Propagating Data Uncertainty and Variability into Flow Predictions in Ungauged Basins

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Abstract:

Explicitly acknowledging uncertainty and variability in model-based hydrological forecasts is a challenging task. Many basins are either ungauged, are undergoing rapid land use change, or are in regions expected to experience significant climate change. These factors, in addition to uncertainty in monitoring data and model structure, collectively contribute to discrepancies between model predictions and observations. Few hydrological modeling studies, however, routinely quantify data uncertainty. Furthermore, few studies compare model forecasts to observations while considering intrinsic uncertainty in the model itself. To bridge this research gap, we test a series of rainfall-runoff models within gauged and ungauged basins in Eastern North Carolina (US). In the model calibration phase, we propagate data uncertainty into model forecasts within a Bayesian framework. We then assess model suitability by examining the distribution of Bayesian posterior p-values (defined as the model-derived probability of a flow measurement as or more extreme than that observed). Evaluating model performance in this way helps identify potential sources of model bias and error, and clearly demonstrates the magnitude of those errors relative to the various potential sources of variability and uncertainty in the model forecast.

Keywords: rainfall-runoff model; ungauged basins; IHACRES; data variability; Bayesian

1 INTRODUCTION

Calibrating continuous rainfall-runoff models is a complicated and often arduous task. Notable challenges include selecting a suitable model (and model error) structure [Young and Beven, 1994; Wagener et al., 2001], identifying a robust set of model parameters [Beven, 1989; Beven and Freer, 2001] and quantifying potential correlation between (and uncertainty within) those parameters [Duan et al., 1992; Kuczera and Parent, 1998; Montanari and Brath, 2004]. Addressing these challenges becomes particularly important when considering how uncertainty and variability might impact (and be incorporated into) hydrological model-based studies.

For example, it is widely recognized that hydrological modeling tools are needed to forecast flows under future land use and climate change scenarios [Nandakumar and Mein, 1997; Anderson et al., 2006], or in basins which are ungauged and for which a model can not be calibrated directly [Seibert, 1999; Kokkonen et al., 2003]. Yet despite the broad range of research on the importance of uncertainty and change in hydrological modeling and water resources research [for further discussion, see Milly et al., 2008], we find that only recently has hydrological modeling research begun explicitly focusing on quantifying forcing data variability *and* propagating that variability into model parameter estimates and flow forecasts using robust (such as probabilistic and Bayesian) procedures [Vrugt et al., 2008; McMillan and Clark, 2009]. Furthermore, we

find that few modeling studies, if any, compare model forecasts to observations while considering intrinsic uncertainty in the model itself.

To help bridge these research gaps, we apply a well-known conceptual rainfall-runoff (CRR) model to gauged basins along the Eastern coast of the United States (U.S.) within a Bayesian framework in order to forecast flows in nearby ungauged basins. We begin by developing parameter probability distributions using an ensemble modeling approach, and then apply the calibrated CRR models to an ungauged basin using recently obtained field data by first assuming that the field data is deterministic (i.e. certain) and then, for comparison, allowing for uncertainty and variability in the forcing data. We apply the derived parameter distributions to generate probabilistic flow forecasts in the ungauged basin, and assess the suitability of the two different assumptions regarding uncertainty in forcing data by comparing the forecasts to field observations using the distribution of Bayesian posterior p-values.

2 MODEL AND DATA

2.1 Model

To address the goals of our study, we apply the IHACRES model, a well-known [see, for example Dye and Croke, 2003; Croke and Jakeman, 2004] version of the more general class of data-based mechanistic (DBM) rainfall-runoff models [Young and Beven, 1994] to coastal watersheds in the Eastern U.S. The IHACRES rainfall-runoff model has been described extensively in previous works, including those providing an introduction to DBM rainfall-runoff models [Whitehead et al., 1979; Jakeman et al., 1990] as well as those which describe and apply the IHACRES graphical user interface software package [Littlewood et al., 1997; Jakeman and Letcher, 2003; Kokkonen et al., 2003; Anderson et al., 2006] and its recent developments [Croke and Jakeman, 2004; Croke et al., 2006]. We provide a brief description of the model here (and in the Appendix) for reference, and direct readers interested in a more detailed description of IHACRES to these earlier works.

