HYDROLOGICAL PROCESSES
Hydrol. Process. **28**, 2033–2045 (2014)
Published online 12 March 2013 in Wiley Online Library
(wileyonlinelibrary.com) DOI: 10.1002/hyp.9721

Application of distributed hydrological models for predictions in ungauged basins: a method to quantify predictive uncertainty

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Abstract:

Stream flow predictions in ungauged basins are one of the most challenging tasks in surface water hydrology because of nonavailability of data and system heterogeneity. This study proposes a method to quantify stream flow predictive uncertainty of distributed hydrologic models for ungauged basins. The method is based on the concepts of deriving probability distribution of model's sensitive parameters by using measured data from a gauged basin and transferring the distribution to hydrologically similar ungauged basins for stream flow predictions. A Monte Carlo simulation of the hydrologic model using sampled parameter sets with assumed probability distribution is conducted. The posterior probability distributions of the sensitive parameters are then computed using a Bayesian approach. In addition, preselected threshold values of likelihood measure of simulations are employed for sizing the parameter range, which helps reduce the predictive uncertainty. The proposed method is illustrated through two case studies using two hydrologically independent sub-basins in the Cedar Creek watershed located in Texas, USA, using the Soil and Water Assessment Tool (SWAT) model. The probability distribution of the SWAT parameters is derived from the data from one of the sub-basins and is applied for simulation in the other sub-basin considered as pseudo-ungauged. In order to assess the robustness of the method, the numerical exercise is repeated by reversing the gauged and pseudo-ungauged basins. The results are subsequently compared with the measured stream flow from the sub-basins. It is observed that the measured stream flow in the pseudo-ungauged basin lies well within the estimated confidence band of predicted stream flow.

KEY WORDS predictions in ungauged basin; predictive uncertainty; distributed hydrologic model; SWAT model

Received 7 March 2012; Accepted 15 January 2013

INTRODUCTION

Human-induced changes, such as climate change, population growth and rapid urbanization, are putting enormous stress on our water resources. The global aim of water management is to avoid or minimize risk of crisis related to water supply to meet various human and ecological needs, such as irrigation, minimum flow for maintaining proper aquatic ecosystem structures and functions, and wastewater treatment. An accurate estimate of the available water resources is a prerequisite to sustainable water resources planning and management. For gauged basins, historical records of hydrological observations are available, but for ungauged basins, the assessment of water availability is a challenging task. Therefore, the major focus of studies pertaining to predictions in ungauged basins is to develop appropriate tools that can accurately quantify hydrologic responses under various land use and climate conditions.

A number of hydrologic simulation models, varying from simple empirical models to complex physics-based distributed models, are available for generating the watershed response (Singh and Prevert, 2002). These models represent the hydrologic processes in forms of various linear/nonlinear mathematical equations. However, most of these complex models have a large number of parameters that are to be estimated prior to their application to a specific watershed. Parameters estimation is generally achieved through calibration of the model by using observed data from the watershed under investigation. Calibration of models for an ungauged basin is not possible because of a lack of observed data. Therefore, there exists some skepticism about the accuracy of model predictions for ungauged basins (Bardossy, 2007; Pokhrel and Gupta, 2010; Hughes, 2010; Jos *et al.*, 2012). The complexities associated with predictions in ungauged basins are evident from the large-scale project initiated by the International Association of Hydrological Sciences, 'Predictions in Ungauged Basins (PUB)', emphasizing the need to examine and improve existing models in terms of their ability to predict flows in ungauged basins (Sivapalan *et al.*, 2003).

Parameter regionalization is one of the most common approaches to predict a hydrologic response of ungauged basins by relating model parameters and catchment descriptors in a statistical manner (Wagener and Wheater, 2006; Buytaert and Beven, 2009). In this approach, the parameters are calibrated in gauged basins and then transferred to hydrologically similar ungauged basins with

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suitable modifications. Vogel (2005) provided a comprehensive overview of regionalization approaches. The methods include bivariate and multivariate regression, clustering, kriging and neural networks (Gotzinger and Bardossy, 2007; Ganora et al., 2009; Samaniego *et al.*, 2010). Regionalization assumes that the model parameters estimated from historical data of gauged basins can afford accurate estimates of stream flow in ungauged basins. However, because every catchment is unique, model parameters need to be adapted for differences between a calibration and a prediction catchment, by either transformation or further selection (Andréassian *et al.*, 2001; Post *et al.*, 1998). This process is inherently uncertain (Buytaert and Beven, 2009). Thus, extrapolating model parameter applicability from one basin to the next may lead to a weak relationship between the model parameters and the catchment descriptors. Yet another concern in regionalization of parameters is associated with the equifinality problem—multiple parameter sets giving equally good simulation results (Beven *et al.*, 2000; Beven and Freer, 2001). This implies that a combination of parameters, which work very well on the gauged basin, may not guarantee a good performance when transferred to ungauged basins (Hundecha *et al.*, 2008). Therefore, it is desirable to relate the catchment response to the model parameters in terms of a likelihood measure (Montanari and Toth, 2007). Consequently, in such cases, stochastic validation of the model in ungauged basin may be preferred.

The stochastic validation evaluates the ability of a model to simulate watershed response by transforming parameter uncertainty into predictive uncertainty by using parameter probability distribution functions (Migliaccio and Chaubey, 2008). Model validation is then performed by estimating the confidence intervals of the model predictions. In the case of ungauged basins, quantification of the predictive uncertainty is only possible through stochastic simulation by transferring parameter probability distribution function from the gauged basins to ungauged basins. The main advantage of transferring the probability distribution function of the parameters to ungauged basins over the conventional regionalization techniques is that the parameter sets are neither averaged nor interpolated; rather, the full information about the parameter behaviour in a gauged basin is transferred to the ungauged basin (Buytaert and Beven, 2009). In addition, by using the probability distribution of parameters, the problem of equifinality can be minimized by creating an ensemble outputs for the model. However, to perform stochastic simulations of any watershed model in an ungauged basin, it is essential to have a priori knowledge about the probability distribution function of the model parameters. Note that the probability distribution function of the parameters depends on the catchment characteristics and therefore can be transferred from a gauged basin only to hydrologically similar ungauged basins.

In this paper, we apply a distributed watershed model (Soil and Water Assessment Tool, or SWAT) to predict the river flow in an ungauged basin. We have accomplished this by deriving the probability distribution function of the sensitive parameters of SWAT and applying them to generate ensemble predictions in an ungauged basin.

THEORETICAL CONSIDERATIONS

Hydrologic simulation models are indexed by parameters, which may (or may not) be physically interpretable. The generalized representation of a hydrologic model is as follows:

$$y = \mathrm{f}(x|\boldsymbol{\theta}) \tag{1}$$

where f(.) is the function described by the model, $\boldsymbol{y}$ is the output from the model (stream flow, sediment concentration, nutrient concentration, etc.) corresponding to the inputs $\boldsymbol{x}$ (rainfall, temperature, evaporation, etc.) and $\boldsymbol{\theta}$ is the vector of parameters of the model. If the model is employed to make temporal predictions, there could be a time subscript added to each of these variables. Some of these parameters such as the area of the watershed and the slope of the watershed are measurable, but many others are to be estimated through the process of calibration. Typically, model parameters are estimated by nonlinear optimization using an objective function, such as the following:

$$\text{Min (sum of squares of errors)} = \min \sum_{t=1}^{n} \left[y_{t,\text{obs}} - y_{t,\text{sim}}(x_t;\theta) \right]^2 \tag{2}$$

where $y_{t,\text{obs}}$ and $y_{t,\text{sim}}$ are observed and simulated system responses at time t, respectively. Calibration of watershed models, however, is a challenging problem because of various levels of uncertainty. Generally, the uncertainty in model simulations are considered to be caused from three different components: (i) structural uncertainty, which is a source of uncertainty that includes processes that are not accounted in the model and model inaccuracy due to oversimplification of the processes considered in the model; (ii) input uncertainty, which is often related to imprecise measurements of model inputs or initial conditions, such as elevation, land use, precipitation and temperature; and (iii) parameter uncertainty , which is attributed to a number of unknown parameters in the model (Beven and Freer, 2001; Srivastav *et al.*, 2007; Renard *et al.*, 2010). Although all the sources of uncertainty should be addressed in any modelling effort, the focus of this paper is to quantify the uncertainty caused by the parameters of the model when applying to an ungauged basin.

