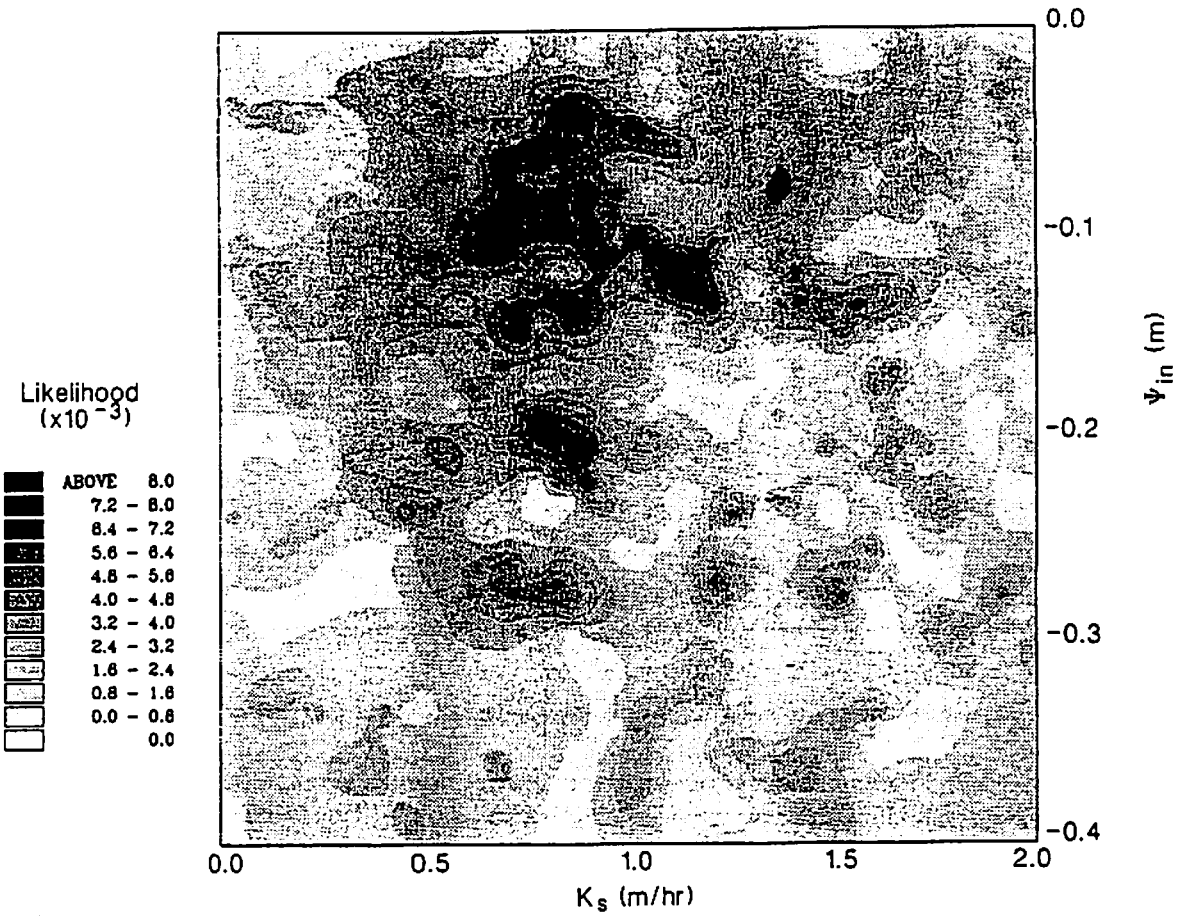


Figure 7. Variation of the likelihood function, prior to storm 3, with K_s and ψ_{in}

not necessarily the case here for two reasons. The GLUE procedure explicitly allows that the 'optimal' set of parameter values may vary from period to period of observation and that this will be reflected in the evolution of the posterior likelihood distribution. It also allows that there may be more than one region of high likelihood values in the parameter space, as shown in Figure 7, where the likelihood distribution has been collapsed onto a two parameter space.