Figure 1: Location of contributing watershed areas (grey regions), weather stations (hollow circles) and USGS flow gauges (inverted triangles) in Eastern Virginia (top portion of figure) and Eastern North Carolina (bottom portion).

The IHACRES model is divided into two components. The first is a non-linear loss module which uses a measure of evaporation (such as temperature t or pan evaporation) to translate incident rainfall (r_k, in units of mm) at time k into effective rainfall (u_k, also in mm). The second component is a linear unit hydrograph-based module which translates effective rainfall (u_k) into streamflow (x_k). The IHACRES model (like many other CRR models) can divide flow into a "quick" and "slow" component. In initial attempts to calibrate the IHACRES model, however, we found that representing flow through a single flow path provided as good or better model performance than representing flow through two parallel flow paths. Furthermore, we do

not expect the catchments in our study area (as described in the following section) to generate a significant base flow, and implement a version of the IHACRES model with only four parameters; c (a mass balance parameter, in 1/mm, often described as an index of watershed wetness capacity), f (a temperature modulation parameter, in 1/deg C), τ_w (the time constant of wetness decline, in days), and τ_f (the flow response time constant, in days).

2.2 Data

The watersheds selected for this study drain into some of the most sensitive coastal embayments in the world, including the Chesapeake Bay (VA) and the Neuse River Estuary (NC), which collectively host a wide range of both natural resources and recreational and commercial uses. Unfortunately, water quality in these embayments is declining due, in part, to elevated pollutant loading levels [see, for example Borsuk et al., 2003; Fries et al., 2007; Gronewold et al., 2008]. Understanding the dynamics of these hydrological systems and applying that understanding to model forecasts is critical to the success of ongoing studies and large-scale planning initiatives addressing these water quality problems, including those being conducted through the United States Environmental Protection Agency (USEPA) total maximum daily load (TMDL) program [National Research Council, 2001; Houck and Environmental Law Institute, 2002; Reckhow, 2003], the most comprehensive and far-reaching water quality management program in the U.S.

Table 1: Summary of land use characteristics for each watershed in the eastern North Carolina and Virginia study area.

Watershed	Area (km^2)	Land use land cover percentage (%) Agricultural	Forested	Urban	Other
Bear Creek	149.4	41.4	26.3	0.8	31.5
Chicod Creek	116.6	56.9	24.9	3.7	14.5
Contentnea Creek	1898.5	42.2	34.4	3.0	20.5
Durham Creek	67.3	11.4	43.9	0.4	44.2
Hood Creek	55.9	5.1	69.5	0.3	25.1
Moccasin Creek	4.9	35.5	49.6	0.0	14.9
Nahunta Swamp	208.2	52.4	29.3	1.6	16.7
Piscataway Creek	72.3	26.0	67.8	0.1	6.1
Potecasi Creek	582.8	31.4	49.4	2.6	16.6
Swift Creek	696.7	34.5	26.7	2.5	36.3
Van Swamp	59.6	5.7	34.1	0.0	60.1

We delineated watersheds for eleven streams and creeks in this region (figure 1) for which the United States Geological Survey (USGS) maintains a permanent flow gauge with a relatively long (i.e. approximately 2-10 years) uninterrupted flow record. Land use and land cover (LULC) information for each contributing watershed (based on 2001 imagery) was obtained from Homer et al. [2004]. A summary of the characteristics of each watershed, including total land area and LULC data, is included in table 1).

Daily precipitation and temperature measurements in the vicinity of the watersheds were collected from the National Oceanic and Atmospheric Administration (NOAA) National Climatic Data Center (NCDC) network of monitoring stations (figure 1). Average daily rainfall for each watershed was calculated using the Kriging model in the `fields` package within the statistics and graphics software program R [Ihaka and Gentleman, 1996]. Average daily temperature in each watershed was assumed equal to the average daily temperature recorded at the nearest NCDC weather station.

