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A computationally efficient method for uncertainty analysis of SWAT model simulations

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Abstract

The physically based distributed hydrological models are ideal for hydrological simulations; however most of such models do not use the basic equations pertaining to mass, energy and momentum conservation, to represent the physics of the process. This is plausibly due to the lack of complete understanding of the hydrological process. The soil and water assessment tool (SWAT) is one such widely accepted semi-distributed, conceptual hydrological model used for water resources planning. However, the over-parameterization, difficulty in its calibration process and the uncertainty associated with predictions make its applications skeptical. This study considers assessing the predictive uncertainty associated with distributed hydrological models. The existing methods for uncertainty estimation demand high computational time and therefore make them challenging to apply on complex hydrological models. The proposed approach employs the concepts of generalized likelihood uncertainty estimation (GLUE) in an iterative procedure by starting with an assumed prior probability distribution of parameters, and by using mutual information (MI) index for sampling the behavioral parameter set. The distributions are conditioned on the observed information through successive cycles of simulations. During each cycle of simulation, MI is used in conjunction with Markov Chain Monte Carlo procedure to sample the parameter sets so as to increase the number of behavioral sets, which in turn helps reduce the number of cycles/simulations for the analysis. The method is demonstrated through a case study of SWAT model in Illinois River basin in the USA. A comparison of the proposed method with GLUE indicates that the computational requirement of uncertainty analysis is considerably reduced in the proposed approach. It is also noted that the model prediction band, derived using the proposed method, is more effective compared to that derived using the other methods considered in this study.

Keywords Uncertainty · GLUE · Mutual Information · Distributed hydrological models · MCMC · SWAT

1 Introduction

Watershed modeling is generally associated with a lot of uncertainties that arise from imprecise representation of the hydrological processes in the model, and also from the measurement error present in the input data. In addition, the spatial heterogeneity of the processes in a watershed makes the model simulations much more uncertain (Beven and Freer 2001), especially in the case of lumped models. Many of the currently used process based models include certain level of empiricism in process representation, and are generally characterized by a multitude of parameters (Cibin et al. 2010; Wu and Liu 2012). Due to the spatial variability of the processes in a watershed, value of many of these parameters will neither be exactly known, nor are directly measurable. Therefore, in most cases model calibration is necessary and is performed to bring the simulations as close as to the measurements (Jeremiah et al. 2012). Nonetheless, the simulations cannot be considered perfect since there could be problems associated with equifinality and identifiability (Beven 2006; Cibin et al. 2014), in addition to the uncertainty caused by model structural and input imprecision. Therefore, an assessment of the uncertainty in model simulation is essential before any decision is made based on the model simulations.

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The importance of accounting for uncertainty in model simulations has been emphasized by various researchers in the past (Beven 2006; Refsgaard et al. 2007; Warmink et al. 2010; Yen et al. 2015), and consequently various methods to quantify the uncertainty have evolved. A comprehensive summary of various techniques available for uncertainty analysis can be found in Li and Wu (2006). The techniques that are generally employed for this analysis include (1) probability theory method (Wiwatenadate and Claycamp 2000), (2) Taylor series expansion (Rastetter et al. 1992), (3) Monte Carlo simulation (Gardner and O'Neill 1983), (4) generalized likelihood uncertainty estimator (GLUE; Beven and Binley 1992), (5) Bayesian statistics (Katz 2002), and (6) sequential partitioning (Rastetter et al. 1992). In this study, we have focused on the uncertainty arising from the model parameters, though the other sources of uncertainty are also equally important.

The GLUE is one of the most commonly used uncertainty estimation method in hydrological modeling; the total uncertainty can be estimated by this technique (Beven and Binley 1992). Zhang et al. (2015) and Uniyal et al. (2015) conducted a study to compare different uncertainty estimation methods (SUFI-2, GLUE, PARASOL, PSO) for hydrological model prediction. They reported that the GLUE could provide reliable uncertainty estimates compared to other methods; however number of model runs required is very high for reliable results. *Despite*, some studies have reported certain limitations of the GLUE method (Christensen 2004; Montanari 2005; Mantovan and Todini 2006; Stedinger and Vogel 2008)—the major criticisms being the use of informal likelihood and subjectivity in the selection of threshold. Jin et al. (2010) and Li et al. (2010) did a comparative study on GLUE that used formal and informal likelihood measures for uncertainty estimation. They reported that posterior distribution of parameters and the error bound for prediction are sensitive to the choice of threshold value. They concluded that when the threshold value in GLUE (that used informal likelihood) is high (acceptable sampling ratio—ASR $< 1\%$), the uncertainty estimates from GLUE is very similar to the estimates derived using a formal likelihood in GLUE.

The design/identification of an evaluation criterion for model evaluation is an important aspect for proper uncertainty estimation in any approach (Beven and Binley 2014). Smith et al. (2008) reported that the marginal posterior distributions resulting from the informal likelihood (such as Nash–Sutcliffe) are conservative and more robust than those derived using an in appropriate formal likelihood. Several studies show that the limit of acceptability approach of GLUE (Beven 2006) and the formal approximate Bayesian computation (ABC) can give similar estimate of uncertainty (Nott et al. 2012; Sadegh and Vrugt 2013) without subjective selection of likelihood. However, the computational requirement associated with the process is high (Alazzy et al. 2015; Mirzaei et al. 2015; Zhang et al. 2015). Vrugt et al. (2003, 2008a, b) introduced Shuffled Complex Evolutionary Metropolis Algorithm (SCEM) and Differential Adaptive Metropolis (DREAM) Algorithm respectively for uncertainty analysis (UA) with adaptive MCMC sampling; both are formal Bayesian based methods. These algorithms were found to be more effective in uncertainty estimation; however there was no significant compromise on the number of model runs required for the analysis. Further, the assumption of uniform prior probability distribution for the parameters (which is generally the case) may require billions of model runs to get better performing parameter sets (Jin et al. 2010). In addition, there is no guideline to define the minimum number of behavioral parameter sets that are required to characterize the model response surface.

