Characterizing Model Error in Conceptual Rainfall-Runoff Models using Storm-Dependent Parameters

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EXTENDED ABSTRACT

Calibration and prediction in conceptual rainfall-runoff (CRR) modelling is affected by input, model and response error (Figure 1a). This study works towards the goal of developing a robust framework for dealing with these sources of error and focuses on model error. The characterization of model error in CRR modelling has been thwarted by poor conceptualizations of error propagation (Figure 1b) and the convenient but indefensible treatment of CRR models as deterministic descriptions of catchment dynamics. It is argued that CRR fluxes are fundamentally stochastic because they involve spatial and temporal averaging. Acceptance that CRR models are intrinsically stochastic paves the way for a more rational characterization of model error. The hypothesis advanced in this paper is that CRR model error can be characterized by storm-dependent random variation of one or more CRR model parameters that affect fluxes. A simple sensitivity analysis is developed to assist in identifying the parameters most likely to behave stochastically. A Bayesian hierarchical model is formulated to explicitly differentiate between input, response and model error – this provides a very general framework for calibration and prediction, as well as the testing of hypotheses regarding model structure and data uncertainty. A case study using daily data from the Abercrombie catchment (Australia) and employing a 6-parameter CRR model demonstrates the considerable potential of this approach. Figure 2 illustrates the excellent fit to the observed data. Of particular significance is the use of posterior diagnostics to test key assumptions about errors. The assumption that the storm-dependent parameters are log-normally distributed is only partially supported by the data, which suggests that the parameter hyperdistributions have thicker tails. Further research is aiming to refine this approach to characterizing model error.
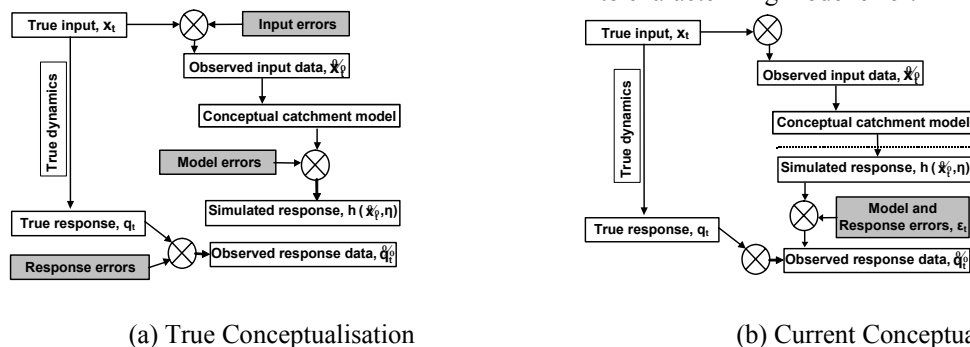
(a) True Conceptualisation   (b) Current Conceptualisation

Figure 1. Errror propagation in CRR models (sources of errors shaded grey) [Kavetski et al. (2002)].
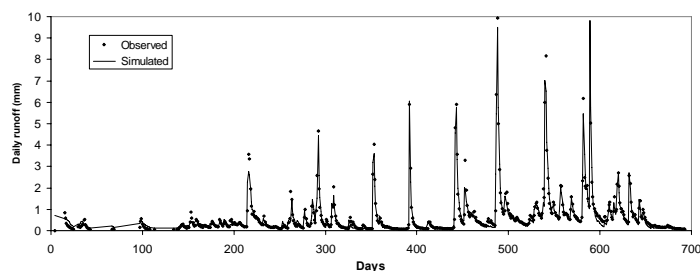

Figure 2. Plot of observed and simulated runoff for Abercrombie River with storm-dependent parameters (Nash-Sutclife statistic = 0.947)

1. INTRODUCTION

Conceptual rainfall-runoff (CRR) models are used to simulate water balance dynamics at the catchment scale. Characterising the uncertainty in streamflow predicted by a CRR model has attracted the attention of hydrologists over many years. Yet in the recent reviews Kuczera and Franks (2002), Kavetski et al. (2002), Vrugt et al. (2005) note that a robust framework that accounts for all sources of error (input, model and response error) remains to be developed. This has a number of implications. The regionalization of CRR model parameters continues to be confounded by bias and unreliable assessment of parameter uncertainty. Furthermore, it remains difficult to discriminate between competing CRR model hypotheses. Poor model performance can "hide" behind the veil of ignorance about the sources of error.