There is, as in any multiparameter calibration problem, a certain difficulty in displaying such results. The GLUE procedure is only sensitive to such complex response surfaces in respect of the number of samples required to define the likelihood distribution adequately. Again, it is worth emphasising that it only works with parameter sets, and the display of the distribution for individual parameters has value only in the sense of evaluating the sensitivity of the model to that parameter. Sensitivity analysis can be carried out using the GLUE results directly using, for example, the Generalized Sensitivity Analysis procedures of Hornberger and Spear (1981), modified to take account of the likelihood weights for the acceptable simulations. Figure 8 shows such a comparison of the cumulative distributions for the behaviour and non-behaviour simulations (the definition of which follows) for the IHDM parameters varied in this study after taking account of the observations from the first storm. This shows a distinct difference between the behavioural and non-behavioural distributions of θ_s and ψ_{in}, which is demonstrated further by the significance of the Kolmogorov-Smirnoff D statistic in each case (Table III).

It is important, however, to retain a proper definition of the areas in the response surface with significant likelihood values as more observations are taken into account. This may be done by excluding those sets of parameter values giving simulations with very low likelihood values (the non-behaviour simulations of

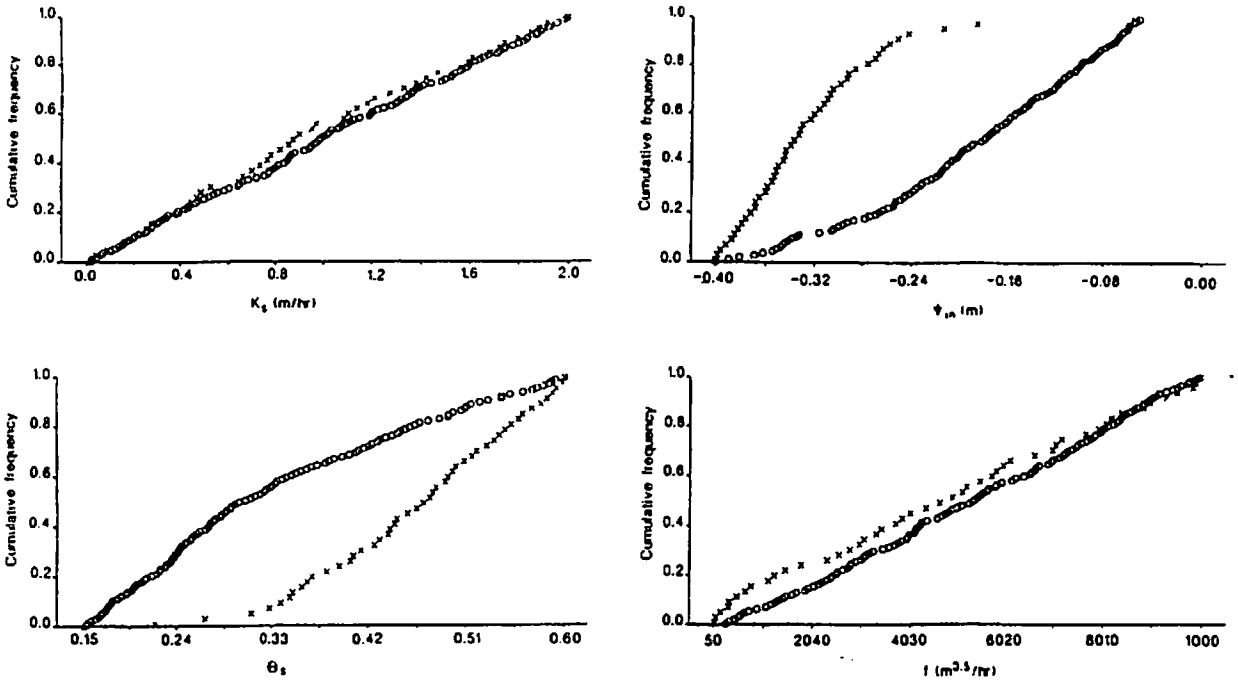


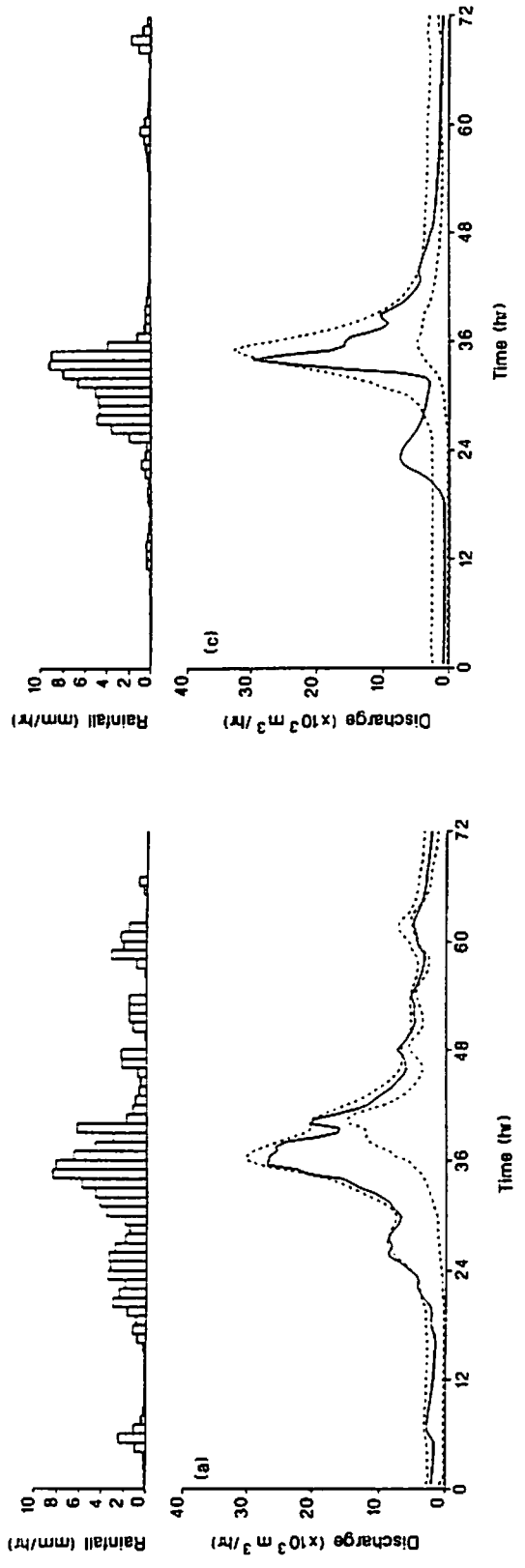
Figure 8. Comparison of behavioural (o) and non-behavioural (x) parameter distributions based on likelihoods after storm 1