Consequently, this study is focused to facilitate the reduction of computational requirement for uncertainty analysis of complex hydrological models. Mutual Information (MI) is a measure that quantifies the stochastic dependency between two random variables without making any assumptions (e.g., linearity) about the nature of their relation (Steuer et al. 2002). There are not many applications of this measure in hydrology; some of the applications are in the input variable selection of artificial neural network modelling (May et al. 2008; Mukund Nilakantan et al. 2015). Athira and Sudheer (2015) used MI along with Latin Hypercube Sampling in GLUE for uncertainty analysis of SWAT model. The current study proposes to use mutual information (MI) along with a better sampling approach, MCMC for sampling the behavioral sets in GLUE approach. The uncertainty estimates from both the approaches are compared and analyzed in this study. The Soil and Water Assessment Tool (SWAT) model is considered in this study for demonstration.

2 Description of the hydrological model

2.1 Soil and water assessment tool (SWAT) model

Soil and water assessment tool (SWAT) model is one of the most popular hydrological models in use (Arnold et al. 1993; Arnold and Fohrer 2005; Confessor and Whittaker 2007; Zhang et al. 2008). The model has gained international recognition as is evidenced by a large number of applications of this model (Zhenyao et al. 2012; Zhang et al. 2011; Gassman et al. 2007; Anand et al. 2007; Barlund et al. 2007). SWAT is a process based distributed simulation model operating on a daily time step. The fundamental SWAT simulations are carried out at hydrological response units (HRU) level. The SWAT model is also characterized by a large number of parameters, and therefore will induce lot of uncertainty in the simulations (Talebizadeh et al. 2010). While existing methods of uncertainty analysis could be employed to understand the associated uncertainty in SWAT simulations, these methods require a lot of computational time in terms of model simulations. The current study concentrates on the stream flow modeling component of SWAT. The parameters of the SWAT model that affect the stream flow computations are identified through a detailed literature review and are presented in Table 1, along with their recommended range of perturbations (Neitsch et al. 2002; Arabi et al. 2007).

3 Uncertainty analysis method

3.1 Modification proposed for the GLUE method

The methodology envisaged in this study is a synergistic combination of the GLUE and MCMC with the inclusion of mutual information while sampling, to reduce the computational requirement. The method starts with Monte Carlo simulations of the hydrological model (SWAT in this study) using ensemble parameter sets generated initially by stratified random sampling within the parameter bounds. Since the parameter probability distribution is not available initially, a uniform distribution is assumed (Freer et al. 1996; Manache and Melching 2008, Freni and Mannina 2010). The rationale behind using stratified random sampling in the initial sampling is to get a full representation of the range of parameters since uniform distribution is assumed. The likelihood value of all the simulations is then computed. There has been several discussions and debates in recent years that has focused on the use of either a formal or informal approach for specifying a likelihood function for uncertainty analysis (Mantovan and Todini 2006; Vrugt et al. 2008b; Stedinger and Vogel 2008; McMillan and Clark 2009; Schoups and Vrugt 2010). The GLUE method is often used to calculate the uncertainty interval of streamflow simulation with a statistically informal likelihood function. A lot of studies compared the use of GLUE with informal likelihood and formal Bayesian approach for uncertainty estimation (Li et al. 2010; Jin et al. 2010; Vrugt et al. 2008b; Nott et al. 2012), and most of them concluded that both these approaches can make very similar estimates of prediction uncertainty. In this study, the Nash Sutcliff (NS) Efficiency is used as the informal likelihood index as it is the most commonly used likelihood index in GLUE; its value is zero or less if the behavior of prediction is away from the characteristics of the system and it monotonically increases to 1.0 as the prediction behavior comes closer to the characteristics of the system. NS efficiency is defined as:

$$NSE = 1 - \frac{\sum_{t=1}^{n}\left(y_{obs}^{t} - y_{sim}^{t}\right)^2}{\sum_{t=1}^{n}\left(y_{obs}^{t} - \bar{y}_{obs}\right)^2} \tag{1}$$

where, n is the number of observed data points, y_{obs} and y_{sim} represent the observation and the model simulation at any given time t respectively, and $\bar{y}_{obs}$ is the average observed value.

The acceptable simulations from the total Monte Carlo ensembles are then selected based on a predefined threshold of the likelihood measure. The current study followed

Table 1 The SWAT parameters that influence stream flow simulation in the model and their range of perturbation

Symbol	Description	Unit	Min	Max	Process	Sensitivity index
ALPHA_BF	Base flow recession coefficient	Days	0	1	Groundwater	0.015
CN_f[a]	Curve number	%	− 25	15	Surface runoff	0.385
ESCO	Soil evaporation coefficient	–	0.001	1	Evapotranspiration	0.421
GW_DELAY	Groundwater delay time	day	1	500	Groundwater	0.000
GW_REVAP	Revap coefficient	–	0.02	0.2	Groundwater	0.000
GWQMN	Depth of water in shallow aquifer	mm	0	5000	Groundwater	0.000
OV_N	Manning's N	–	0.1	0.3	Overland flow	0.000
SFTMP	Snowfall temperature	°C	− 5	5	Snow	0.002
SLOPE[a]	Slope	%	− 0.5	1	Surface runoff	0.018
SLSUBBSN[a]	Slope sub basin	%	− 0.5	1	Surface runoff	0.000
SOL_AWC[a]	Available water capacity	%	− 0.3	2	Groundwater, evaporation	0.162
SOL_K[a]	Saturated hydraulic conductivity	%	− 0.5	1	Groundwater	− 0.003
SURLAG	Surface lag	Day	1	12	Surface runoff	0.001

[a]These parameters were changed as a percentage of their default values to maintain heterogeneity

the suggestions of Jin et al. (2010), Li et al. (2010) and Zhang and Li (2015) in selecting the threshold when informal likelihood such as NS efficiency is employed. Li et al. (2010) after an extensive numerical exercise for identifying an appropriate threshold for GLUE, suggested that the threshold be fixed in such a way to select less than 1% of the total ensembles (acceptable sampling ratio—ASR) as behavioral sets. Therefore, the selected threshold depends on the performance of the individuals in the ensemble. Jin et al. (2010) reinforced this recommendation for fixing up the threshold. They further concluded that the selection of a higher threshold value (with ASR $< 1\%$) can result in similar estimates of parameter probability distributions functions and corresponding predictive uncertainty bounds in GLUE, as compared to formal Bayesian methods of analysis. The threshold value of likelihood, which is considered to define the acceptable simulations, helps size the parameter range, thereby reducing the uncertainty caused by parameters. The posterior probability distributions of the parameters are then derived using the Bayesian approach, as follows:

$$P(\theta|\varphi) = \frac{L(\varphi|M(\theta)) \times P(\theta)}{C} \tag{2}$$

where $P(\theta)$ denotes the prior probability density for model parameters, $P(\theta|\varphi)$ denotes a posterior probability density after conditioning the observations via the likelihood function, L, and C is a scaling constant so that cumulative probabilities sum to one.