The focus of this study is a more rigorous characterisation of the uncertainty associated with CRR models. The study builds on the Bayesian total error analysis (BATEA) framework of Kavetski et al. (2002, 2005c,d). The main contribution is an explicit characterisation of model error. This is linked with models of input and response error to produce a rudimentary total error framework.

The paper is organised as follows: Following a brief review of CRR modelling, the need for characterising model error is motivated by an example. It is argued that the notion of a deterministic CRR model is indefensible. To make the CRR model stochastic a simple approach is assumed where the parameters vary randomly from storm to storm. A Bayesian inference framework is developed where hypotheses for model, input and response error are explicitly assumed and tested. A case study explores the viability of this approach and highlights the role of diagnostic checks of key assumptions.

2. TRADITIONAL VIEW OF CRR MODEL ERROR

CRR models are characterized by:

$$\mathbf{q_t} \leftarrow h(\mathbf{x_t}, \boldsymbol{\eta}) \qquad (1)$$

where $\mathbf{q_t}$ is the true response vector, which is typically the observed streamflow at time t. The vector $\mathbf{x_t}$ is the true input and contains observable point or spatially averaged quantities (typically rainfall and ET). The function h() is a probability density function (pdf) which represents the catchment response to forcing inputs. The true response $\mathbf{q_t}$ is a random sample from the pdf h().

The vector $\boldsymbol{\eta}$ represents the conceptual parameters which determine the magnitudes of $\mathbf{q_t}$ for a given external forcing $\mathbf{x_t}$. These parameters are inferred by the process of calibration.

All calibration methods make some assumption, either explicit or implicit, about how errors propagate through the CRR model. (see Kavetski et al. (2002) for an overview). Figure 1a summarizes the three distinct sources of error in CRR models. The catchment responds to forcing inputs such as rainfall and ET. The observation of forcing inputs, particularly rainfall, is subject to measurement error due to instrument inaccuracy and incomplete sampling of the spatial field. The streamflow is also subject to measurement error. Even with error-free forcing and response observations the CRR model would not be expected to reproduce exactly the true response - this is called model error.

In stark contrast, Figure 1b presents the conceptualisation that underpins calibration methods that dominate practice. The defining features are (a) observed forcing $\tilde{\mathbf{x}}_t$ equals the true forcing $\mathbf{x_t}$ (input error is assumed negligible) and (b) the model and response error are represented by a pseudo-additive random process, the simplest being the simple least squares (SLS) error model:

$$\tilde{\mathbf{q}}_\mathbf{t} = h(\mathbf{x_t}, \boldsymbol{\eta}) + \boldsymbol{\varepsilon_t} \qquad (2)$$

where $\boldsymbol{\varepsilon_t}$ is a random independent, constant variance Gaussian error.

3. SIGNIFICANCE OF MODEL ERROR

The conceptualisation of error propagation shown in Figure 1b is known to be a crude approximation of reality. This is illustrated by calibrating the Sacramento model to daily runoff using daily rainfall for the 2770 km^2 Abercrombie River at Abercrombie (412028) in New South Wales, Australia. Thirteen parameters were calibrated to two years of data using the SLS criterion with the runoff data was square-root transformed to account for the heteroscedasticity of the runoff errors.

Figure 3 presents a scatter plot of observed and simulated daily runoff along with the 90% confidence and prediction limits. The confidence limits (based on linear approximation) only account for the uncertainty in the parameters, while the prediction limits account for parameter, model and response uncertainty. The Nash-Sutcliffe (NS) statistic was 0.73. The striking feature is that most of the predictive uncertainty is dominated by model, response (and input) error.