3 METHODOLOGY

3.1 Parameter estimation

We calibrate the IHACRES model to the eleven watersheds using the IHACRES v2.1 software package [Littlewood et al., 1997; Croke et al., 2005] and flow, temperature, and precipitation data

as described above (figure 1). Here, we evaluate the model over a uniform sampling grid, similar to the exhaustive gridding (EG) procedures introduced in Duan et al. [1992], with $\tau_w \in [2, 300]$ and $f \in [0, 12]$. A common criticism of this approach, of course, is the potential computational effort of evaluating the model over a multi-dimensional grid. A distinct advantage of using the IHACRES v2.1 software package to implement this procedure, however, is that for any given pair of parameters τ_w and f, IHACRES implements an instrumental variable (IV) procedure to calculate the other two parameters (i.e. c and τ_s), thus greatly reducing the dimensionality of the problem.
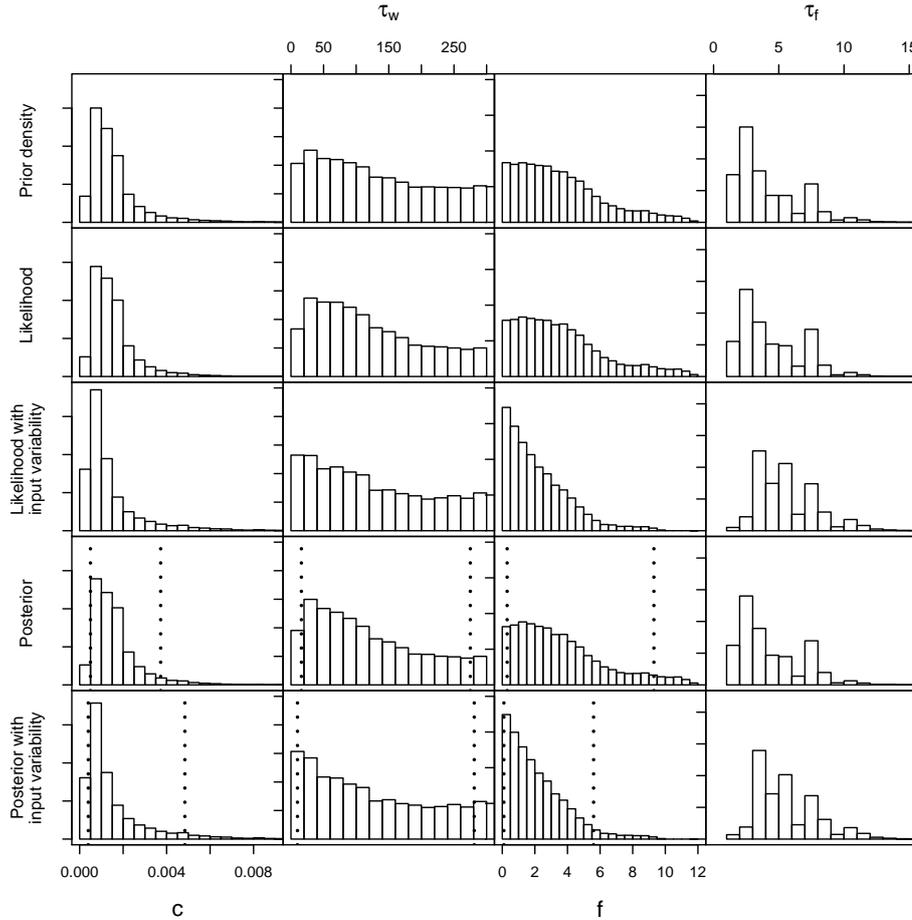
Figure 2: Histograms of simulated samples from marginal prior distributions (first row), normalized likelihood functions (second and third rows), and posterior probability density functions (fourth and fifth rows) for four IHACRES model parameters. Likelihood functions and posterior probability density functions are presented based on a both fixed (second and fourth rows) and variable (third and fifth rows) data inputs. Vertical dashed lines in the fourth and fifth rows indicate 95% credible intervals.