The effectiveness of the estimated uncertainty using GLUE highly depends on the choice of the prior marginal distribution for parameters (Zhang 2012). If one could clearly express the uncertainty as a prior distribution, and have observed data, there would be no need for statistical analysis at all. But, if uncertainty is not clearly expressible as a prior, then a major requirement for Bayesian updating seems to be questionable. Therefore, GLUE in this study is envisaged to be applied in an iterative way by replacing the prior with derived posterior in each iteration (Zhang 2012; West 1993). Since the prior is conditioned and approximated in successive iterations, the uncertainty is considered to be better described in each iteration. The iteration can be stopped when the derived posterior converge with the prior.

A large number of parameter values (sample length of 1000 in this study) for each parameter are independently sampled from the derived marginal probability distribution function using MCMC sampling method. A simple random walk MCMC algorithm, Metropolis Hasting method (Kuczera and Parent 1998), is employed for sampling in this study. The essential requirement for improving the computational efficiency of GLUE is that one should increase the number of behavioral parameter sets in the analysis. In this study, in order to increase the number of behavioral parameter sets, only those sets which preserved the mutual relationship between the parameters are accepted for further analysis. The inter-relationship between the parameters can be ascertained using various indices, and mutual information (MI) is used in this study as it considers both linear and nonlinear dependence (Steuer et al. 2002). So the next step was to generate a group of parameter sets (combination of parameters) from the independently sampled parameter values such that the inter-relationship between the parameters is similar to that is already estimated with the behavioral parameter sets.

The MI of the parameters, which gives an indication about the inter-dependency of parameters, is estimated from the screened behavioral sets. Mutual information is a quantitative measure of how much one variable is dependent on the other one (MacKay 2003). For a set of N bivariate measurements $\mathbf{z}_i = (\mathbf{x}_i, \mathbf{y}_i)$, i = 1,2,…,N, which are assumed to be interdependent and identically distributed realizations of a random variable $\mathbf{z} = (\mathbf{x},\mathbf{y})$, mutual information (MI) is defined as

$$\mathrm{MI(x,y)} = \sum_{i=1}^{N} f_{x,y}(x_i, y_i) \log_e \frac{f_{x,y}(x_i, y_i)}{f_x(x_i) f_y(y_i)}, \tag{3}$$

where $f_x(x)$ and $f_y(y)$ are the marginal probability density functions of **x** and **y**, respectively, and $f_{x,y}(x, y)$ is the joint probability density function of **x** and **y**. Herein, the marginal probability density function of the parameters is the posterior distribution derived from Bayes' theorem and the joint probability density function is derived from the likelihood.

The increase in number of behavioral parameter sets was achieved with the help of an optimizer. With 1000 samples for each parameter, the total number of possible parameter sets becomes 1000^4. From this possible pool of parameter sets, a group of 200 parameter sets, which satisfied the MI criteria, were randomly sampled using an optimization algorithm. The criteria used for this selection was the proximity of mutual information between parameters. Accordingly, the objective function for the optimizer was defined as minimum deviation between the MI computed for the selected group of 200 parameter sets and that for the behavioral parameter sets. The mutual information was estimated using the marginal probability distribution functions (derived using Bayes' theorem) and joint probability distribution of the parameters. While any optimization algorithm can be employed for this, the current study used Genetic Algorithm (GA) with sum of the squared difference between the respective MI values as objective function. The finally selected 200 parameter sets were used for the simulations in the next iteration, and the method is iteratively repeated until the prior and posterior distribution converged. The Kullback–Leibler (KL) divergence criterion (Carota et al. 1996) was used to check the convergence of the distributions. It is a non-negative, non-symmetric measure of difference between two distributions and is an expectation of the logarithmic difference between two distributions. The sum of the probabilities should be one for estimating the KL divergence criteria. The KL divergence of the distribution P on Q is estimated as:

$$D_{KL}(P||Q) = \frac{1}{n} ln\left(\frac{P(i)}{Q(i)}\right) P(i) \tag{4}$$

Here, n is the number of data used for the analysis and P(i) and Q(i) are the corresponding probabilities. A flow diagram of the computational procedure is presented in Fig. 1. The proposed methodology is illustrated through a case study of SWAT simulations in Illinois River basin in the USA.

In the proposed method of uncertainty analysis, the probability distribution function of the parameters has to be conditioned using the observed information. For a direct comparison with the proposed method, the results of standard GLUE and the results of uncertainty analysis without using the mutual information between parameters are also presented and discussed in this study. In addition, the results of GLUE with LHS (instead of MCMC) along with Mutual information are also presented for the