Noting that the 90% prediction limit interval represents ±(60 to 80)% of the simulated runoff, it is highly unlikely this uncertainty is due to errors in estimating runoff – a well maintained gauging station is unlikely to have a coefficient of variation (CV) in errors exceeding 5 to 10%. This evidence suggests the bulk of the uncertainty is due to model and forcing error (which was ignored).

Inspection of the observed and simulated time series revealed the model error is highly structured and completely at odds with the SLS assumption of independence. There are long runs of systematic over- and under-estimation, recessions are mis-specified, peaks are spuriously simulated or completely missed. These qualitative features are well known to practitioners and researchers – it is generally recognised that model and input errors induce a complex uncertainty structure in the model parameters and predictions.
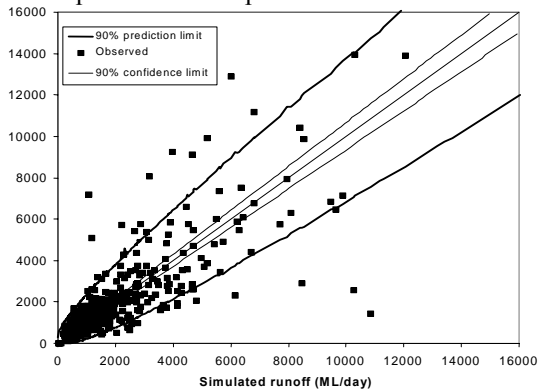

Figure 3. Scatter plot for Sacramento model calibrated to daily runoff from the Abercrombie river.

4. STORM-BASED CHARACTERISATION OF MODEL ERROR

CRR models focus on the dominant catchment dynamics and are deliberately constructed to be parsimonious to ease the burden of calibration. Therein lies a likely major source of model error, namely the ever-present simplification of catchment processes.

CRR models typically route water through one or more conceptual storages. These one-dimensional stores represent two or three-dimensional features of the catchment and therefore the contents of conceptual stores are almost always spatially averaged. The observed forcing input is typically a spatial and temporal average of a random field. There are an infinite number of spatially distributed rainfall fields that yield the same catchment average rainfall. However, each rainfall field creates a spatially different hydrologic response. Models based on spatial and temporal averaging cannot replicate such behaviour. As a result, CRR fluxes based on spatial and temporal averaging will, almost always, be in error. Because the CRR model may have interconnected stores, an error in one flux can propagate through "downstream" stores and thus affect other fluxes. This induces a persistent error in the fluxes dependent on the downstream store.

This suggests it is unreasonable to expect a CRR model to deterministically simulate catchment response even if the true forcing were known. Spatial and temporal averaging induces unavoidable errors in fluxes. We argue that the notion of a deterministic CRR model needs to be relaxed if a rational description of model error is to be developed.

The central question, therefore, is how to relax the determinism that is currently embedded in the CRR paradigm. The approach taken is to allow some of the CRR parameters to be random variables over some characteristic time scales. This will induce stochastic variations in the fluxes. This notion of time-varying parameters is not new. The state-space formulation underlying the Kalman filter naturally allows for time variation in parameters – in the extended Kalman filter CRR parameters can be treated as state variables which can be randomly perturbed at every update step [see Bras and Rodriguez-Iturbe (1985) for an overview of hydrologic applications]. However, as Kavetski et al. (2002) observe, the extended Kalman filter approach is hampered by assumptions of linearity in the state equation and Gaussian errors.

The critical question to address is the temporal variation of the random perturbations of the model fluxes. The persistence in the flux errors previously discussed indicates that some form of persistence in the flux random perturbation is required. The rainfall during a storm event represents the primary (and spatially the most heterogeneous) forcing of the catchment water balance. It is therefore reasonable to suggest as a working hypothesis that flux perturbations should persist over storm-event time scales. One logical way to introduce this persistence is to randomly perturb flux parameters at the beginning of each storm event – this is consistent with the idea of storm-dependent parameters explored by Kuczera (1990). Hence the CRR conceptual parameter vector is partitioned as $\eta = (\theta, \omega)$, where ω is the vector of time-invariant (deterministic) parameters and θ is the vector of storm-dependent (stochastic) parameters.