One way to quantify the parameter uncertainty is to introduce suitable probability distributions (Thiemann *et al.*, 2001). The available methods for such assessment of uncertainty can be grouped into two: formal Bayesian approach and informal Bayesian approach (Li *et al.*, 2010). Many studies that compared the uncertainty estimates derived using both the methods have reported merits and demerits of both the approaches (Vrugt *et al.*, 2009;

Jin *et al.*, 2010; Mantovan and Todini, 2006; Yang *et al.*, 2008; Stedinger *et al.*, 2008). The informal approach, generalized likelihood uncertainty estimator (GLUE) proposed by Beven and Binley (1992), is popular for its conceptual simplicity, ease of implementation and flexibility of using the hydrological models without modifications (Li *et al.*, 2010). In GLUE, uncertainty is expressed in terms of probability distributions and is considered to be one of the defining features of Bayesian inference. Concepts behind GLUE framework are discussed later. Let p($\boldsymbol{\theta}$) denote the probability density function of the possible parameter sets, which is an unconditional distribution, as it does not depend on currently available values of the inputs ($\boldsymbol{x}$) or outputs ($\boldsymbol{y}$). Note that the probability distribution of parameters is not known initially. Beven and Binley (1992) suggested restricting attention to a large range of parameter values and initially imposing a uniform distribution on that range. These initial probability distributions can be conditioned (or modified) by considering the measured values of inputs and outputs by using a Bayesian approach. Let p($\boldsymbol{y} \mid \boldsymbol{x}$, $\boldsymbol{\theta}$) denote the conditional probability of output $\boldsymbol{y}$ given the inputs $\boldsymbol{x}$ and the parameters $\boldsymbol{\theta}$, whose functional form has to be specified from a plausible family of distributions for the model residuals. Then the conditional probability density function for the outputs and the model parameters, given only the inputs, can be determined as follows:

$$p(\boldsymbol{y}, \boldsymbol{\theta}|\boldsymbol{x}) = p(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta}) * p(\boldsymbol{\theta}) \tag{3}$$

In a deterministic calibration procedure, a single optimal parameter that is most likely to reproduce the set of observed outputs is sought. Aim of Bayesian approach, on the other hand, is to infer the posterior probability distribution of the parameter p($\boldsymbol{\theta} \mid \boldsymbol{x}$, $\boldsymbol{y}$) given the observed data of inputs and outputs. Accordingly, a region of highest posterior density describes a set of plausible models. The marginal posterior density function of parameter p($\boldsymbol{\theta} \mid \boldsymbol{x}$, $\boldsymbol{y}$) can be computed as follows:

$$\begin{aligned} p(\boldsymbol{\theta}|\boldsymbol{x}, \boldsymbol{y}) &= \frac{p(\boldsymbol{y}|\boldsymbol{x}, \ \boldsymbol{\theta}) * p(\boldsymbol{\theta})}{p(\boldsymbol{y}|\boldsymbol{x})} \\ &= \frac{p(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta}) * p(\boldsymbol{\theta})}{\int p(\boldsymbol{y}|\boldsymbol{x}, \ \boldsymbol{\theta}) * p(\boldsymbol{\theta}) * d(\boldsymbol{\theta})} \end{aligned} \tag{4}$$

The term p($\boldsymbol{y} \mid \boldsymbol{x}$, $\boldsymbol{\theta}$) is usually known as the likelihood function (Yang *et al.*, 2008). The specific requirement of a good likelihood measure to be employed in the GLUE framework is that the likelihood value should be close to zero to indicate dissimilarity with the actual system, and the measure should monotonically increase as the similarity with the actual system increases (Beven and Binley, 1992). In recent years, several researchers have discussed/debated on the use of either a formal or an informal approach for specifying a likelihood function for uncertainty analysis (Mantovan and Todini, 2006; Beven *et al.*, 2008; Vrugt *et al.*, 2008; Stedinger *et al.*, 2008; McMillan and Clark, 2009; Schoups and Vrugt, 2010). Despite this, no clear guidelines are available for specifying the form of likelihood function. The most frequently used likelihood measure in literature is the Nash–Sutcliffe (NS) efficiency (Freer *et al.*, 1996; Beven and Freer, 2001) defined as follows:

$$NS = 1 - \frac{\sum_{t=1}^{n} (y_t(\boldsymbol{\theta}) - y_t)^2}{\sum_{t=1}^{n} (y_t - \bar{y})^2} \tag{5}$$

where n is the number of observed data points, y_t and $y_t(\boldsymbol{\theta})$ represent the observation and model simulation with parameters $\boldsymbol{\theta}$ at any given time, t, respectively, and $\bar{y}$ is the average observed value. It may be noted that similar to any likelihood measure, use of NS as likelihood is also limited by its inherent assumptions of homoscedasticity, independence and Gaussian distribution on model residuals. Therefore, according to Bayes' theorem, the probability density of the posterior distribution can be derived from the prior density and measured data using Equations (4) and (5). Subsequently, the probability density function of the parameter can be iteratively updated so that a distribution that gives a maximum likelihood value can be identified.

METHODOLOGY

The proposed methodology works on concepts very similar to that of the GLUE approach and employs Monte Carlo simulation of the hydrologic model by using ensemble parameter sets generated by Latin hypercube sampling (LHS) (McKay *et al.*, 1979). A major difference between the proposed methodology and the GLUE is that in our methodology, GLUE is considered in an iterative loop, until the probability distributions of the parameters converge in successive iterations. The flowchart of the proposed methodology is presented in Figure 1.

Because the parameter probability distribution is not available initially, a uniform distribution is assumed (Freer *et al.*, 1996; Manache and Melching, 2008). Subsequently, the sensitivity of the model parameters is computed using the method of Sobol', a global sensitivity analysis technique (Sobol', 1993; Tang *et al.*, 2007; Cibin *et al.*, 2010). A detailed description of LHS and the sensitivity analysis of Sobol' for the SWAT model are described by Cibin *et al.* (2010) and are not presented here.

The posterior probability distributions of the sensitive parameters are computed using a Bayesian approach described earlier. In order to arrive at the posterior probability distribution, an informal Bayesian approach in the GLUE framework is employed in this study. In addition, preselected threshold values of likelihood measure of simulations are employed for sizing the parameter range, which helps reduce the predictive uncertainty.