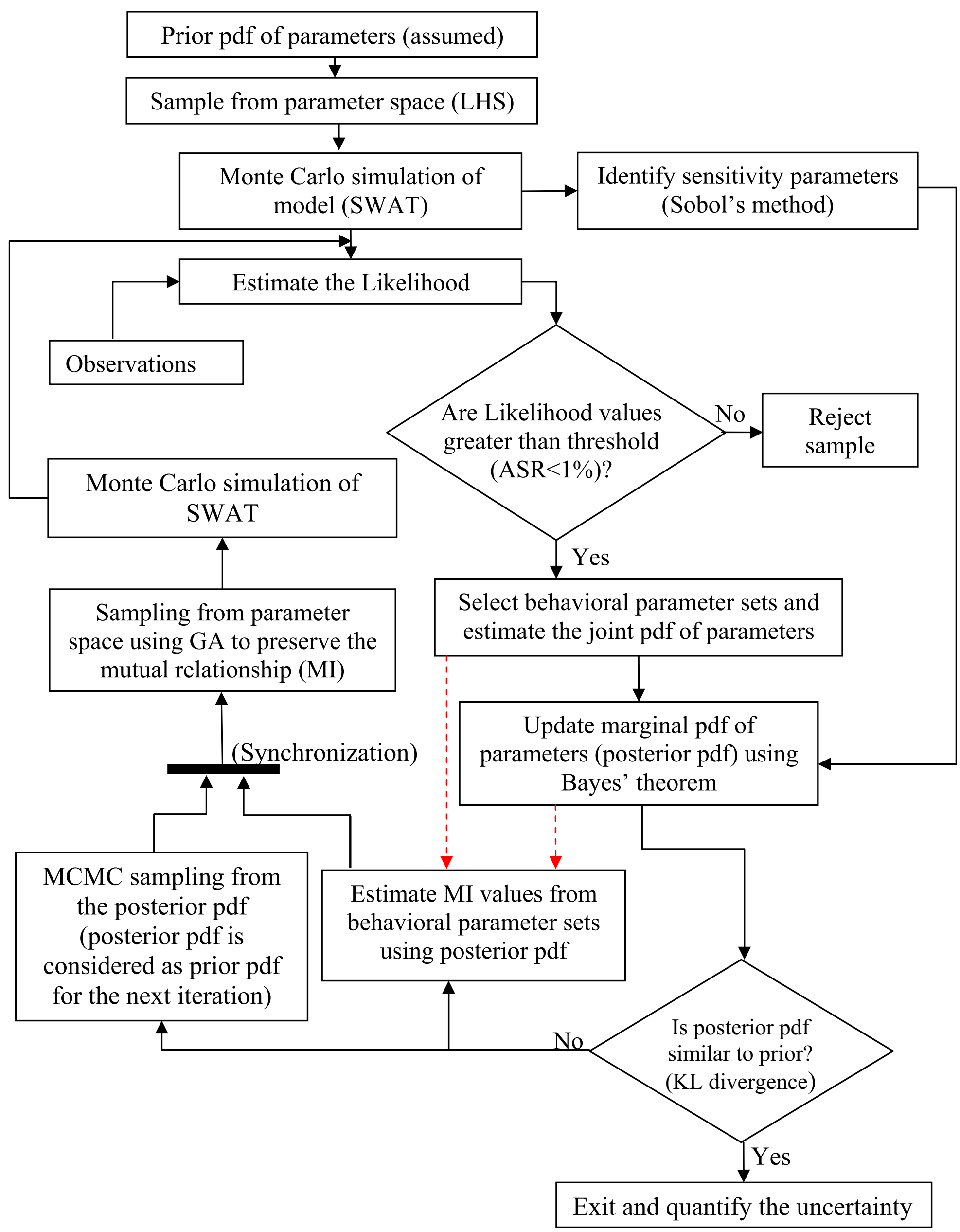

Fig. 1 Flow chart of the proposed computational scheme for assessing the uncertainty. The 'synchronization' block indicates that the tasks after this block start only when both the inputs to the block (estimation of MI and MCMC sampling) are completed. The dotted lines indicate that the flow of information will take place only when the decision box output is 'NO'. *ASR* acceptance sampling rate, *GA* genetic algorithm, *MI* mutual information, *pdf* probability distribution function

comparison of effect of sampling methods on the model predictions. For the clarity of further discussion, the different approaches are named in this study as follows: Case1—the proposed approach (MCMC with MI), Case 2—MCMC without MI, Case 3—LHS with MI and Case 4—standard GLUE. The probability distribution of parameters are quantified using the Best Fit program (Palisades Corp. CA, USA), which considered 28 different distributions to the data, and ranked them according to a specified 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.

4 Details of the study area

The SWAT model has been applied to Illinois River basin in Arkansas, USA, which is one of the major watersheds of the Northwest Arkansas. Illinois River, flowing west across the Arkansas–Oklahoma border into Oklahoma, crosses the state line just south of Siloam Springs at the Arkansas Highway 59 Bridge. This watershed is used in this study for the demonstration of the proposed method. The outlet of the watershed is the USGS gauging site 07195430 on Illinois River, South of Siloam Springs, Arkansas. The georeference for the gauging site is 36°06′33.32″ Latitude and 94°32′04.3″ Longitude (NAD83). The drainage area of the watershed up to this gauging site is 1490 km^2. The watershed boundary, delineated using SWAT model (with ArcView interface), is shown in Fig. 1 for reference.

The elevation of the watershed varies from 279.6 to 600.0 m with a mean elevation of about 380.5 m. The digital elevation map obtained from United States Geological Survey (USGS) at 30-m resolution is used to provide the GIS file of elevation in the SWAT model. The land use information of the Illinois watershed has been obtained from the 'Arkansas Land-use/Land-cover, 1999' data prepared by Center for Advanced Spatial Technologies (CAST), University of Arkansas. Major land use categories of the watershed are pasture under tall fescue and Bermuda followed by forests and residential areas (Table 2). United States Department of Agriculture (USDA), Natural Resources Conservation Service (NRCS) database, Soil Survey Geographic (SSURGO), for Benton County and Washington County, Arkansas are used for extracting soil information in the watershed. Major soil types in the watershed are Nixa, Captina, Clarksville, and Enders covering an area of more than 5% (Table 2). There are several minor soil types having a share of less than 5% in the watershed. Weather data from stations within the region, Fayetteville Experiment Station, and Bentonville, are incorporated to provide the most representative precipitation and temperature data available. Other meteorological data required by SWAT (solar radiation, wind speed, and relative humidity) are estimated using the SWAT weather generator.

The SWAT model is setup to run for a period of 9 years, 1995–2003, for the watershed, with the first 3 years being considered the warm up period. Thus, effectively 6 years' data were considered for the analysis. The HRU definition was done based on the landuse, soil, and slope and the threshold values used was 5, 10 and 10% to define the minimum coverage of landuse, soil, and slope respectively for the classification of HRUs. The measured daily stream flow values from USGS gauging station 07195430 (Fig. 1) were used for the analysis. Illinois basin experiences an average annual rainfall of 90.5 cm. The daily flow ranged from a minimum of 2.4 m^3/s to a maximum of 538 m^3/s during the period of analysis. The mean flow during the period was 16.5 m^3/s with a standard deviation of 33.7 m^3/s. The Illinois River basin lies in the southern region of the USA and experiences high temperature, and evaporation is a dominant hydrological process in this basin, with average annual potential evaporation of 105 cm. The SWAT setup for Illinois River watershed had 26 sub basins and 286 HRUs (Fig. 2).