5. AN EXAMPLE WITH STORM DEPENDANT PARAMETERS

Our hypothesis is that a significant part of model error can be described by randomly sampling one or more parameters from a probability distribution at the start of each storm. This section uses an example to demonstrate the plausibility of this mechanism and introduces a useful tool for identifying the CRR parameters suitable for characterization as storm-dependent.

Figure 4 illustrates a typical CRR model, a member of the saturated path modelling (SPM) family [Kavetski et al., 2003], hereafter referred to as logSPM. The logSPM has 7 parameters (Table 1) and three stores operating at a daily time step. The seventh parameter, rMult, needs further comment. Kavetski et al. (2002, 2005c,d) use storm-dependent rainfall depth multipliers as an explicit (albeit approximate) representation of input uncertainty, which corresponds to the assumption that rainfall errors are multiplicative (i.e., $rain_{true}=rain_{obs}*rMult$). The same approach is used in this paper to compensate for catchment rainfall error.
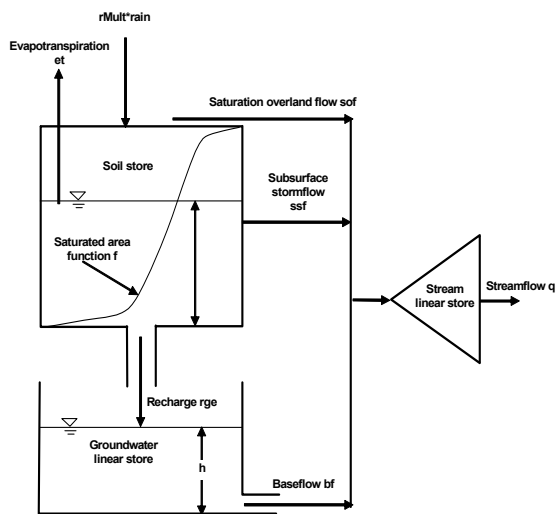
$$\frac{ds}{dt}=rMult*rain-quick(f)-ssf(f)-rge(f)-et(s)..\text{ surface store water balance}$$

$$f=\frac{1}{1+(sF+99)e^{-ks}}-\frac{1}{sF+100}\quad......\text{saturation}-\text{soil depth function}$$

$$quick(f)=f*rMult*rain.................quickflow$$

$$ssf(f)=f*ssfMax.........................subsurface stormflow$$

$$rge(f)=f*rgeMax.......................groundwater recharge$$

$$et(s)=pet*(1-e^{-s}).........................actual evapotranpiration$$

$$\frac{dh}{dt}=rge-bf(h)............................\text{ groundwater store water balance}$$

$$bf(h)=kBf*h........baseflow$$

$$\frac{dS}{dt}=quick+\ ssf+\ bf-q(S).........\text{streamflom store water balance}$$

$$q(S)=kStream*S........................stream runoff$$

Figure 4. Schematic of the 7-parameter logSPM CRR model.

The effects of storm-dependent parameter stochasticity were explored using a daily runoff time series $\mathbf{Q_o}$ derived from the two-year daily rainfall record for Abercrombie River assuming all the logSPM parameters were deterministic with values given in Table 1 (obtained by fitting the logSPM model to the Abercrombie streamflow record with a NS statistic of 0.73). Given the same rainfall a new runoff time series $\mathbf{Q_i}$ was generated with the ith logSPM parameter, θ_i selected as being stochastic with a log-normal distribution with expected value given by Table 1 and a given CV. A new value of θ_i is sampled at the beginning of each storm. The remaining parameters remain deterministic with values given by Table 1. The NS statistic, NS(i) is then evaluated treating $\mathbf{Q_o}$ as the "observed" and $\mathbf{Q_i}$ the "simulated" time series.