We then, following "ensemble modeling" procedures outlined in McIntyre et al. [2005] and McMillan and Clark [2009], combine the resulting parameter sets to form a joint probability distribution potentially suitable for application to both gauged and ungauged watersheds throughout the region. Following guidance presented in similar studies on hydrological model uncertainty [for example, the rainfall-runoff models presented in Duan et al., 1992; Beven, 2001; McMillan and Clark, 2009], we remove from the IHACRES-generated ensemble of calibrated parameter sets those with a Nash-Sutcliffe index of model efficiency (NSE) less than 0.6 [Nash and Sutcliffe, 1970]. We repeat this calibration procedure by modifying the rainfall data using an event multiplier [for details, see Vrugt et al., 2009]. While some recent studies [Kavetski et al., 2006; Stedinger et al., 2008, for example] promote more formal Bayesian approaches to addressing uncertainty (which, among other differences, address variability from all forcing data), our focus on variability and uncertainty in precipitation data is a reasonable simplifying step for this particular

study. This approach leads to two joint parameter posterior distributions, each based on a different assumption regarding input data variability, which can subsequently be used to forecast flows in Ware Creek (and, potentially, in similar ungauged basins).
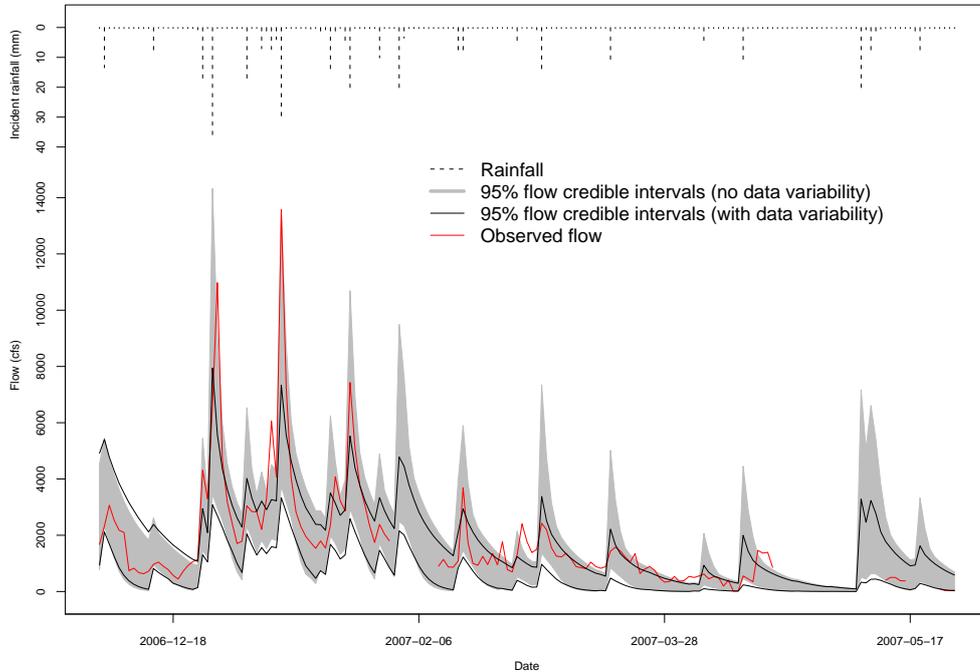
Figure 3: Comparison between observed flow in Ware Creek (red line) and 95% credible intervals based on model calibration without (grey region) data variability and with (black lines) data variability.

3.2   Assessing model performance

In order to evaluate potential benefits of propagating forcing data uncertainty into IHACRES model parameters (and model forecasts), we apply the parameter sets from each approach to generate 100,000 daily simulations of flow in Ware Creek, a small tributary of the Newport River Estuary in Eastern NC (see figure 1). Ware Creek does not have a permanent flow gauge, however field-scale flow measurements were collected for model validation between 2007 and 2008 [Kirby-Smith, 2008]. We assess the impact of each assumption regarding forcing data variability using the Bayesian posterior predictive p-value, calculated for each flow observation as the area under the curve of the predictive probability distribution (for a particular observation) which equals or exceeds the observed value [for details, and for a similar application, see Gelman et al., 2004; Gronewold et al., 2009].