5 Results and discussion

5.1 Sensitivity of SWAT parameters

The parameters of the SWAT model that affect the streamflow simulations are identified through a detailed literature review, and are presented in Table 1, along with their recommended range of perturbations (Neitsch et al. 2002; Arabi et al. 2007), and all of them are considered in this study. Initially a sensitivity analysis was performed using Sobol's method (Cibin et al. 2010) to identify the most influencing parameters. Monte Carlo simulations of the SWAT model for the study watershed have been performed considering uniform probability distribution for all the 13 parameters. A base sample size of 2000 for each parameter was considered in this study, the base sample has been rearranged for each parameter with a shift in the position of first- and second- thousand values in the 2000 samples. Hence, the parameter combinations to be evaluated became 28,000 (13 × 2000 + 2000) to get the sensitivity index for each parameter. The major limitation of this method is the higher computational demand; the number of model runs required is very high. While it is true that the length of base sample affects the results of the analysis, it is expected that 28,000 simulations are reasonably sufficient for the current study (Cibin et al. 2010).

Table 2 The major landuse and soil categories and their corresponding areal coverage in the Illinois river basin

Landuse	Percentage of areal coverage	Soil name	Percentage of areal coverage
Forest-mixed	35.86	CAPTINA	23.71
Tall fescue	28.68	NIXA	21.26
Bermuda grass	25.36	CLARKSVILLE	14.12
Residential area	9.75	ENDERS	13.02
Agricultural land	0.35	PICKWICK	9.22
		TONTI	4.97
		PERIDGE	2.88
		HECTOR	2.65
		Others	8.17

Fig. 2 Map of the Illinois River Watershed with stream network and USGS gauging stations

As mentioned earlier, stratified random sampling has been adopted for initial sampling from the parameter space. For each of the simulation, the RMSE and Nash–Sutcliffe efficiency were computed using the observed and simulated values of river flow from the watershed. The model performance in terms of NS efficiency was ranging from − 0.2412 to 0.5282.

The sensitivity analysis ranked the parameter ESCO at first position, followed by CN_f; the corresponding sensitivity indices are 0.421 and 0.385, respectively (Table 1, sensitivity index column). It may be noted that the Illinois River watershed, being located in the southern parts of the USA, experiences greater values of temperature and radiation, and therefore the evaporation losses are more. Consequently, the parameter ESCO, which is directly influencing the evapotranspiration losses from the watershed, is expected to be sensitive in Illinois. This is in agreement with the results reported by Migliaccio and Chaubey (2008), wherein they reported that ESCO is a sensitive parameter in Illinois River watershed. As discussed earlier, the CN_f is the major driving parameter in runoff estimation and is found to be sensitive in this watershed also. The third sensitive parameter in Illinois watershed is SOL_AWC, which accounts for the available soil water in the HRU. While this parameter can be expected to be sensitive in most of the watersheds, the ranking may vary from one watershed to another (Cibin et al. 2010). While SURLAG was not very sensitive in this watershed, this parameter was identifiable and was also considered for further analysis in addition to the first 3 sensitive parameters. The remaining 4 parameters, though were found to be slightly sensitive, were kept at the recommended values since they were not identifiable. Identification of non-identifiable parameters is difficult because of the equifnality nature of the parameter sets (Demaria et al. 2007; Cibin et al. 2010). In this study, these parameters were assigned values considering their importance in the concerned hydrological processes and also considering the watershed characteristics.

5.2 Probability distribution and range compression of parameters

The current study considered a base simulation of 28,000 and the performance range of NS efficiency was found to vary within − 0.2412 to 0.5282. This study considered 0.45 NS efficiency as the threshold with an acceptance sample rate of 0.8%. The parameter sets which produced NSE above the threshold limit (behavioral set) were selected, and the probability distribution of the parameter variability in the behavioral sets was determined. At this stage, the acceptable simulations were the same for all the four cases (Case 1 through Case 4), and hence the probability distribution too. The Mutual Information index between the parameters were estimated from the behavioral sets by considering the joint probability distribution of parameters that was derived using the likelihood values. Using the derived probability distribution of parameters, 1000 samples of parameters were selected using MCMC procedure. From these samples, 200 parameter sets that preserved the mutual information have been selected using Genetic Algorithm. It should also be noted that the quantity of behavioral sets for further analysis (200 in this case) was not randomly selected, but through a trial and error exercise. Monte Carlo simulation of the model was performed using this sampled parameter set, and the behavioral sets for further analysis are identified again by filtering (using threshold of 0.45).

After the first iteration, the model performance (in terms of NSE) was found to be ranging from 0.3033 to 0.6609 in Case 1. It is to be noted that the original range of NSE, prior to updating of the probability distribution is − 0.2412 to 0.5282, which indicates an improvement in the model performance. The NS ranged from − 0.0690 to 0.6618 after the updating for Case 2. In the instance of Case 3, the performance range was from − 0.4450 to 0.6302. As expected, 96% of the new samples (after GA) were above the threshold in Case 1, which suggests that the MCMC with MI help improve the number of behaviuoral samples. In other cases, it was found to be 22% (Case 2), 28% (Case 3) and 17% (Case 4).

The derived posterior probability distribution of the parameters is found to be converged after second cycle of iteration in Case 1 (MCMC with MI), while, additional iterations were required for other cases. The characteristics of the finally converged probability distribution in all four cases are presented in Table 3. From Table 3 it is apparent that all the parameters followed Beta general distribution, but with varying shape and location parameters. As mentioned earlier, the value of Kulback–Leibler divergence index (KL) was used for assessing the convergence of probability distribution, whose ideal value is zero. In the proposed approach (Case 1), the posterior and prior distributions converged after the second updating of the probability distribution with a corresponding KL value of 0.007 for SURLAG, 0.140 for ESCO, 0.051 for CN_f, and 0.038 for SOL_ AWC. In Case 2 and Case 3, the parameter probability distributions converged after three iterations. It is also noted that the cases that considered MI (Case 1 and Case 3) required less number of simulations (200 per iteration), while other cases required 1000 simulation per iteration for probability distribution convergence. This result suggests that employing MI while sampling of parameters help significantly reduce the computation requirement for the analysis.