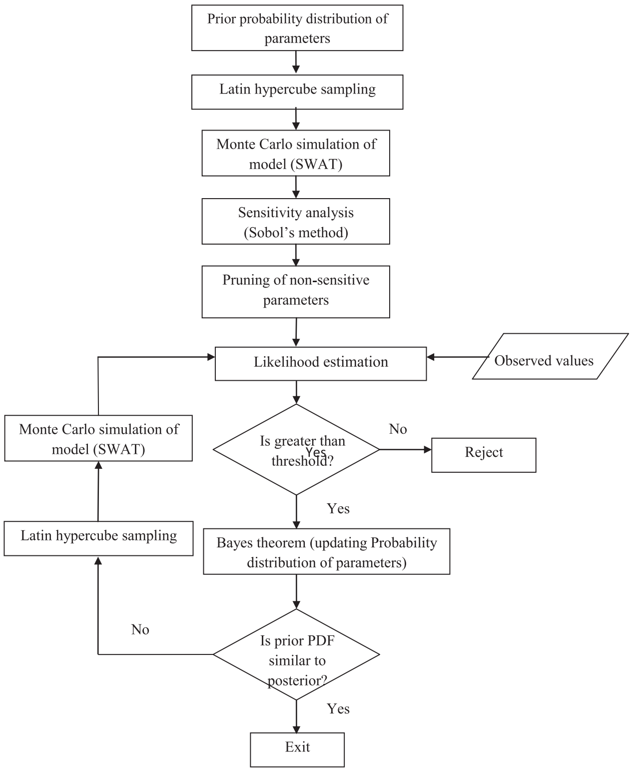

Figure 1. Flowchart of the proposed methodology for deriving the probability distribution function of parameters

Probability distribution updating is continued till both the distributions (prior and posterior) converge in successive Monte Carlo simulations. (The criteria used for testing the convergence are discussed in later sections where a case study is illustrated). Although majority of the GLUE studies have used simple uniform random sampling, we propose to use LHS, which is accepted to be an efficient alternative to random sampling (Tolson and Shoemaker, 2008). Even though other sampling methods such as Markov chain Monte Carlo and importance sampling can also be used for this study, LHS is considered to be simple and computationally efficient. One concern with the LHS is its inability to improve the sampling frequency of the behavioural parameter sets. However, in the current study, the probability distributions of the parameters are modified using the behavioural parameter sets every time before the LHS is performed; therefore, sampling frequency of the behavioural parameters sets are not limited.

To facilitate stochastic simulation of the model in ungauged basin, the distribution of the parameters are obtained for a gauged basin and transferred to hydrologically homogenous ungauged basins. It may be noted that the larger the ensembles, the higher will be the frequency of behavioural parameter sets; however, in the current study, the high computational requirement for SWAT simulation restricted us to arrive at a compromising number of simulations in the ensemble. One thousand ensembles of predictions were obtained for the ungauged basin by using the transferred parameter probability distribution and were used for quantifying predictive uncertainty.

Illustrative case example

The proposed methodology is illustrated through an application of the SWAT model for simulating river flow in an ungauged basin. In this study, two hydrologically independent sub-catchments of Cedar Creek watershed, Texas (Figure 2), are considered: (i) Cedar Creek and (ii) King's Creek. Although both the basins are gauged, one of them is considered as ungauged for the analysis, making it a pseudo-ungauged catchment. Two numerical exercises were conducted in this study by considering the following: (i) King's Creek basin as gauged and Cedar Creek basin as pseudo-ungauged, and (ii) Cedar Creek basin as gauged and King's Creek basin as pseudo-ungauged. As discussed earlier, the probability distribution of the model parameters are derived using the data corresponding to the gauged basin and are applied for stochastic simulations in the pseudo-ungauged basin. The two exercises mentioned earlier help evaluate if the quantified uncertainty is biased towards the data pertaining to the gauged basin that is used for deriving the distribution of parameters.

SWAT model. The SWAT model is a complex physics-based distributed hydrologic model that operates on a daily time step, developed by the United States Department of Agriculture (Arnold *et al.*, 1993). SWAT has been proven to be an effective tool for assessing water resource and nonpoint source pollution problems for a wide range of scales and environmental conditions across the globe. The SWAT spatially divides the watershed into sub-watersheds or sub-basins on the basis of the topographical information. The sub-watersheds are further divided into smaller spatial modelling units called hydrologic response units. Hydrologic response units are lumped areas within sub-basin that are composed of unique land cover, soil and management practices, in which the simulations are carried out and are aggregated at the sub-basin level. Major hydrological processes modelled in SWAT are surface runoff, soil and

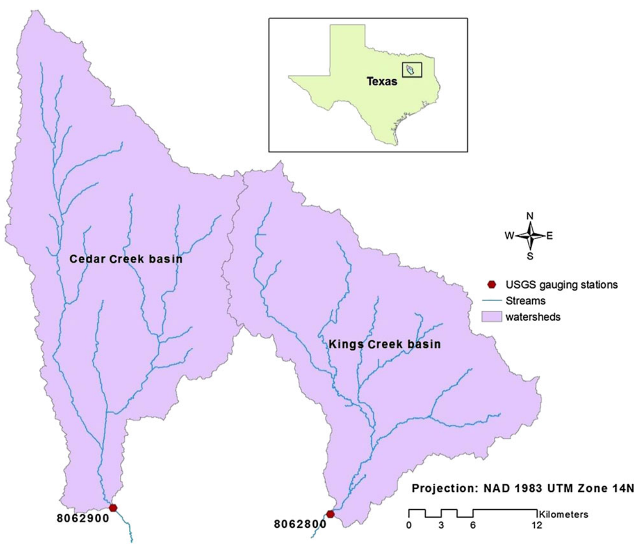

Figure 2. The location map of the study area

root zone infiltration, evapotranspiration, soil and snow evaporation and base flow (Arnold *et al*., 1998). The current study concentrates on the steam flow modelling component of SWAT. More detailed mathematical description about the SWAT model is available in Neitsch *et al*. (2002).

SWAT parameters affecting stream flow generation. The parameters of the SWAT model that affect stream flow predictions are identified through a detailed literature review and are presented in Table I, along with their recommended range of perturbations (Neitsch *et al*., 2002; Arabi *et al*., 2007). Note that some of these parameters have been perturbed as a percentage of their default values to maintain their heterogeneity. In this study, 13 important parameters related to stream flow generation are considered (Table I).

The parameters SFTMP and SURLAG are sub-basin level parameters. SFTMP is the snowfall temperature, mean air temperature at which precipitation is equally likely to be rain as well as snow. SURLAG controls the fraction of the total water that will be allowed to enter the reach on any specific day. In large basins, with a time of concentration of more than one day, only a portion of surface runoff will reach the main channel on the same day. Parameters such as ALPHA_BF, GW_DELAY, GW_REVAP and GWQMN are groundwater simulation parameters of SWAT. ALPHA_BF, the base flow recession coefficient, is a direct index of groundwater flow response to changes in recharge. GW_DELAY is the lag between the times that water exits the soil profile and enters the shallow aquifer. GW_REVAP, groundwater revap coefficient, controls the reverse water movement from shallow aquifer to the unsaturated soil layers. GWQMN is the threshold depth of water in the shallow aquifer for return flow to occur. The parameter that is related to evaporation is ESCO, soil evaporation compensation factor. The parameter ESCO controls the soil evaporative demand that is to be met from different depths of the soil. With the value of ESCO smaller, the model allows extracting more of the evaporative demand from lower soil profiles. The parameters OV_N (overland Manning's roughness coefficient), SLOPE, SLSUBBSN and CN_f (curve number) contribute directly to the surface runoff component of SWAT. Soil moisture characteristics in the model are represented by SOL_AWC and SOL_K. SOL_AWC, plant available water or available water capacity, is estimated as the difference between the field capacity and the wilting point. SOL_K, saturated hydraulic conductivity, relates soil water flow rate to the hydraulic conductivity.