Table 1. Summary of logSPM parameters.

| Parameter	Description	Expected value
k	Exponent controlling saturated area fraction	0.02
sF	Shift parameter controlling saturated area fraction	2300
ssfMax	Subsurface stormflow at full saturation	0.62 mm/day
rgeMax	Groundwater recharge rate at full saturation	5.6 mm/day
kBF	Groundwater discharge constant	6.3×10^{-5}
kStream	Stream discharge constant	0.47
rMult	Observed storm depth rainfall multiplier	1.21
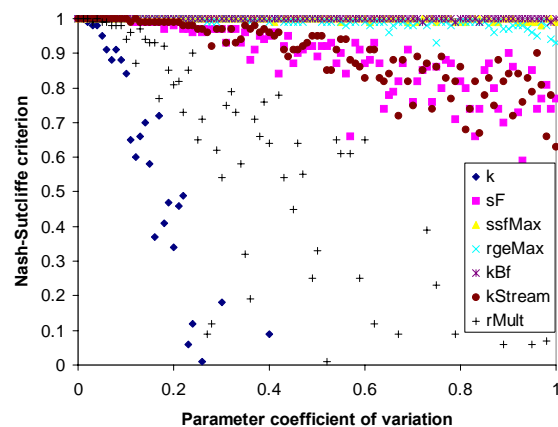
Figure 5. Sensitivity of Nash-Sutcliffe criterion to storm-dependent parameter variability.

Figure 5 presents a plot of NS(i), i=1,..,8, for a range of CVs. The NS criterion is most sensitive to storm-dependent variation in the parameter k. This regulates the production of saturation overland and

subsurface stormflow. The second most sensitive parameter is the rainfall multiplier parameter rMult. This regulates the magnitude of the error in the rainfall, the primary forcing. The remaining parameters display limited, if any, sensitivity to storm-dependent variation strongly suggesting they are best treated as time-invariant.

6. INCORPORATING MODEL UNCERTAINTY INTO BATEA

The BATEA framework, proposed by Kavetski et al. (2002, 2005c,d) to deal with forcing or input uncertainty can be readily extended to accommodate model uncertainty, expressed in the form of storm-dependent parameters. This formulation leads to posing BATEA in terms of a Bayesian hierarchical model (Figure 6).

The hydrologic time series is partitioned into n epochs $\{(t_i, t_{i+1}-1), i=1,..n\}$ where t_i is the time step index corresponding to the beginning of the ith epoch. Each epoch is characterized by a storm event at its beginning followed by a dry spell. At the beginning of each epoch the storm-dependent parameters for the input error and model error components are sampled from their hyperdistributions, $p(\phi | \alpha)$, and $p(\theta | \beta)$ respectively. The parameters for the hierarchical BATEA are therefore the deterministic parameters, ω, the hyperparameters, β for the storm-dependent model error component, the hyperparameters α for the storm-dependent input error component, and the parameters for the response error component, γ. For a full description refer to Kuczera et al (2005).
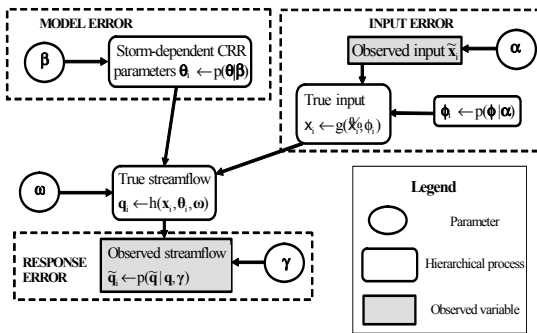

Figure 6. Hierarchical BATEA model.

6.1. BATEA Inference Problem

The objective of BATEA inference is to identify the parameters α, β, ω and γ given the streamflow $\tilde{Q} = \{\tilde{q}_i, i=1,..,n\}$ and forcing $\tilde{X} = \{\tilde{x}_i, i=1,..,n\}$ data. Following Kavetski et al. (2002), the most probable (modal) parameters are found by maximizing the posterior pdf:

$$p(\alpha, \beta, \omega, \gamma, \theta_{1:n}, \varphi_{1:n} | \tilde{Q}, \tilde{X}) \qquad (3)$$

where $\theta_{1:n} = \{\theta_1,...,\theta_n\}$ is the vector of CRR storm-dependent parameter realizations for all the storms, $\varphi_{1:n} = \{\varphi_1,...,\varphi_n\}$.