4   RESULTS, DISCUSSION, AND CONCLUSIONS

The results of our parameter estimation procedure indicate that the joint parameter likelihood function (and posterior probability density function) derived from a stochastic representation of forcing data differs considerably from the joint parameter likelihood function based on an assumption of "exact" forcing data (figure 2). For example, the marginal normalized likelihood for τ_f based on an assumption of no data uncertainty (second row, fourth column) is noticeably different from the marginal normalized likelihood for τ_f based on an assumption of data variability (third row, fourth column). Similar differences are noticeable for other model parameters as well and propagate into differences in marginal posterior probability density functions for each parameter (fourth and fifth row in figure 2, with dashed lines indicated 95% credible intervals) as well as (see following paragraph) into flow forecasts. While not an explicit goal of this paper, these results

support the widely recognized view [see, for example Kuczera and Parent, 1998] that uniquely determined model parameter values are effectively unreliable, and that appropriate assessment of model parameter uncertainty is critical to model performance.
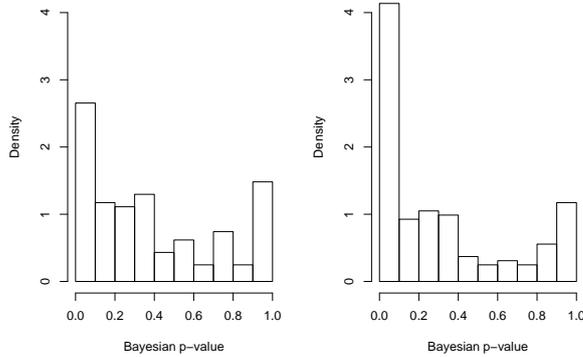
Figure 4: Histogram of Bayesian p-values based on model calibrated without (left panel) and with (right panel) forcing data uncertainty.

Our analysis of flow forecasts in Ware Creek (figure 3) indicates that 95% prediction intervals derived from a modeling approach which explicitly acknowledges forcing data uncertainty (black lines in figure 3) are considerably narrower than those derived from a modeling approach which assumes invariable data (grey region in figure 3). Furthermore, our results indicate that the prediction intervals derived from the model acknowledging data variability may, in fact, fail to include a significant portion of the observed flow measurements (red line in figure 3). Our analysis of Bayesian posterior p-values (figure 4) further supports this observation (indicated by the relative weight of each histogram at a p-values of 0, and of p-values less than 0.5).

While these results suggest that the approach of ignoring precipitation data variability might provide a better explanation of observed flow, we suspect that our results may be somewhat biased based on our exclusive focus on variability in precipitation measurements alone [an approach consistent with similar studies by Nandakumar and Mein, 1997; Vrugt et al., 2008; Biemans et al., 2009]. We leave analysis of flow measurement error and other forcing data for future research, and conclude by acknowledging the potential advantages of our proposed model evaluation procedure which, unlike more common approaches based on point estimates of flow [such as the Nash-Sutcliffe index of model performance, Nash and Sutcliffe, 1970], highlights potential sources of model bias and error and indicates the magnitude of those errors relative to the various potential sources of variability and uncertainty in the model forecast.

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REFERENCES

Anderson, R. M., B. F. Hobbs, and J. F. Koonce. Modeling effects of forest cover reduction on larval walleye survival in Lake Erie tributary spawning basins. *Ecosystems*, 9(5):725–739, 2006.

Beven, K. How far can we go in distributed hydrological modelling? *Hydrology and Earth System Sciences*, 5(1):1–12, 2001.

Beven, K. Changing ideas in hydrology: the case of physically-based models. *Journal of Hydrology*, 105(1-2):157–172, 1989.

Beven, K. and J. Freer. Equifinality, data assimilation, and uncertainty estimation in mechanistic modelling of complex environmental systems using the GLUE methodology. *Journal of Hydrology*, 249(1-4):11–29, 2001.

Biemans, H., R. Hutjes, P. Kabat, B. Strengers, D. Gerten, and S. Rost. Effects of precipitation uncertainty on discharge calculations for main river basins. *Journal of Hydrometeorology*, 10 (4):1011–1025, 2009.

Borsuk, M. E., C. A. Stow, and K. H. Reckhow. Integrated Approach to Total Maximum Daily Load Development for Neuse River Estuary using Bayesian Probability Network Model (Neu-BERN). *Journal of Water Resources Planning and Management*, 129:271, 2003.