Details of the study area and data availability. The Cedar Creek watershed (hydrologic unit code #12030107) with an area of 1623 km^2 is located in the Trinity River basin, in East Central Texas, USA. Two independent sub-basins of the Cedar Creek watershed (Figure 2) are considered. The sub-watershed Cedar creek has a catchment area of 490 km^2 and one gauging station near Kemp, TX [United States Geological Survey (USGS) gauging station #08062800]. The second sub-basin, King's Creek with its outlet near Kaufman, TX (USGS Gauging station #08062900), has a catchment area of 603 km^2. Environmental Protection Agency BASINS3.0 interface was used for watershed delineation and developing input data for the SWAT model of both sub-watersheds. The elevation data Digital elevation model (DEM) from the National Elevation Dataset, 30-m resolution, developed by USGS, was used to delineate the sub-watersheds. The soils database used for this project was developed from two sources from the Natural Resources Conservation Service, namely Soil Survey Geographic (SSURGO) and Computer Based Mapping System (CBMS). The land use/land cover input was obtained from the1992 USGS National Land Cover Dataset.

The geomorphological characteristics, climatic characteristics and land use characteristics of the sub-basins are given in Table II, from which it can be observed that

Table I. The SWAT parameters that influence stream flow simulation in the model, range of perturbation and their relative sensitivity rank

Symbol	Description	Unit	Range	Hydrologic process affected by the parameter	Sensitivity rank	
					Cedar Creek	King's Creek
ALPHA_BF	Base flow recession coefficient	Days	0–1	Groundwater	9	9
CN_f*	Curve number	%	−25–15	Surface runoff	2	2
ESCO	Soil evaporation coefficient	—	0.001–1	Evapotranspiration	1	1
GW_DELAY	Groundwater delay time	day	1–500	Groundwater	9	9
GW_REVAP	Revap coefficient	—	0.02–0.2	Groundwater	9	9
GWQMN	Depth of water in shallow aquifer	mm	0–5000	Groundwater	9	9
OV_N	Manning's *N*	—	0.1–0.3	Overland flow	5	6
SFTMP	Snowfall temperature	^{0}C	−5–5	Snow	8	8
SLOPE*	Slope	%	−0.5–1	Surface runoff	6	7
SLSUBBSN*	Slope sub-basin	%	−0.5–1	Surface runoff	7	5
SOL_AWC*	Available water capacity	%	−0.3–2	Groundwater and evaporation	3	3
SOL_K*	Saturated hydraulic conductivity	%	−0.5–1	Groundwater	9	9
SURLAG	Surface lag	Day	1–12	surface runoff	4	4

*These parameters were changed as a percentage of their default values to maintain heterogeneity.

Table II. Hydrologic characteristics of the study basins

CA	Cedar Creek	King's Creek
Area (km^2)	490	603
Drainage density (m/m^2)	0.0012	0.0011
Annual precipitation (mm)	984.45	1065.70
Slope (%)	3.2	4.7
Bifurcation ratio	2.41	2.40
Shape factor	2.485	4.179
Mean elevation (m)	95	100
% of area – agriculture	67	67
% of area – forest	17	17
% of area – urban	7	7
% of area – miscellaneous	9	9

CA, Catchment Attributes.

all characteristics are similar except the shape factor. The shape factor of a watershed is expected to influence the time of concentration of the watershed and, in turn, may influence the time-to-peak characteristics of hydrograph. Because the proposed method envisages transfer of parameter probability distribution to ungauged basin for simulations, it does not account for the variability in watershed characteristics and can be applied to hydrologically similar watersheds only. The similarity in the hydrological responses of the sub-basins is analysed using the concept of L-moments introduced by Hosking and Wallis (1993). In these sub-watersheds, the dispersion statistic is less than 1 ($H1 = -1.7264$, $H2 = -0.3536$, $H3 = -0.3508$), so these basins are relatively homogenous according to Hosking and Wallis (1993).

The weather data from six weather stations and the daily stream discharge data from two stream gauge stations were obtained from the National Climatic Data Center and USGS websites. The model was set up for 10 years from 1977 to 1986, out of which the first three years were considered as the model's warm-up period. Thus, effectively 7 years of data were considered for the analysis. These 7 years (1980–1986) in King's Creek basin were characterized with a minimum daily flow of 0.0 m^3/s and maximum daily flow of 433.22 m^3/s. The mean daily flow during this period was 4.34 m^3/s with a standard deviation of 20.47 m^3/s. The watershed response in Cedar Creek basin was characterized with a minimum daily flow of 0.0 m^3/s and maximum daily flow of 269.22 m^3/s. The mean daily flow during this period was 3.16 m^3/s with a standard deviation of 13.84 m^3/s.

RESULTS AND DISCUSSIONS

Case study 1: Cedar Creek as gauged and King's Creek as pseudo-ungauged

The sensitivity analysis of Sobol' on the SWAT parameters in study watersheds suggested SURLAG, CN_f, ESCO and SOL_AWC as the most sensitive parameters (Table I). The sensitivity analysis also indicated that five parameters, namely, ALPHA_BF, GW_DELAY, GW_REVAP, GWQMN and SOL_K, did not significantly influence the runoff generation by the SWAT model in the Cedar Creek watershed. Hence, these five parameters were assumed to have a fixed value in the analysis and were not considered in further sampling. The sensitivity analysis also indicated that only three parameters (SURLAG, SOL_AWC and CN_f) were identifiable in the first stage (Figure 3) of