To expedite this inference problem the following simplifications are made: 1) The input error model is $x_i = \phi_i \tilde{x}_i$ for each storm epoch, with ϕ_i (denoted as rMult in Figure 4) being storm-dependent. 2) The response error parameters γ are assumed known. This is a reasonable assumption for streamflow from a well-maintained gauging station

7. CASE STUDY

The Abercrombie catchment is revisited to explore the hypothesis that storm-dependent parameters adequately describe rainfall input and model uncertainty. Storm epochs were defined by dry spells of 2 or more days with a 0.5mm rainfall threshold defining a wet day. In the two-year daily record, 71 storm epochs were identified.

The distributional assumptions used in BATEA to characterise the input, model and response error are summarized in Table 2. Uniform non-informative priors were specified for deterministic parameters ω, while weakly informative priors were prescribed for the hyper parameters β, since otherwise the posterior pdf becomes ill-posed (unbounded) (Kavetski et al., 2005c). The chosen streamflow response error model [N(0,0.25^2)] was selected for convenience for this case study. The key point is that the response error model is inferred independently of BATEA, typically by analysis of rating curve residuals. This assists the inference because the focus is on input and model error rather than all three sources of uncertainty.

Table 2. Distributions used in BATEA.

Variable	Probability Model	Prior Distribution
K	log k $\sim N(\mu_k, \sigma_k^2)$	$\mu_k \sim N(-3.88, 0.5^2)$ $\sigma_k^2 \sim$ Inv-$\chi^2(1, 0.5^2)$
sF	deterministic	Uniform
ssfMax	deterministic	Uniform
rgeMax	deterministic	Uniform
kBF	deterministic	Uniform
kStream	deterministic	Uniform
rMult	log rMult $\sim N(\mu_r, \sigma_r^2)$	$\mu_r \sim N(0, 0.1^2)$ $\sigma_r^2 \sim$ Inv-$\chi^2(1, 0.2^2)$
Stream-flow	$\tilde{q} \sim N(q, 0.25^2)$	-

2929

The logSPM model was first calibrated using SLS, which yielded a NS statistic of 0.736 (same as the Sacramento model). Due to its high correlation with ssfMax and rgeMax, the parameter sF was fixed at its SLS value for BATEA inference – this avoids the confounding effects associated with strong parameter interaction (which are important in practice but lie beyond the scope of this paper). The natural logarithm of the parameters was calibrated to guarantee the positivity constraint and reduce the parameterization nonlinearity of the objective function surface.

The posterior mode for parameters $\boldsymbol{\beta}$, $\boldsymbol{\omega}$ and $\boldsymbol{\theta}_{1:n}$ was identified using a quasi-Newton optimization scheme (Kavetski et al, 2005a,b). Table 3 presents the posterior modal values and shows that the NS statistic climbs to 0.947 from 0.736 for the SLS. Figure 2 shows the fit is excellent with only small discrepancies at peaks and in recessions. Comparison of the SLS and BATEA parameters reveals a marked shift. This suggests a considerable bias can be induced by SLS calibration and is consistent with Kavetski et al. (2002) who conclusively demonstrate bias in a synthetic example with corrupt inputs and no model error. However, without assessing parameter uncertainty, the suspected bias in this case study cannot be confirmed.

Table 3. Modal posterior parameter summary

Parameter	Posterior mode (NS=0.947)		SLS values (NS=0.736)
	Mean	SD	
$\log_e k$	-2.1	0.075	-3.9
$\log_e sF$	7.7	-	.7
$\log_e ssfMax$	4.5	-	-0.56
$\log_e rgeMax$	3.4	-	1.72
$\log_e kBF$	-8.9	-	-10.2
$\log_e kStream$	0.97	-	-0.767
$\log_e rMult$	-0.3	0.27	0.19

7.1. Posterior Diagnostics

Although the results are encouraging, it is necessary to test the assumptions underpinning the BATEA analysis using a variety of posterior diagnostics. The major assumption is that the storm-dependent parameters are independent and log-normally distributed. The normal probability plots (not shown) for log rMult and log k reveals that although the normal distribution is a reasonable approximation there are clear departures from normality in the tails. This suggests distributions more kurtotic then normal may be required to accommodate outliers. The time series plots (not shown) of the storm-dependent parameters reveals that outliers tend to

cluster. Although the runs test statistics do not reject the hypothesis that the storm-dependent parameters are independent there does appear to be second-order effects which suggest the definition of storm epochs may require further consideration.