It is to be noted that filtering the parameters using the threshold value of likelihood help reduce the active range of parameters of model in this basin. The effective range of parameters obtained after the analysis in all cases is presented in Table 4. The reported range shows a better performing parameter region as compared to single optimal parameter value obtained in conventional calibration method. During each cycle of analysis parameters are sampled from the compressed range using the derived probability distribution. The results indicate that in cases where MCMC is used for sampling (Case 1 and Case 2), the effective range of parameters is small, and lesser compared to that obtained for other cases. This can be plausibly attributed to the characteristics of the MCMC sampling since it samples more from high probability region of the parameter. Further, when MI is employed along with MCMC (Case 1), the method identifies a further reduced range of parameter compared to that in Case 2. However, the methods that used LHS (Case 3 and Case 4) do not show considerable reduction in parameter range plausibly due to the sampling from entire range of parameter irrespective of the probability density (property of LHS). Nonetheless, Case 3 (LHS with MI) has obtained a reduced range compared to Case 4 (LHS alone).

The finally derived probability distribution of the parameters is presented in Fig. 3 for all cases. It is noted from Fig. 3 that the methods that used MCMC (Case 1 and Case 2) identified maximum probability density for SURLAG near a value close to 1.0. The Illinois River basin has smaller time of concentration as the length of the main channel is not very large, and hence will have a smaller value for SURLAG as the value of SURLAG is correlated to the time of concentration of the basin (Neitsch et al. 2002). The results indicates that the proposed method (Case 1) is able to effectively identify the performing range in less number of iterations since maximum probability density for SURLAG is found close to the theoretical minimum value of 1.0. When the evaporative demand in the system is high, the parameter ESCO takes a value close to 1.0 in order to account for the soil moisture redistribution in different layers due to evapotranspiration (Neitsch et al. 2002). As explained earlier the evaporative demand in Illinois River basin is high, and consequently ESCO would take values in higher ranges of the possible values (upper limit being 1.0), and this validates the high probability density obtained in all approaches for ESCO at a value close to 1.0. The method Case 1 identified a range from 0.79 to 0.97 for ESCO in the Illinois River basin. The probability distribution identified for SOL_AWC has multiple peaks in the methods except for Case 1. This may be plausibly due to the identification of less uncertain range

Table 3 Location and shape characteristics of the probability distribution of SWAT parameters for different cases

	Probability distribution							
	Case 1		Case 2		Case 3		Case 4	
SURLAG	Beta general	1.1894	Beta general	1.0374	Beta general	0.4441	Beta general	1.5196
		2.278		1.4096		0.9090		3.0653
		1.0000		1.0203		1.0197		1.0000
		1.2501		1.5012		2.0955		1.3590
ESCO	Beta general	1.2566	Beta general	2.8399	Beta general	2.8411	Beta general	1.0700
		1.0212		1.2365		0.6894		0.9216
		0.7750		0.8185		0.7690		0.3210
		0.9850		0.9806		0.9728		0.9950
CN	Beta general	1.2566	Beta general	3.3228	Beta general	1.5526	Beta general	1.6421
		1.0212		1.9958		1.0585		1.3411
		0.0614		0.0690		− 0.170		− 0. 180
		0.1200		0.1410		0.1200		0.1492
AWC	Beta general	1.2874	Beta general	0.4061	Beta general	0.5423	Beta general	0.5655
		1.873		0.5733		0.8679		0.6765
		0.1508		− 0.054		− 0.127		− 0.263
		1.335		1.9895		1.420		1.950

Table 4 Identified effective range of parameters for different cases

Parameter	Initial range	Final range			
		Case 1	Case 2	Case 3	Case 4
SURLAG	1.00–12.00	1.02–1.23	1.02–1.48	1.00–5.7	1.02–7.685
CN_f	− 0.25–0.20	0.06–0.12	0.06–0.14	− 0.17–0.12	− 0.18–0.14
SOL_AWC	− 0.30–2.00	0.15–1.33	− 0.05–1.98	− 0.12–1.42	− 0.26–1.95
ESCO	0.00–1.00	0.77–0.97	0.81–0.98	0.76–0.97	0.32–0.98

of parameters with the help of MCMC and MI together in Case 1. In the case of CN_f, the effective range identified by Case 1 is considerably less (0.06–0.12) compared to that obtained from other methods.

The likelihood value plotted against their normalized frequency in the ensemble generated from the finally converged frequency distribution is shown in Fig. 4 for all cases. The standard GLUE (Case 4) with maximum possible ranges for all the parameters has shown very high uncertainty with Nash–Sutcliffe efficiency varying from of − 3.8 to 0.57. The variation in model performance with different cases can be seen from Fig. 4. Compared to LHS based methods (Case 3 and Case 4), MCMC based methods (Case 1 and Case 2) gave more behavioral parameter sets as the likelihood is found to have higher frequency towards higher value of NS. Further, the range of performance in Case 1 is better compared to Case 2 since sampling from marginal probability distribution may not preserve the inter relationship between the parameters (Case 2). The highest number of better performing samples are obtained from Case 1.

5.3 Prediction band of the SWAT model output

Figure 5 depicts the prediction interval of SWAT modeled stream flow derived from the ensemble of simulations generated in Case 1. The ensembles have been created using the final probability distribution of the model parameters. The measured flow during the same period is also presented in Fig. 5 for comparison. The prediction interval derived from the ensemble is an indication of the acceptable level of plausible error due to an uncertainty in the model parameters. It can be observed that measured flow is mostly contained in the prediction interval. The shape of the prediction band closely follows the measured hydrograph indicating the validity of the derived probability distribution and the final parameter range. The stream flow prediction band is analyzed using two popular indices, viz. average band width, containing ratio (Xiong et al.