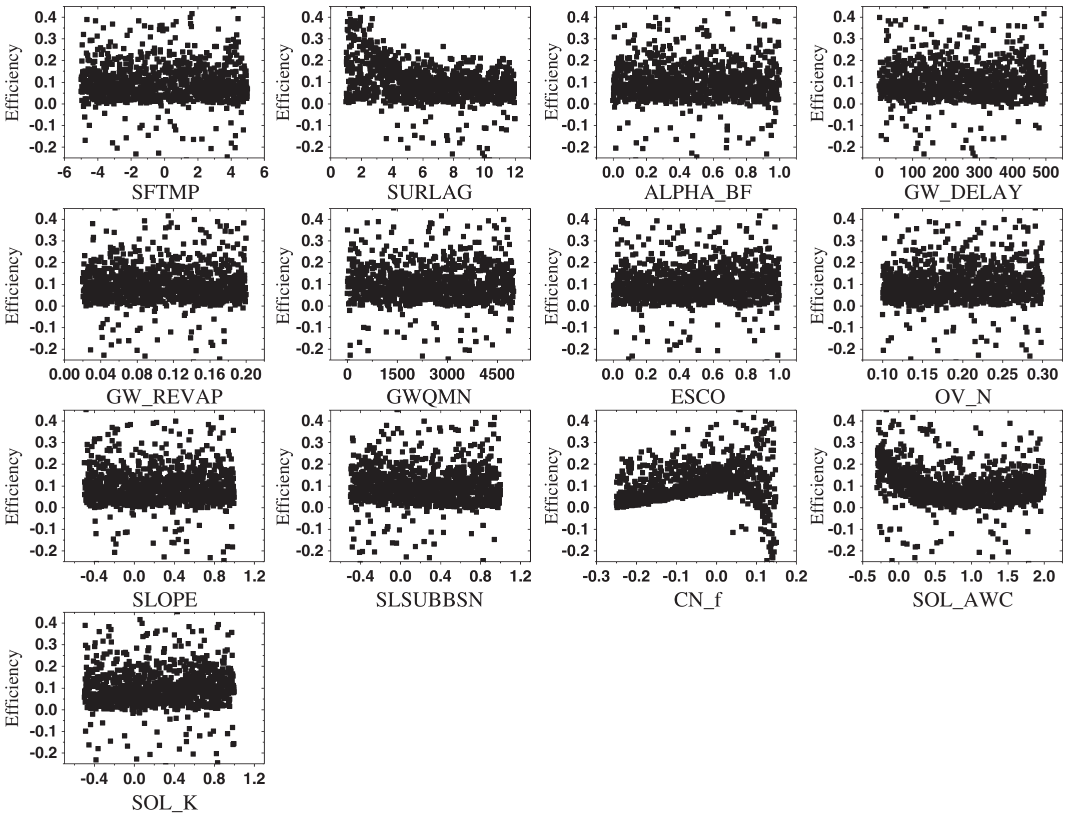

Figure 3. Scatter plot of Nash–Sutcliffe efficiency against the variation of the parameters in the Monte Carlo simulations in Cedar Creek watershed (base simulation)

iteration in the Cedar Creek watershed. Consequently, in the first iteration of modifying the probability distribution of parameters, SURLAG, SOL_AWC and CN_f were only considered for Bayesian updating of probability distribution functions of parameters in the Cedar Creek watershed. The remaining five parameters, although were found to be slightly sensitive, were kept at the recommended values because they were not identifiable. A calibration of nonidentifiable parameters is difficult, as they can lead to equifinality of parameters (Damaria *et al.*, 2007; Cibin *et al.*, 2010). In this study, these parameters were assigned values considering their importance in the concerned hydrologic processes and also considering the watershed characteristics. The procedure employed a threshold value for the likelihood to accept/reject simulations: initially, all simulations resulting in positive values of NS efficiency is considered acceptable. Accordingly, the range for SURLAG was reduced to 1–3.0 from the original rage of 1–12 in the first iteration of the derivation of probability distribution. After the first updating of the probability distribution of parameters, the ensemble simulations were created and a threshold value equal to 0.20 as NS efficiency was used to reduce the range of parameter. The threshold value was modified further at every iteration such that only the top 50% of the ensembles are considered in further analysis. In the final iteration, the threshold used was 0.45.

The basic assumption during the updating of probability distribution was that the highest probability density for the parameter should be at points of high model performance (likelihood). Accordingly, the total parameter range was divided into a number of bins (100 numbers), and the maximum likelihood value corresponding to each bin was considered as the likelihood measure for that bin. These likelihood values along with the corresponding prior probability distribution were employed to compute the posterior probability distribution using Bayes theorem (Equation (4)). The iterations were continued using the posterior probability distribution for further sampling through LHS (1000 samples). The derived probability distribution of individual parameters was compared with corresponding prior probability distribution for similarity in terms of their characteristics. The updating of the probability distribution continued till both the distributions (prior and posterior) converged in successive Monte Carlo simulations. Note that the identifiability of parameters is analysed with scatter plots in each of the iterations.

Probability distribution of SWAT parameters. The probability distribution of parameters was quantified, after every iteration, using the Best Fit program (Palisades Corp., CA, USA), which considered 28 different distributions to the data and ranked them according to a specified goodness-of-fit criterion. The parameters of the probability distributions were estimated using maximum-likelihood estimator (Haan, 2002). The Chi-square goodness-of-fit test was performed to evaluate and rank the distributions that best described the data. Probability distribution of some of the model parameters could not be derived because they were not identifiable (e.g. ESCO), indicating that identifiability of the parameter is a major requirement for derivation of probability distribution. More discussion on the identifiability of SWAT parameters can be obtained from Cibin *et al.*, (2010). The progressive modification of probability distribution of SWAT parameters obtained from Monte Carlo analysis is shown in Figure 4. As mentioned earlier, SURLAG, CN_f and SOL_AWC were identifiable and assumed to have ‘uniform distribution’. It is also to be noted that as the probability distribution was updated, the range of parameters in which region of high probability density falls was reduced, suggesting that the uncertainty associated with the parameter was also reduced. The proximity of parameters of the probability distribution is used as the convergence criteria for stopping the modification of the probability distribution of SWAT parameters.

Kullback–Leibler Divergence (KLDive) test (Cover and Thomas, 1991; Veldhuis *et al.*, 2003, Burnham *et al.*, 2001) was used to check convergence of the posterior probability distribution of parameters on the prior. KLDive index close to zero confirms the convergence of probability distributions. The probability distribution functions of different parameters were found to converge at different iterations. After the convergence of the probability distribution function, the sampled values of sensitive parameters were kept unchanged. The parameters SURLAG and CN_f converged after four iterations, with index values of 0.00099 and 0.0027, respectively. The SOL_AWC converged in the sixth iteration with an index value of 0.016. The probability distribution of the SWAT parameters was found to have no significant change after six iterations, indicating that the prior and posterior distributions had converged. The change in parameters of the distribution of SOL_AWC is presented in Table III, which clearly illustrates that the characteristics of the probability distribution are very similar.

Probability distributions of the model parameters were identified, and the parameters of the corresponding distribution are presented in Table IV. All parameters followed Beta general distribution in general with varying shape and location parameters (Table IV). Final ranges of model parameters were considerably different from the original range considered for the analysis. This implies that any calibration effort of the SWAT model that considers the probability distribution of parameters may lead to efficient convergence.

Progressive improvement in uncertainty reduction. A lack of information about the output uncertainty is the main concern that prevents the application of hydrological models in ungauged basin. The first simulation with maximum possible ranges for all the parameters showed a very high output uncertainty, with NS efficiency varying from −0.88 to 0.45. As mentioned earlier, during the first iteration, the actual probability distribution of the parameters was not available; therefore, uniform distribution was assumed for all the parameters. It is observed that in the subsequent iterations, as the parameter probability