Croke, B., F. Andrews, A. Jakeman, S. Cuddy, and A. Luddy. IHACRES Classic Plus: A redesign of the IHACRES rainfall-runoff model. *Environmental Modelling and Software*, 21(3):426, 2006.

Croke, B., F. Andrews, J. Spate, and S. Cuddy. IHACRES user guide. Technical Report 2005/19. Second edition. iCAM, School of Natural Resources, Environment and Society, The Australian National University, Canberra. 2005.

Croke, B. and A. Jakeman. A catchment moisture deficit module for the IHACRES rainfall-runoff model. *Environmental Modelling and Software*, 19(1):1–5, 2004.

Duan, Q., S. Sorooshian, and V. Gupta. Effective and efficient global optimization for conceptual rainfall-runoff models. *Water Resources Research*, 28(4), 1992.

Dye, P. and B. Croke. Evaluation of streamflow predictions by the IHACRES rainfall-runoff model in two South African catchments. *Environmental Modelling and Software*, 18(8-9):705–712, 2003.

Fries, J., R. Noble, G. Kelly, and J. Hsieh. Storm Impacts on Potential Pathogens in Estuaries. *Eos Trans. AGU*, 88(8):93, 2007.

Gelman, A., J. B. Carlin, H. S. Stern, and D. B. Rubin. *Bayesian Data Analysis*. Chapman & Hall/CRC, Boca Raton, Florida, 2004.

Gronewold, A., S. Qian, R. Wolpert, and K. Reckhow. Calibrating and validating bacterial water quality models: A Bayesian approach. *Water Research*, 43(10):2688–2698, 2009.

Gronewold, A. D., M. E. Borsuk, R. L. Wolpert, and K. H. Reckhow. An assessment of fecal indicator bacteria-based water quality standards. *Environmental Science & Technology*, 42 (13):4676–4682, 2008.

Homer, C., C. Huang, L. Yang, B. Wylie, and M. Coan. Development of a 2001 national landcover database for the United States. *Photogrammetric Engineering and Remote Sensing*, 70:829–840, 2004.

Houck, O. A. and Environmental Law Institute. *The Clean Water Act TMDL program: law, policy, and implementation*. Environmental Law Institute, Washington, DC, 2nd edition, 2002.

Ihaka, R. and R. Gentleman. R: A language for data analysis and graphics. *Journal of Computational and Graphical Statistics*, 5(3):299–314, 1996.

Jakeman, A. J. and R. A. Letcher. Integrated assessment and modelling: Features, principles and examples for catchment management. *Environmental Modelling & Software*, 18(6):491–501, 2003.

Jakeman, A. J., I. Littlewood, and P. Whitehead. Computation of the instantaneous unit hydrograph and identifiable component flows with application to two small upland catchments. *Journal of Hydrology*, 117(1):275–300, 1990.

Kavetski, D., G. Kuczera, and S. Franks. Bayesian analysis of input uncertainty in hydrological modeling: 1. Theory. *Water Resources Research*, 42(3):W03407, 2006.

Kirby-Smith, W. W. Study on flow patterns in Ware Creek, North Carolina, 2008.

Kokkonen, T., A. Jakeman, P. Young, and H. Koivusalo. Predicting daily flows in ungauged catchments: model regionalization from catchment descriptors at the Coweeta Hydrologic Laboratory, North Carolina. *Hydrological Processes*, 17(11):2219–2238, 2003.

Kuczera, G. and E. Parent. Monte Carlo assessment of parameter uncertainty in conceptual catchment models: the Metropolis algorithm. *Journal of Hydrology*, 211(1-4):69–85, 1998.

Littlewood, I., K. Down, J. Parker, and D. Post. IHACRES v1.0 user guide. *Centre for Ecology and Hydrology, Wallingford, UK and Integrated Catchment Assessment and Management Centre, Australian National University, Canberra*, 1997.

McIntyre, N., H. Lee, H. Wheater, A. Young, and T. Wagener. Ensemble predictions of runoff in ungauged catchments. *Water Resources Research*, 41:3307–3323, 2005.

McMillan, H. and M. Clark. Rainfall-runoff model calibration using informal likelihood measures within a Markov chain Monte Carlo sampling scheme. *Water Resources Research*, 45(4): W04418, 2009.