Hornberger and Spear, 1981) and replacing them with a new set of simulations which are expected to have significant likelihood values by resampling the response surface. This is done quite easily within the GLUE procedure since the shape of the likelihood distribution is always defined with respect to a uniform sampling of values along each parameter axis. For the current purpose this has advantages over the more common Monte Carlo procedure of taking samples to reproduce the expected density function in the parameter space, so that each sample is then equally weighted. Excluding a set of parameter values is equivalent to setting the likelihood at that point in the parameter space to zero. New sample sets may be added by continuing to sample uniformly along each axis and interpolating a likelihood value from the posterior distribution defined by the existing sets of values. If the interpolated value results in a negligible likelihood value, a new sample is taken until the required number of sample parameter sets is available.

This resampling procedure is computationally quite efficient in that new sets of parameter values can be chosen before the model runs are made. The search area might also be limited if it is clear that there are areas of the parameter space that are not expected to yield significant likelihood values, but experience would suggest that excluding such areas is difficult if the parameters are considered individually and should only be done with care. The estimated likelihood values for the resampled parameter sets can be added to the existing prior likelihood distribution to be used in the next application of the Bayesian updating of Equation 8. They represent, in effect, our best prior knowledge of the shape of the likelihood distribution before taking account of any additional observations. In this study we treat all realisations within the lower 5 per cent tail of the cumulative likelihood distribution as non-behavioural and adopt a simple distance squared interpolation procedure for resampled, taking account of the 10 nearest neighbours in the parameter space to each resampled point. All the results presented here have made use of this resampling technique.