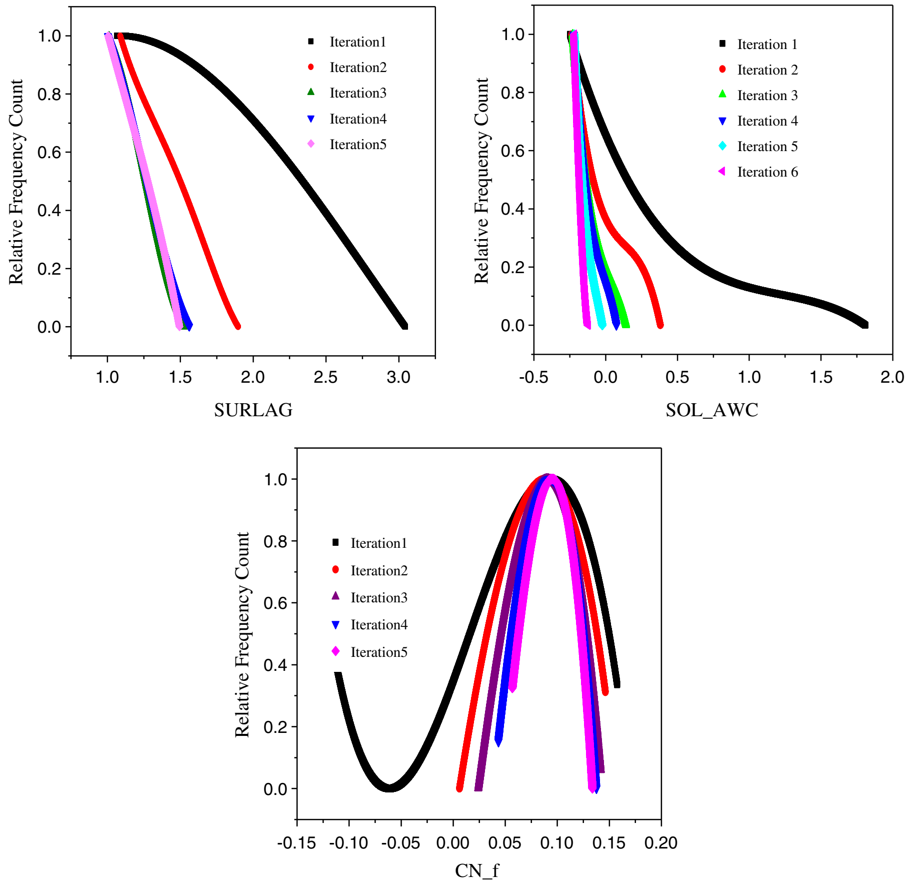

Figure 4. Progressive updating of parameter probability distributions for the three parameters in Cedar Creek River watershed considered along the iterations

Table III. Variation of parameters of probability distribution function along the iteration for the SWAT parameter SOL_AWC in basins of Cedar Creek watershed

	Iteration	a_1	a_2	min	max
Cedar Creek basin	4	0.5134	1.1275	−0.2223	0.0744
	5	0.5126	1.2049	−0.2188	−0.0235
	6	0.7660	1.9469	−0.2177	−0.0223
King's Creek basin	3	0.56756	1.1479	−0.2383	−0.03199
	4	0.56459	1.0760	−0.2366	−0.17830
	5	0.61530	1.2895	−0.2358	−0.19690

Beta general distribution: $f(x) = \frac{1}{(\max - \min)} \frac{\Gamma(a_1+a_2)}{\Gamma a_1 \Gamma a_2} \left(\frac{X-\min}{\max-\min}\right)^{a_1-1} \left(\frac{\max-X}{\max-\min}\right)^{a_2-1}$.

distribution become updated, the acceptable simulations were within a compressed range of parameter values, thereby reducing parameter uncertainty. The progressive improvement in the uncertainty, with the likelihood value plotted against their normalized frequency in the entire simulations is shown in Figure 5. In the first simulation, where uniform distribution for parameters is considered, the likelihood values are found to have high occurrence close to zero (Figure 5a). As the probability distributions converge (Figure 5b), the frequency distribution of likelihood values is found to be shifting towards higher values. For the final iteration, the uncertainty in terms of output efficiency varies from 0.3 to 0.53 (Figure 5c). In other words, once the distribution of the parameters was identified, the final ensemble predictions resulted in considerably improved NS efficiency of 0.30 compared with −0.88 during the base simulation, which employed uniform distribution for all the parameters. This certainly is a substantial improvement obtained because of the reduction in parameter uncertainty obtained through the updating of the probability distribution of the model parameters. Therefore, considering the progressive updating of distribution of parameters (Figure 4) and the reduction in uncertainty (Figure 5), it can be observed that Bayesian updating of the parameter probability distribution helped in compressing the range of likely parameter values and in reducing output uncertainty.

The frequency histogram of the NS efficiency is presented in Figure 6 for four different cases, namely, (i) the base simulation, which assumed that all the parameters follow uniform distribution; (ii) simulations generated

Table IV. Derived probability distribution of SWAT parameters and their characteristics in Cedar Creek watershed

SWAT parameter	King's Creek basin			Cedar Creek basin		
SURLAG	Beta general distribution	a_1	0.7778	Beta general distribution	a_1	0.8781
		a_2	2.1438		a_2	1.6246
		min	1.0000		min	1.0000
		max	1.6350		max	1.5000
CN_f	Beta general distribution	a_1	1.5165	Beta general distribution	a_1	1.2065
		a_2	1.0086		a_2	1.3080
		min	−0.0198		min	0.0560
		max	0.0154		max	0.1338
SOL_AWC	Beta general distribution	a_1	0.6153	Beta general distribution	a_1	0.7661
		a_2	1.2895		a_2	1.9469
		min	−0.2358		min	−0.2177
		max	−0.1969		max	−0.1223
ESCO	Beta general distribution	a_1	1.0624	Not identifiable		
		a_2	1.1994			
		min	0.8605			
		max	0.9783			

Beta general distribution: $f(x) = \frac{1}{(\max-\min)} \frac{\Gamma(a_1+a_2)}{\Gamma a_1 \Gamma a_2} \left(\frac{X-\min}{\max-\min}\right)^{a_1-1} \left(\frac{\max-X}{\max-\min}\right)^{a_2-1}$.

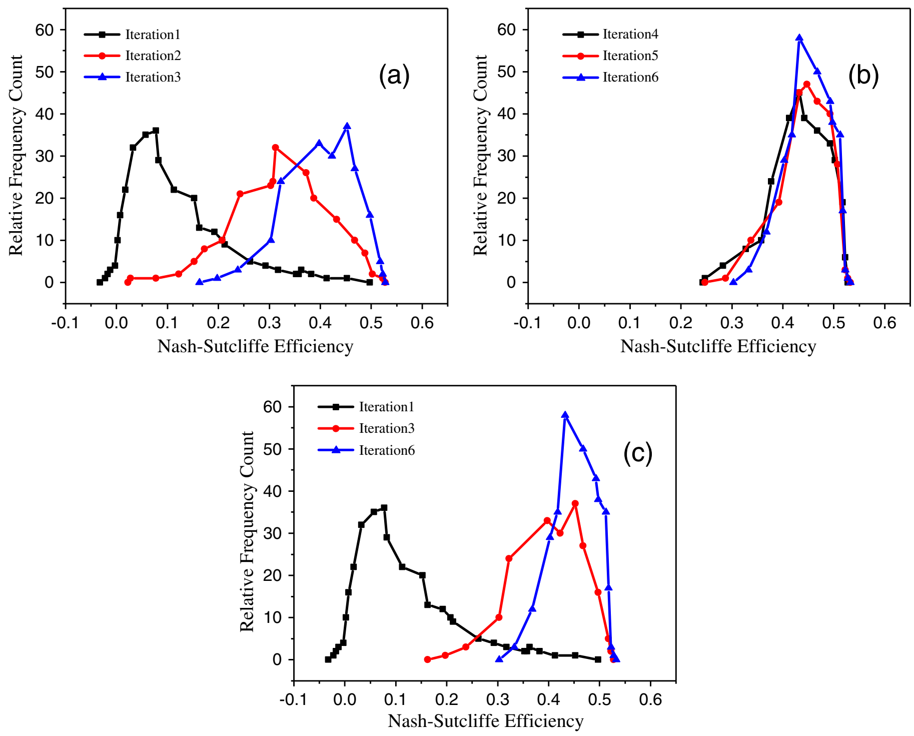

Figure 5. Progressive improvement in model prediction and reduction in uncertainty in Cedar Creek watershed: (a) normalized frequency plot of the Nash–Sutcliffe efficiency for iterations 1, 2 and 3 during the updating of the probability distribution function in Cedar Creek watershed; (b) normalized frequency plot of the Nash–Sutcliffe efficiency for iterations 4, 5, and 6 during the updating of the probability distribution function in Cedar Creek watershed; and (c) normalized frequency plot of Nash–Sutcliffe efficiency during the first, third and final iterations

using the standard GLUE approach; (iii) simulations generated using reduced parameter range by employing a threshold value of NS efficiency equal to 0.30 – no updating of probability distribution; and (iv) simulations that used the finally identified (converged) probability distribution of the parameters (proposed methodology). The number of simulations for all test cases was the same (1000 ensembles), except for the base simulations which was 32 000, and this large number of simulations during base simulations were from Sobol' sensitivity analysis. The threshold of NS efficiency for identifying the acceptable simulations was kept the same for Cases 2 and 3. For Case 4, the threshold value was progressively increased to identify the sensitive range of parameter and to ensure uncertainty reduction.