Milly, P. C., J. Betancourt, M. Falkenmark, R. M. Hirsch, Z. W. Kundzewicz, D. P. Lettenmaier, and R. J. Stouffer. Stationarity is dead: Whither water management? *Science*, 319(5863): 573–574, 2008.

Montanari, A. and A. Brath. A stochastic approach for assessing the uncertainty of rainfall-runoff simulations. *Water Resources Research*, 40(1):W01106, 2004.

Nandakumar, N. and R. Mein. Uncertainty in rainfall-runoff model simulations and the implications for predicting the hydrologic effects of land-use change. *Journal of Hydrology*, 192(1-4): 211–232, 1997.

Nash, J. and J. Sutcliffe. River flow forecasting through conceptual models part I–A discussion of principles. *Journal of hydrology*, 10(3):282–290, 1970.

National Research Council. Assessing the TMDL approach to water quality management, 2001.

Reckhow, K. H. On the need for uncertainty assessment in TMDL modeling and implementation. *Journal of Water Resources Planning and Management-ASCE*, 129(4):245–246, 2003.

Seibert, J. Regionalisation of parameters for a conceptual rainfall-runoff model. *Agricultural and Forest Meteorology*, 98(1):279–293, 1999.

Stedinger, J., R. Vogel, S. Lee, and R. Batchelder. Appraisal of the generalized likelihood uncertainty estimation (GLUE) method. *Water Resources Research*, 44, 2008.

Vrugt, J., C. ter Braak, M. Clark, J. Hyman, and B. Robinson. Treatment of input uncertainty in hydrologic modeling: Doing hydrology backward with Markov chain Monte Carlo simulation. *Water Resources Research*, 44(W00B09), 2008.

Vrugt, J., C. ter Braak, H. Gupta, and B. Robinson. Equifinality of formal (DREAM) and informal (GLUE) bayesian approaches in hydrologic modeling? *Stochastic Environmental Research and Risk Assessment*, 23(7):1011–1026, 2009.

Wagener, T., D. Boyle, M. Lees, H. Wheater, H. Gupta, and S. Sorooshian. A framework for development and application of hydrological models. *Hydrology and Earth System Sciences*, 5 (1):13–26, 2001.

Whitehead, P., P. Young, and G. Hornberger. A systems model of stream flow and water quality in the bedford ouse river. 1. stream flow modelling. *Water Research*, 13(12):1155–1169, 1979.

Young, P. Top-down and data-based mechanistic modelling of rainfall-flow dynamics at the catchment scale. *Hydrological Processes*, 17(11):2195–2217, 2003.

Young, P. C. and K. J. Beven. Data-based mechanistic modelling and the rainfall-flow non-linearity. *Environmetrics*, 5(3):335–363, 1994.

APPENDIX A

The IHACRES model derives effective rainfall u_k (in mm) at time k from incident rainfall r_k (in mm) through a unitless catchment wetness index s_k as follows [Jakeman et al., 1990]:

$$
\begin{aligned}
u_k &= r_k s_k \\
s_k &= c r_k + \left(1 - \frac{1}{\tau_w(T_k)}\right) s_{k-1}; s_0 = 0 \text{ and (ideally) } 0 < s_k < 1 \\
\tau_w(T_k) &= \tau_w \exp\left\{(R - T_k)f\right\}
\end{aligned}
$$

where,

$$
\begin{aligned}
c &= \text{volume-forcing constant (1/mm)} \\
\tau_w(T_k) &= \text{mean soil storage residence time at temperature } T_k \text{ (unitless)} \\
T_k &= \text{mean daily temperature (deg C)} \\
\tau_w &= \text{catchment drying time constant at reference temperature } R \\
R &= \text{reference temperature} = 20 \text{ (deg C)} \\
f &= \text{temperature modulation factor (1/deg C)}
\end{aligned}
$$

Streamflow x_k at time k is then calculated from effective rainfall u_k through recursive application of the following [Young, 2003]:

$$
x_k = \alpha x_{k-1} + \beta u_k
$$

where α and β are model coefficients such that $\beta = 1 - \alpha$ and $\tau_f = \frac{1}{-\ln \alpha}$.