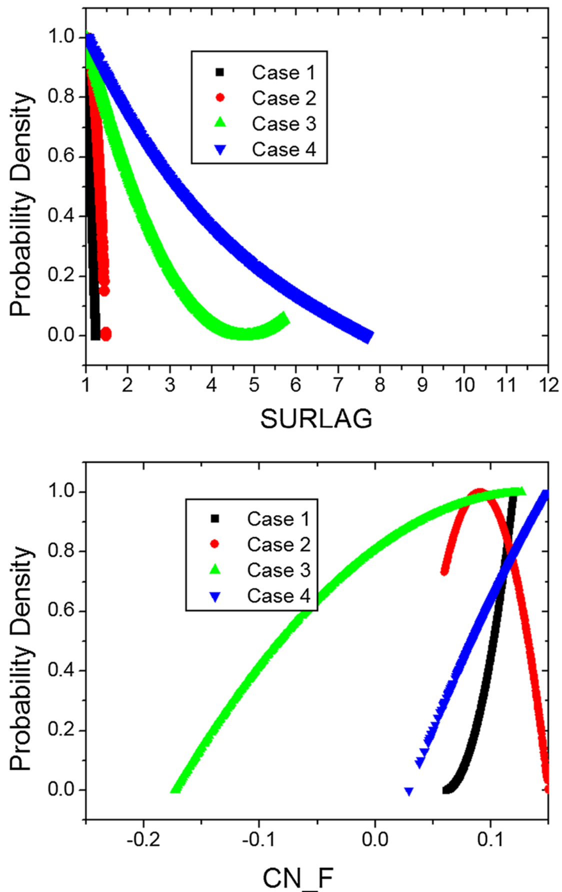

Fig. 3 Shape of derived probability distribution of parameters in different cases

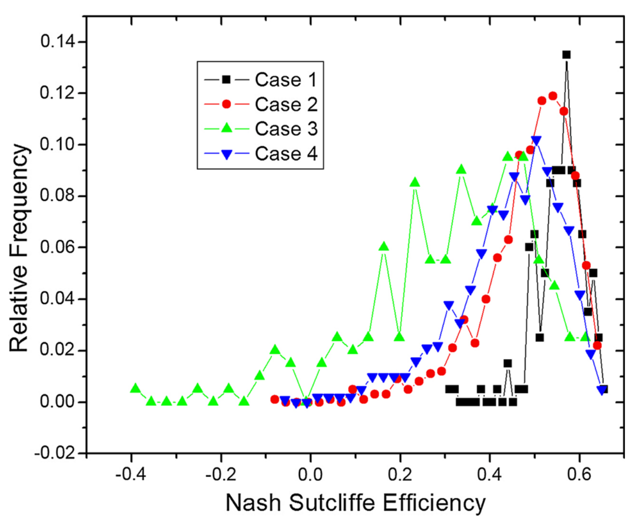

Fig. 4 Plot of frequency histogram of Nash–Sutcliff efficiency in the final ensemble simulation for different approaches

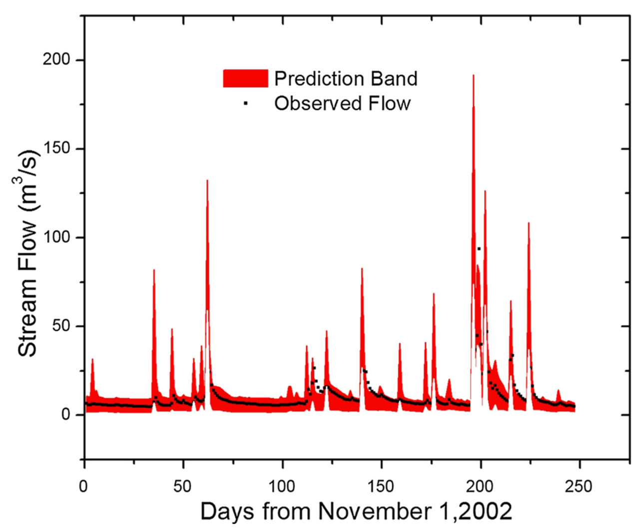

Fig. 5 Streamflow prediction interval estimated from the ensemble generated using the proposed method for Illinois River basin (simulations during November 2002–June 2003)

2009), and the results are presented in Table 5. In theory, if the width of prediction band is wider, it covers most of the observed values. However, in order to include more observed values in the prediction band, compromising on the width of the prediction band is not desirable. Since these measures are conflicting, a desired solution is to have maximum coverage with a narrow prediction band.

Table 5 Performance indices of the prediction band derived from each case

Indices	Case1	Case2	Case3	Case4
Average band width (m^3/s)	14.96	17.61	21.89	23.96
Containing ratio (%)	84	86	82	58.15

It can be noted from Table 5 that the proposed method (Case 1) provides minimum average width for the prediction band (14.96 m^3/s) with a reasonably good containing ratio (84%). The Case 2 provides a slightly higher average width (17.61 m^3/s) with a containing ratio of 86%. The increase in containing ratio (2%) is not very significant in Case 2 when compromised on the increase in average width. The standard GLUE (Case 4) provides an average prediction band width of 23.63 m^3/s with 58% of the observations falling within it. The average width obtained for Case 3 (LHS with MI) is high compared to the other methods (21.89 m^3/s) with a relatively low containing ratio (82%). These results suggest that the proposed method (Case 1) produces relatively better prediction band with less number of simulations. Figure 6 depicts the performance of the SWAT model simulation in different ranges of flow for all the cases. It can be observed that methods that use MCMC (Case 1 and Case 2) provide better performance compared to the other two methods that used LHS for sampling. Across all the methods, Case 1 requires less number of simulations to arrive at the similar performance that is obtained from other method (Case 2).

The finally derived probability distribution function in Case 1 was used for the performance evaluation of the model at the locations upstream of the watershed outlet (*see* Fig. 1). It is to be noted that the results were encouraging: the performance range of NSE was found to be between 39 and 47.6% in the gauging station 07195000 and within 42–49% in the gauging station 07194800. The SWAT simulations with less than 50% NSE cannot be generally considered as behavioral. However, the acceptability of the current simulations can be justified in two aspects (1) this model performance is from a non-calibrated model—calibration of the model starting from this parameter combinations can give a better estimate of model output with minimum computational requirement (2) these upstream gauging stations can be considered as ungauged