From Figure 6, it is evident that the proposed methodology results in high frequency of occurrence of the high value of NS efficiency. It is clear that the base simulation that assumes uniform distribution generates more number of simulations that have NS efficiency close

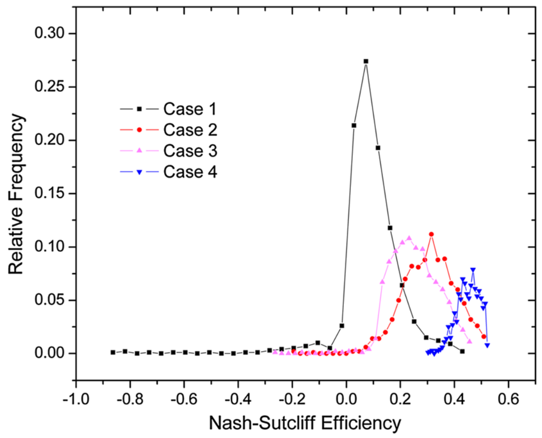

Figure 6. Frequency histogram of Nash–Sutcliff efficiency for different cases: (i) the base simulation, which assumes that all the parameters follow uniform distribution; (ii) simulations generated using the standard GLUE approach; (iii) simulations generated using reduced parameter range by employing a threshold value of NS efficiency equal to 0.30 – no updating of probability distribution; and (iv) simulations that used the finally identified (converged) probability distribution of the parameters

to 0.10. When the range of parameters were reduced using a threshold value of NS efficiency of 0.30 (Case 3, Figure 6), the ensemble simulations tend to marginally improve the high-frequency region of the high value of NS efficiency. The high frequency is focused in the region around a value of efficiency slightly more than 0.20. It may be noted that during this exercise, after the behavioural sets have been identified using an NS efficiency threshold value of 0.30, 1000 ensembles of parameter combinations were generated using LHS without any updating of the probability distribution function of the parameter (i.e. the parameter was assumed to be uniformly distributed). It is noted that although a value of 0.30 is considered as the threshold, the maximum relative frequency of the NS efficiency of simulations during Case 3 is observed to be less than 0.30. A plausible reason for this behaviour is that the stratified sampling (LHS in this study) does not ensure the appropriate combination of the parameters that gives a better performance while sampling. Case 2 is the standard GLUE approach (using a threshold value of 0.30 NS efficiency), where the initial probability distributions of the parameters (uniform) were conditioned using the likelihood value of simulations, and the results indicate that the high-frequency region of the NS efficiency is found to be centred around 0.30. This result indicates that the uncertainty can be reduced by modifying the probability density function of parameters. In the proposed methodology (Case 4), it is found that after an acceptable convergence of the probability distribution is arrived, the high frequency of the NS efficiency of ensemble simulations focuses around a value of 0.50. The results clearly illustrate that the proposed methodology has certain advantages over the currently employed methods.

The average band width of simulations is an index that is generally employed for analysing the performance of ensemble simulations (Xiong *et al.*, 2009). Figure 7 depicts the variation of average band width of simulations along the updating of probability distribution. It is evident

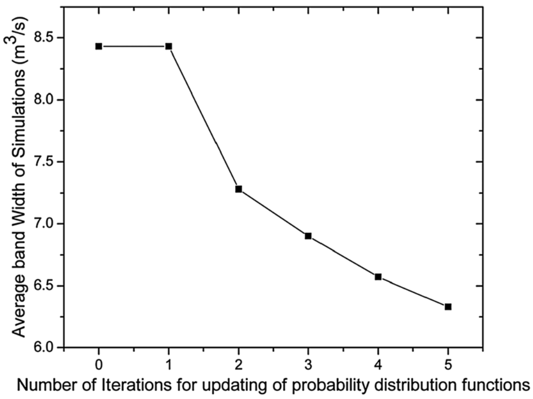

Figure 7. Plot of variation of average band width of simulations over the updating of probability distribution functions of parameters

from Figure 7 that the simulations are improving as the probability distribution becomes converged. The foregoing discussions clearly illustrate that the proposed method simultaneously improved model performance and minimized parameter uncertainty.

Simulations in King's Creek (pseudo-ungauged basin). The probability distribution of SWAT parameters derived from the gauged basin was used for the hydrologic simulation in the ungauged basin (King's Creek watershed, herein the pseudo-ungauged basin). An ensemble of 1000 simulations was generated using LHS in the parameter space using their corresponding probability distributions. A plot of the 1000 ensemble simulations of the pseudo-ungauged basins for 2 years of study is presented in Figure 8(a,b). Note that the observed flow values of the pseudo-ungauged basin during this period are also presented in Figure 8. It is evident from Figure 8 that the ensemble simulations closely follow the hydrologic response of the watershed in terms of the stream flow production (shape of the hydrograph), suggesting the validity of the derived probability distribution of parameters and their suitability in the ungauged basin. It is also evident from Figure 8 that an uncertainty band (in terms of average band width) of the ensembles is narrow for the period of study. It may be noted that the containing ratio

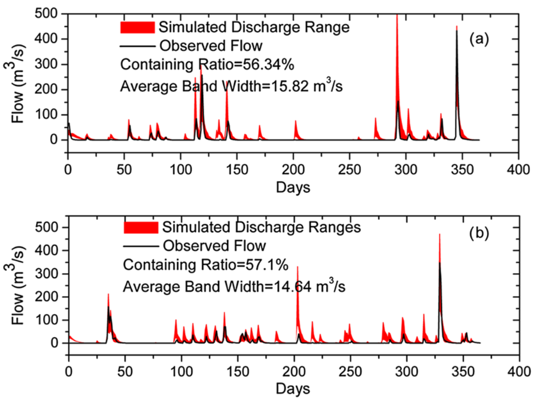

Figure 8. Comparison of the observed stream flow and simulated prediction band of stream flows for the ungauged basin (King's Creek basin) for the years (a) 1985 and (b) 1986

(Xiong *et al.*, 2009) for the ensemble simulations in the ungauged basin (Figure 8a,b) is more than 50%, indicating a good performance of the model.

In order to evaluate the performance of the SWAT model in the pseudo-ungauged basin, various statistical indices are computed using the observed flow record and the simulated flows. Because ensemble mean is considered to be a good approximation of prediction in hydrology, the statistics are initially computed using the ensemble mean simulation and are presented in Table V. Note that these statistics were computed for daily stream flow values. Table V also presents a similar statistics for the gauged basin. The results indicate a maximum efficiency of 0.647 (0.41 average), with an RMSE of 12.26 m^3/s and a correlation coefficient of 0.81 in the pseudo-ungauged basin. In general, the performance of the SWAT model in the ungauged basin is observed to be satisfactory and is reasonably good for planning of water resources management in this basin.