MODEL VALIDATION AND PREDICTION WITHIN THE LIMITS OF UNCERTAINTY

The GLUE procedure allows the modeller to be realistic about the uncertainties associated with his modelling in a way that is conceptually very simple to understand. The posterior likelihood distribution may be used directly to evaluate the uncertainty limits for future events for which observed data may not be



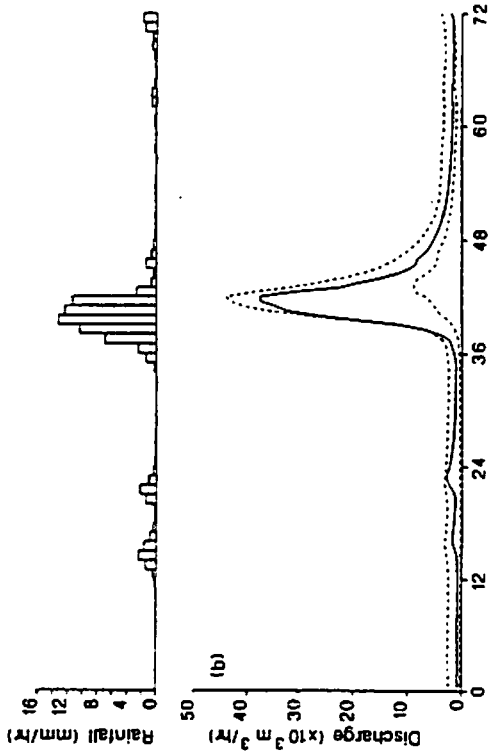


Figure 9. Predictive uncertainty for three storms based on *a priori* parameter distribution. Solid line indicates observed flow, dashed line indicates 5 and 95 per cent simulation limits. (a) Storm 6. (b) Storm 8. (c) Storm 9

Table III. Kolmogorov-Smirnoff D statistic calculated for behavioural and non-behavioural IHDM parameter distributions for storms 1 to 5. Values underlined are significant at the 5 per cent level

Parameter	K_s	θ_s	ψ_{in}	f
Storm 1	0·076	0·497	0·674	0·111
Storm 2	0·190	0·214	0·303	0·260
Storm 3	0·184	0·129	0·437	0·290
Storm 4	0·354	0·162	0·248	0·064
Storm 5	0·270	0·185	0·323	0·116

available or, in a split sample test, to validate a model by comparison with observed data that have not been used in the likelihood updating. This has been done for five further storms on the Gwy catchment, using the posterior likelihood distribution following storm 5. The results are shown in Figure 9 for storms 6, 8 and 9. The uncertainty bands for storm 8 fail to enclose the minor peak for storm 8 due to inconsistency between observed precipitation and discharge. Such a feature, which is not uncommon, should be recognized if the observations of storm 8 were to be used for further refinement of the likelihood distribution.

Physically-based models, such as the IHDM are increasingly being used to predict the results of land-use and climatic change in a catchment. In general, this has been done by a variation on scenario modelling without any consideration being given to the uncertainties associated with individual runs of the model (but see Binley *et al.*, 1991 for an exception in the context of land-use change). If the changed conditions to be considered involve changing parameters or boundary conditions of the model, then there will clearly be additional uncertainty associated with the changed conditions relative to a model 'calibrated' using the GLUE procedure to the present condition of the catchment. This will require a subjective definition of prior likelihood weights associated with the realizations used to model the new catchment condition.

EVALUATING THE VALUE OF ADDITIONAL DATA

The refinement of the uncertainty limits as new data become available provides a measure of the value of that data in the model calibration, and an opportunity to evaluate the value of different types of data in the modelling procedure. To do this objectively, requires some measure of the uncertainty associated with the predictions. The calculated 90 per cent uncertainty limits may not be an adequate measure in this respect, since it is likely that they will display some sensitivity to the sampling limitations of the Monte Carlo procedure. Various integral measures of uncertainty are available (see for example Klir and Folger, 1988), for example the probabilistic Shannon Entropy measure, H,

$$H = -\sum_{i=1}^{M} \mathcal{L}_i \log_2 \mathcal{L}_i \tag{9}$$

where the likelihoods $\mathcal{L}_i$, $i = 1, 2, \ldots M$ are scaled such that $\sum \mathcal{L}_i = 1$ and M is the total number of realizations. This is a maximum ($= \log_2 M$) when all the realizations are equally likely (the case of the uniform prior distribution). It has a minimum of 0 when one single realization has a likelihood of 1 and all others have a likelihood of zero (the case of the 'optimal' parameter set). The way in which the value of H changes with the use of more observations will depend upon the specific definition of the likelihood function $\mathcal{L}_i$ and the value of the observations in constraining the predictive uncertainty.