Another assumption that requires testing is that the residuals were independently and normally distributed with zero mean and a standard deviation of 0.25 mm. The normal probability plot (not shown) of the residuals reveals that while the sample mean and standard deviation are 0.001 and 0.245 mm respectively, the distribution has tails considerably fatter than expected for a normal distribution – the generalization of the normal model described by Box and Tiao (1973) would be a logical extension. The autocorrelation of the residual time series was not significantly different from zero however the runs test strongly rejected the assumption of independence. Nonetheless, given the small magnitude of the residuals, this is viewed as a relatively minor issue.

8. DISCUSSION

The astute reader would be interested in how BATEA differs from the GLUE formalism of Beven and Binley (1992). GLUE exposed the shortcomings of traditional statistical models such as nonlinear regression and the Kalman state-space formulation that assume the errors are additive and Gaussian. However, these shortcomings are not deficiencies of the Bayesian paradigm itself, but are brought about by a failure to recognise that a robust CRR framework must not only describe hydrologic processes, but also error processes.

GLUE and BATEA share in common the recognition that model error is significant and difficult to characterize. However, the conceptual frameworks are fundamentally different. While BATEA incorporates the error propagation framework shown in Figure 1a in which input, response and model error are differentiated, GLUE effectively treats all error as parameter uncertainty. GLUE remains rooted to the deterministic CRR model, whereas BATEA allows parameters to evolve stochastically from storm to storm. The exclusive focus on parameter uncertainty in GLUE creates conceptual difficulties in its derivation. For example, although GLUE uses Bayesian updating, its likelihood functions are not proper – indeed they are often termed "pseudo-likelihood functions" in recognition that subjective goodness-of-fit criteria are used to assemble the likelihood function. In contrast BATEA directly represents input, response and model error (expressed as storm-dependent parameters) within the standard Bayesian framework. As a result, all assumptions

are explicit and open to challenge. Seen in this light, BATEA combines the philosophical basis of GLUE (which abandons the notion of single 'true' parameters) and improves on it by explicitly disaggregating input, model and response error using formal Bayesian strategies.

9. CONCLUSIONS

The characterization of model error in CRR modelling has been thwarted by the convenient but indefensible assumption that CRR models are deterministic descriptions of catchment dynamics. Explicit acceptance that CRR models are fundamentally stochastic paves the way for a more rational characterization of model error. In this study we argued that CRR fluxes are fundamentally stochastic because they involve spatial and temporal averaging. We proposed the hypothesis that CRR model error can be characterized by storm-dependent random variation of one or more CRR model parameters. A simple sensitivity analysis was developed to identify the parameters most likely to vary between storms. A Bayesian hierarchical model was developed to explicitly differentiate between input, response and model error in the form of storm-dependent parameters. The hypothesis that independent and log normally distributed storm-dependent parameters can account for model and input error was evaluated in a case study. Posterior diagnostics showed this hypothesis was partially supported, though the need to deal with outliers was recognised.

This study moves a step closer to a total error formalism which will enable rational assessment of predictive uncertainty and potentially remove some of the factors that confound regionalization of CRR parameters and enable more rigorous testing of competing CRR model hypotheses.

Nonetheless, significant problems remain. The greatest challenge is the characterization of the inherent stochasticity in CRR models. In this study, an intuitive approach was adopted. Further research is needed to develop more rigorous stochastic formulations of CRR models. The computational issues of accommodating storm-dependent parameters are also formidable. Further research is aiming to develop more efficient techniques to resolve these issues.

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