Case study 2: King's Creek as gauged and Cedar Creek as pseudo-ungauged

The general applicability of the methodology was analysed by interchanging the gauged and the pseudo-ungauged basins in Case Study 1. In other words, the procedure was repeated by considering the King's Creek basin as the gauged one and the Cedar Creek basin as pseudo-ungauged. The identifiability of the parameters after the first iteration (base simulation) indicated that SURLAG and CN_f are the only identifiable parameters in this basin. It is noted that as the updating of the probability distribution progresses, two more parameters, ESCO and SOL_AWC, became identifiable, indicating a reduction of uncertainty. The characteristics of the derived probability distribution functions are presented in Table IV, and the derived probability distribution of the SWAT parameters for King's Creek watershed are presented in Figure 9. Similar to that in Case Study 1, the effective parameter ranges were narrowed as the iterations progressed.

Table V. Performance statistics of SWAT model with mean of the 1000 ensemble simulations in gauged and ungauged basins; bracketed values are the best performance values for these 1000 ensemble simulations

Performance evaluation criteria	Daily simulation			
	Gauged	Ungauged	Gauged	Ungauged
	(Cedar Creek)	(King's Creek)	(King's Creek)	(Cedar Creek)
Coefficient of correlation	0.69 (0.73)	0.75 (0.81)	0.82 (0.86)	0.70 (0.73)
Nash–Sutcliffe efficiency	0.47 (0.53)	0.48 (0.65)	0.67 (0.68)	0.48 (0.51)
Mean absolute error	2.78 (2.54)	5.6 (3.63)	3.53 (3.2)	2.67 (2.5)
Mean bias error	−0.59 (−0.013)	3.5 (−0.004)	0.43 (−0.005)	−0.66 (−0.095)
RMSE (m^3/s)	10.26 (9.53)	15.54 (12.26)	12.13 (8.61)	10.1 (9.65)

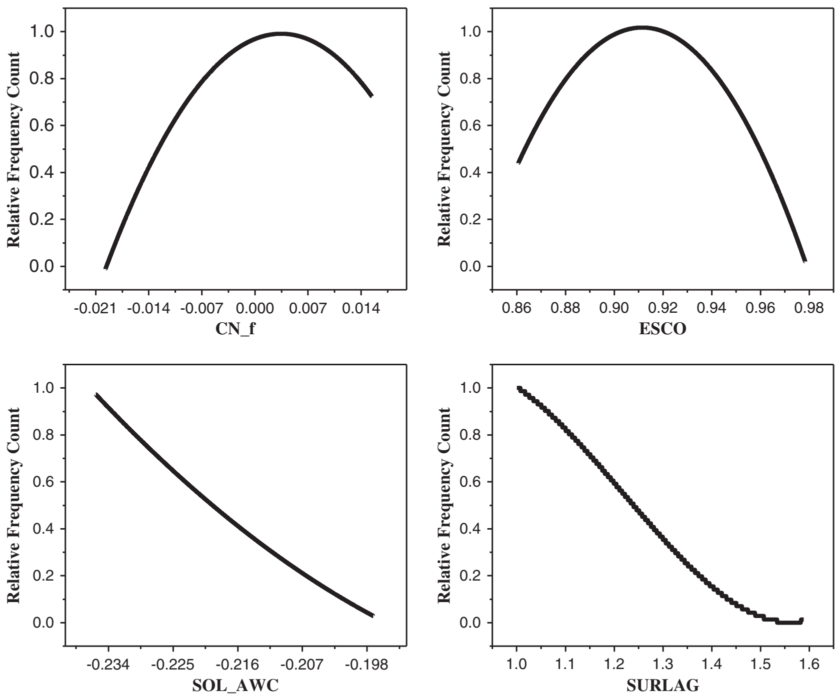

Figure 9. Final parameter probability distributions for the four parameters in King's Creek River watershed

The performance indices with these derived distributions are presented in Table V for both basins. The daily time scale simulations for pseudo-ungauged basin using the derived probability distribution of parameter indicate an efficiency of 0.51 (average of 0.47), with an RMSE of 9.65 m^3/s and correlation coefficient of 0.73.

The foregoing discussions clearly illustrate that the stochastic validation, which employs the probability distribution of model parameters, helps to quantify the uncertainty in model predictions and can be employed for simulations in ungauged basins. One of the advantages of the proposed method is that it recognized the issue of equifinality because it relies on an ensemble of simulations that are generated using the derived parameter probability distributions. Also, any averaging or interpolation of parameter values is avoided in this approach as opposed to the methods of regionalization. Nonetheless, a regionalization of probability distribution of parameters may result in better simulations and could be considered for future studies.

SUMMARY AND CONCLUSIONS

The problem of predictions in ungauged basins and suggestions for quantifying the predictive uncertainty are presented in this study. The objectives of this study were to (i) derive the probability distribution function of the sensitive parameters of a distributed hydrological model; and (ii) demonstrate the stream flow simulation with reduced uncertainty in ungauged basins by using this model. The proposed methodology employs simulations of the hydrologic model using samples of parameter sets generated by the LHS. Initially, a uniform probability distribution function for the model parameters is assumed in the absence of a known probability distribution, for the LHS. The sensitivity method of Sobol' is employed to prune the number of parameters used for subsequent analysis. The posterior probability distributions of the sensitive parameters are computed using a Bayesian approach. In addition, likelihood values of simulations are used for sizing the parameter range, thereby reducing the predictive uncertainty. The updating of the probability distribution is continued till both the distributions (prior and posterior) converge in successive cycles of simulations. To facilitate stochastic validation of the model in ungauged basins, the probability distribution function of the parameters are obtained for a gauged basin and transferred to hydrologically similar ungauged basins.

The proposed methodology is illustrated through a case study of two independent sub-basins in the Cedar Creek watershed, Texas. The SWAT model is considered for the application. The sensitivity analysis of Sobol' was performed for 13 parameters that influenced the stream flow simulation in the SWAT model. The appropriate ranges of parameters, which resulted in minimum uncertainty, were identified for the three most sensitive parameters, and the corresponding probability distribution functions were derived. Using the derived probability distribution and compressed ranges of parameter values, we performed the simulations of the second sub-basin, thereby facilitating a stochastic validation of the model. The study suggests that updating the probability distribution of parameters can considerably reduce the uncertainty of model predictions. Further, it is also observed that transferring the probability distribution of the parameter to the hydrologically similar ungauged basin eliminates the problems associated with equifinality, because an ensemble of model predictions can be employed for the analysis. Further, it eliminates any averaging or interpolation of parameter values as is carried out in the regionalization approaches. The results of the study are highly encouraging and suggest that the proposed method can be a viable approach to minimize and quantify the uncertainty in ungauged basin predictions.

In this study, the probability distribution of parameters was derived from a likelihood computed for the entire flow range consisting of high and low flows. Therefore, the derived distribution of parameters may be biased towards the prominent flow characteristics. Moreover, the current model structures are incapable of simultaneously simulating high-flow and low-flow behaviour of a catchment with a single parameter set (Gupta *et al*., 1998). Consequently, a multicriteria approach, considering the dynamics of the process in different ranges of flow, for deriving the probability distribution of parameters may help reduce the total predictive uncertainty and should be evaluated in future studies. In addition, the current study employed transferring of the derived probability distribution to a hydrologically similar ungauged basin. Instead, a regionalization of the probability distribution can be envisaged in future research so that the regional probability distribution can be applied to any basin in the region for simulations.

ACKNOWLEDGEMENTS

This study was funded by Purdue University through the Visiting Indian and Chinese Scholars programme and USDA-CSREES through an Integrated Water Quality project (Grant No. 07-51130-03876).

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