A second measure, the U-uncertainty, is classed by Klir and Folger (1988) as a possibilistic measure of

non-specificity. It is defined as

$$U = \sum_{i=1}^{M} (\mathscr{L}_i - \mathscr{L}_{i+1}) \log_2 i \tag{10}$$

where the $\mathscr{L}_i$ are the scaled likelihoods ranked from highest to lowest (with $\mathscr{L}_{M+1} = 0$ by convention). The U-uncertainty has a maximum for a uniform distribution ($= \log_2 M$) and a minimum of 0 when a single realization has a likelihood of $\mathscr{L}_1 = 1$.

Both the Shannon entropy and U-uncertainty measures are difficult to apply in the current context when resampling procedures gradually increase the number of realizations M. We have modified both measures to make use of a discretization of the cumulative ranked likelihood function based on M^* increments. The incremental likelihood is calculated by interpolation for each of the M^* increments after which both Equations 9 and 10 can be applied in this rescaled form. In the resampling procedure we have followed based on uniform sampling in the parameter space, it is necessary to keep track of those resampled parameter sets that are rejected as well as those added to the number of realizations retained, both add to effective number of realizations used, even though those rejected are never actually run.

In this study we have evaluated only the utility of additional discharge data in this respect, since only minimal internal state data is available for the Gwy catchment. Figure 10 shows the change in the uncertainty measures (9) and (10) calculated with the posterior likelihood distributions after the application of Bayes equation for each storm. It is worth noting that the uncertainty calculated in this way does not always decrease with the addition of further information. This should surely be expected with hydrological models, where further storms with different specific hydrological responses (such as storm 4 in this study), may not always be reproduced by the same sets of parameter values that have appeared optimal up to that time.

The same procedures may be used to evaluate the value of different types of hydrological data. In particular, for the distributed models that have been under discussion here, the value of distributed observations of internal states of the catchment, such as water table levels or soil moisture profiles, can be considered. Some initial work reported in Binley and Beven (1991) using a hypothetical data set suggests that the use of such data may not be straightforward. In particular, such observations are typically point

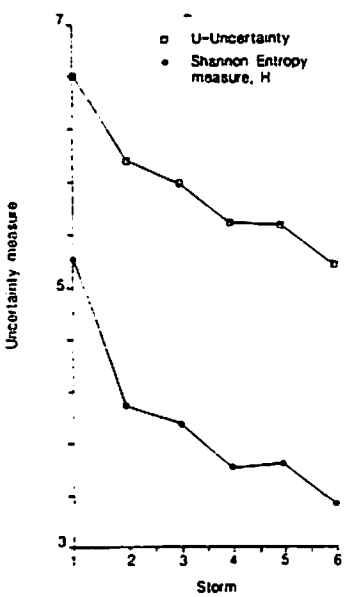


Figure 10. Change in estimated H and U uncertainty measures based on the posterior likelihoods for the sequence of storms in Table I. Likelihood distributions were discretized into $M^* = 100$ increments

observations and, in the same way as measurements of parameter values, may not correspond to the state variables that are being predicted at the model grid scale. Binley and Beven (1991) suggested that for their application, the calculated uncertainty values were dominated by limitations in the model structure and discretisation in reproducing the behaviour of the catchment, rather than the availability of observed data.

COMPUTING REQUIREMENTS

All of the simulations reported here have been run on a parallel computer, the Lancaster University Meiko Computing Surface, which contains some 80 transputers, each of which provides about 1 Mflop average performance. The GLUE procedure is very easily adapted to a distributed memory parallel processor, particularly where each realization may be loaded onto a single processor, as was the case with the IHDM. In general 500 realizations of the IHDM were run for each storm using a 50 transputer array. Each set of runs for each storm took between 30 and 60 hours of computing time on the 50 processors. There is therefore a significant computing burden associated with this technique, but one that is not unreasonable even at the present time. Faster, affordable parallel processing systems, for example based on the Intel i860 (typically 15 or more times the speed of a transputer), are already available. The intention of the GLUE procedure has been to use this type of computing power in a way that presents highly complex nonlinear calculations to a user in a conceptually very simple way and with a minimum of assumptions.