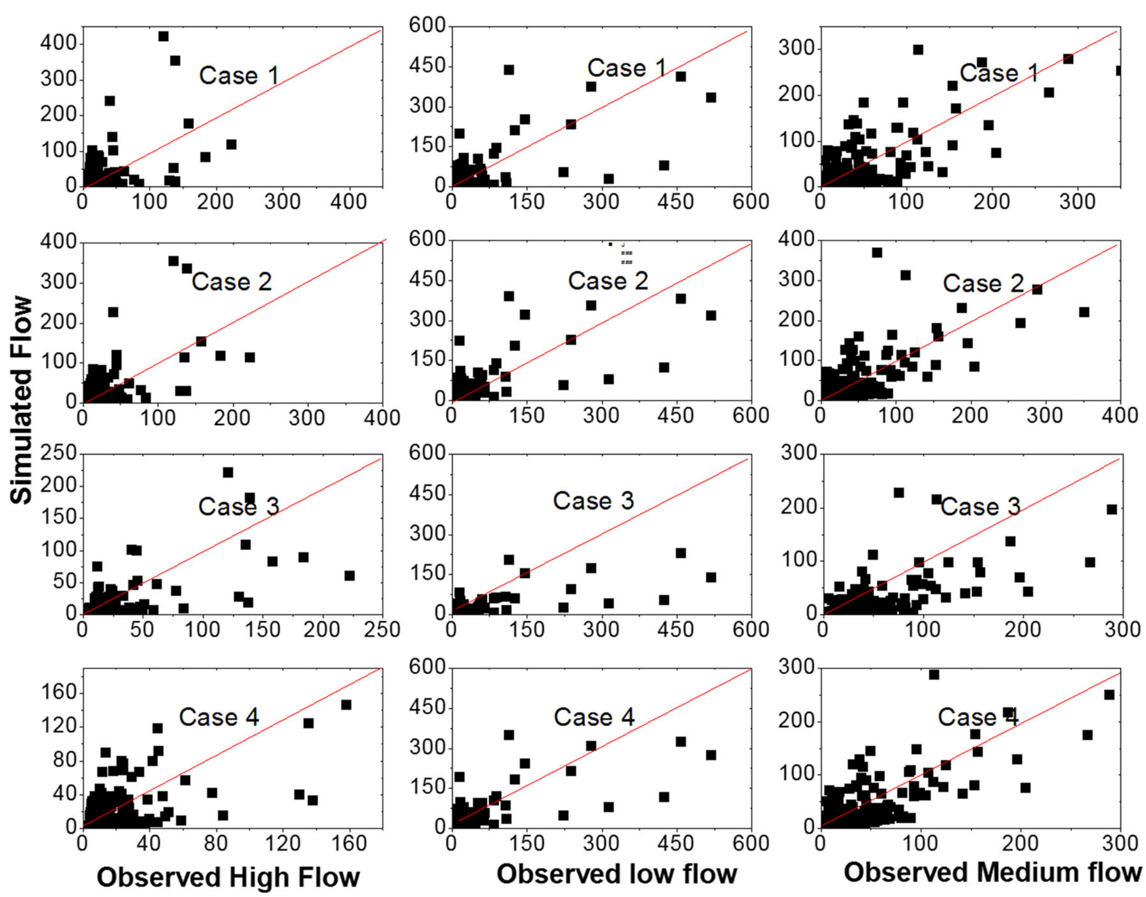

Fig. 6 Scatter plot depicting model performance at different flow ranges for all the approaches

locations in the basin—for a basin which does not have measured data for calibration, and therefore these derived distributions can give a better estimate of model output with less uncertainty. The performance range that found in the watershed outlet was 30–66%. This indicates that the derived probability distribution (at watershed outlet) is able to provide reasonably good simulations at the upstream locations also.

5.4 Computational requirement of the proposed method

It is worth mentioning that the proposed method (Case 1) took only a single iteration to converge the probability distribution of parameters, while the method that did not use MI (Case 2) took two iterations. After a lot of trials, it was observed that Case 2 required a minimum of 1000 model simulations to develop a proper behavioral set, whereas the minimum required simulations in the proposed method was only 200 ensembles. The results indicate that there is a considerable reduction in the number of model simulations (200 against 2000) when MI is used in the analysis. As mentioned earlier, after the first iteration 96% of the total ensembles were found to fall in the behavioral set in Case 1, as compared to 22% in the Case 2. It is also noted that the maximum frequency of likelihood was obtained close to a value of 0.66 from 200 simulations in the case of the proposed approach, while it was close to 0.65 from 2000 simulations in Case 2. This suggests that the use of MI during sampling of parameter helps in reducing the computational requirement of the uncertainty assessment.

6 Summary and conclusions

The distributed hydrological models are ideal for the watershed simulations, but the major skepticism involved in their application is the over-parameterization, the difficulty in calibration process and the uncertainty associated with the predictions. While there are different methods available for uncertainty analysis of hydrological models, the high computational requirement for such analysis makes the modeler skeptic for their application. In this study, a method for uncertainty analysis is presented that uses the mutual information between the parameters in a behavioral set. The analysis starts with an assumption of prior distribution and conditions it on the observed information through successive cycles of simulations. In each iteration the samples were selected which preserves the mutual relationship between the sensitive parameters.

The method is demonstrated through a case study of SWAT model in Illinois River basin. A comparison with the method that did not use MI between parameters indicated that computational requirement can be considerably reduced in the proposed approach. Also, it is noted that the prediction band derived using the proposed method is found to be relatively better compared to the other methods considered in this study. In the case of Illinois River basin, more than 80% of the measured flow was found to fall within the prediction band, and the width of the prediction band was reasonably small. The results of the analysis in general suggests that the number of samples in the behavioral sets can be considerably increased by employing MI during sampling for Monte Carlo simulation to perform uncertainty analysis, and also the analysis require less number of model simulations.

While there are a lot of variants of GLUE (e.g. Vrugt et al. 2003; Beven 2006; Blazkova and Beven 2009; Sadegh and Vrugt 2013; Cibin et al. 2014) that derive the probability distribution of parameters, none of them have explicitly addressed the issue of high computational requirement in the analysis. While most of these variants of GLUE focused on increasing the number of behavioral parameter sets by introducing various filtering criteria, which was very effective, they failed to consider simultaneous reduction of number of simulations required for the analysis. On the contrary, this study considers selection of behavioral sets from relatively less number of simulations, however uses the traditional likelihood measure. Therefore it appears that a synergic combination of the current methods (existing GLUE variants and that proposed in this study) may still help improve the uncertainty analysis procedure for complex hydrological models.

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