THE FUTURE OF DISTRIBUTED MODELS: CRITICAL EXPERIMENTS, VISUALIZATION, AND QUALITATIVE LIKELIHOOD MEASURES

Looking to the future, we envisage a number of ways that the GLUE procedure might lead to a constructive evaluation of both model results and data in the process of distributed modelling. Given that the procedure allows the estimation of the uncertainty associated with a particular set of predictions, we might perhaps expect that with the current generation of distributed models the uncertainty limits will be large. The question then arises as to whether the availability of additional data would help to constrain those uncertainty limits. Within the GLUE framework, this question could be posed in the context of whether there are (cost effective) critical experiments that would yield likelihood functions which would significantly reduce the predictive uncertainty, always subject, of course, to the ultimate constraints of model structural error. Experiments could be designed, for example, to evaluate the relative value of a series of spatial hydraulic conductivity/transmissivity measurements, a number of observation wells in different locations or additional raingauge sites.

The additional data need not always be quantitative. The advantages of distributed models in producing distributed predictions can be used to effect by allowing the modeller to evaluate the process responses predicted by the model in their correct spatial context. Modern visualization techniques on graphics workstations allow the rapid display of distributed data in a way that allows the pattern of response to be qualitatively evaluated. A qualitative likelihood measure could be designed in this way, comparing patterns of response with field understanding and giving zero likelihood to those simulations not considered to behave in a way consistent with knowledge of field processes. The information content to be processed within a multiple simulation context is, of course, immense and, rather than a visual evaluation, might require the initial setting of performance criteria (likelihood measures) based on field understanding even where there are no direct internal state measurements.

CONCLUDING DISCUSSION

The Generalized Likelihood Uncertainty Estimation (GLUE) procedure described above provides a formal framework for taking into account some of the particular difficulties associated with the calibration and application of distributed hydrological models. In particular, the procedure incorporates:

1. The possibility that different sets of parameter values may be equally likely as simulators of a catchment

system within the limitations of a given specific model structure and errors in the definition of boundary conditions and observed variables;
2. The expectation that the errors between observed and predicted responses may be biased, non-Gaussian, autocorrelated, and heteroscedastistic;
3. The possibility of updating the likelihood weight associated with a particular set of parameter values as more observations become available by a simple application of Bayes equation;
4. The possibility of evaluating the value of different types of data by examination of the effect on the likelihood distribution;
5. Procedures for evaluating the sensitivity of the model to individual parameter values as an extension of the Generalized Sensitivity Analysis of Hornberger and Spear (1981).

The GLUE procedure requires of the modeller two formal definitions in any particular application. These are:

A. A joint prior distribution of parameter values;
B. A definition of a likelihood function, with appropriate weights for different predicted variables;

In many applications of distributed models in the past such requirements in model calibration have not been made explicit and this is, we believe a significant feature of the procedures we propose. However, the reader should note that the use of different definitions should be expected to lead to different results in terms of the predicted uncertainty limits.

It is also worth noting, finally, that the GLUE procedure allows not only different parameter sets, but also different model structures to be incorporated into the uncertainty analysis, where by model structure we can subsume the use of different discretizations or sets of boundary conditions as well as different models. In the future of distributed modelling, such considerations and the evaluation of predictive uncertainty must be given prominence in addition to the gradual improvements that we might expect in model definition and the development of solution techniques. We hope that the GLUE procedure might provide the basis for a proper technology for the formal evaluation of both models and observations. We accept that the application of the procedure with its requirement of multiple simulations is currently limited by the general availability of advanced computing facilities but expect this to change over time with the increasing availability of dedicated parallel processing workstations. In the future we intend to address some of the issues raised in the preceding text, in particular the use of field measured internal state data in the calibration of distributed models.

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