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A framework for propagation of uncertainty contributed by parameterization, input data, model structure, and calibration/validation data in watershed modeling

Haw Yen[a,b,*], Xiuying Wang[b], Darrell G. Fontane[a], R. Daren Harmel[c], Mazdak Arabi[a]

[a] *Department of Civil and Environmental Engineering, Colorado State University, Fort Collins, CO 80523, USA*
[b] *Blackland Research & Extension Center, Texas A&M Agrilife Research, 720 East Blackland Road, Temple, TX 76502, USA*
[c] *Grassland, Soil & Water Research Laboratory, USDA-ARS, 808 East Blackland Road, Temple, TX 76502, USA*

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A B S T R A C T

Failure to consider major sources of uncertainty may bias model predictions in simulating watershed behavior. A framework entitled the Integrated Parameter Estimation and Uncertainty Analysis Tool (IPEAT), was developed utilizing Bayesian inferences, an input error model and modified goodness-of-fit statistics to incorporate uncertainty in parameter, model structure, input data, and calibration/validation data in watershed modeling. Applications of the framework at the Eagle Creek Watershed in Indiana shows that watershed behavior was more realistically represented when the four uncertainty sources were considered jointly without having to embed watershed behavior constraints in auto-calibration. Accounting for the major sources of uncertainty associated with watershed modeling produces more realistic predictions, improves the quality of calibrated solutions, and consequently reduces predictive uncertainty. IPEAT is an innovative tool to investigate and explore the significance of uncertainty sources, which enhances watershed modeling by improved characterization and assessment of predictive uncertainty.

Software availability

Name of software: IPEAT
Program language: MATLAB
Developer: Haw Yen, research associate of the Texas A&M University, developed and completed the code of IPEAT in August, 2012.
The source code: Available from Haw Yen, 720 East Blackland Road, Temple, Texas 76502, USA.
Tel: +1 254 774 6004, hyen@brc.tamus.edu

1. Introduction

The ability of watershed models to simulate and predict real world phenomena has been considerably advanced in recent years. Simultaneously, the number of model parameters in empirically or physically based functions has also increased (Yang et al., 2008; Bai et al., 2009), which increases the difficulty of manual calibration. Fortunately, through the progressive improvement of computer science and development of auto-calibration techniques, computational expense of model calibration is no longer a major challenge (Duan et al., 1992; Tolson and Shoemaker, 2007; Vrugt et al., 2009a; Yen, 2012). Thus, modelers can now focus more attention on appropriate representation of watershed phenomena and improved modeling methodology.

However, models are only simplified representations of natural systems. Actual watershed processes are more complex and variable than what can be generally represented in even most sophisticated models (Haan et al., 1995). Uncertainty due to model parameterization, input data, model structure, and observations used for model calibration can significantly impact the accuracy of model outputs. For clarification in this study the uncertainty from forcing inputs (input data) should not be regarded as a part of error contributed from model parameterization. As pointed by Ajami et al. (2007) that it is not appropriate to assume all prediction uncertainty is contributed by model parameterization as it is typical in watershed calibration/validation. On the other hand, even when uncertainty from parameterization, input data, and/or model structure is included, the commonly used goodness-of-fit statistics

* Corresponding author. Blackland Research & Extension Center, Texas A&M Agrilife Research, Texas A&M University System, 720 East Blackland Road, Temple, TX 76502, USA. Tel.: +1 254 774 6004.
E-mail addresses: hyen@brc.tamus.edu, haw.yen@gmail.com (H. Yen).

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which are calculated relative to observational data need to be modified considering measurement uncertainty. Because of imperfect observation, Harmel and Smith (2007) and Harmel et al. (2010) have proposed to consider measurement uncertainty in the evaluation of goodness-of-fit statistics in hydrologic and water quality modeling. In fact, failing to consider one or more sources of uncertainty may cause biased model calibration results and corresponding model predictions.

In review of literature, parameterization uncertainty has received the most attention in previous studies (e.g., Kuczera and Parent, 1998; Osidele et al., 2006; Gallagher and Doherty, 2007; Hassan et al., 2009; Loosvelt et al., 2011; Rasmussen and Hamilton, 2012; Joseph and Guillaume, 2013). The parameter-calibration approach indicates that parameter errors are the ultimate attribution of all possible sources (Ajami et al., 2007). Predictive uncertainty contributed by model input data has been explored and proven to have significant impact on model calibration (Kavetski et al., 2002; Ajami et al., 2007; Strauch et al., 2012). Wang (2008) applied the Bayes inferences to stochastically conduct data generation with non-concurrent, missing input data. In addition, other studies incorporate input uncertainty explicitly during the calibration processes (Kavetski et al., 2002; Ajami et al., 2007). A further source of uncertainty is model structure. The importance of structural uncertainty was demonstrated by Refsgaard et al. (2006) and Clark et al. (2008). One of the most frequently cited approaches for exploring the structural uncertainty is to aggregate different models through the Bayesian Model Averaging (BMA) technique, where the significance of simulation performance for each implemented model can be stated by BMA weights (Kavetski et al., 2006a, 2006b; Ajami et al., 2007; Duan et al., 2007). The contribution of uncertainty in calibration/validation data has only recently been incorporated into evaluation of watershed models. For example, Ullrich and Volk (2010) investigated the influence of uncertainty in NO_3–N monitoring data on model calibration and evaluation. Prior to work by (Harmel et al., 2006, 2009), no comprehensive framework for estimation of uncertainty in measured discharge and water quality data was available. Following the development of this framework, methods were further developed by Harmel and Smith (2007) and Harmel et al. (2010) to modify goodness-of-fit indicators to consider uncertainty in measured data used for model calibration/validation evaluation. Uncertainty has also been explored in associated with other techniques. A Bayesian-based framework assisted by the Morris global sensitivity analysis method was developed to evaluate performance of two models (Minunno et al., 2013), and a set-membership approach was implemented to identify parameter and prediction uncertainty while conducting sediment yield simulations (Keesman et al., 2013).

The main contribution of this study is the development of a framework that facilitates simultaneous evaluation of parameterization, input data, model structure, and calibration/validation data uncertainty and their contribution to predictive uncertainty, entitled Integrated Parameter Estimation and Uncertainty Analysis Tool (IPEAT). The specific objectives of this study were to: (i) quantify predictive uncertainty while propagating different sources of uncertainty and (ii) calibrate the Soil and Water Assessment Tool (SWAT) model with the consideration of four sources of uncertainty (as opposed to typical model calibration of considering only parameter uncertainty) to understand the role and importance of uncertainty source on model prediction (best solution) and predictive uncertainty. In this study, the model structural uncertainty analysis was limited to the two modified SCS, now the Natural Resource Conservation Service (NRCS), curve number method (USDA Soil Conservation Service, 1972; USDA–NRCS, 2004) for calculating surface runoff within the SWAT2009 model. A set of other models can also be included in the analysis, which is not the focus of this study.

2. Methods and materials

2.1. Framework of incorporating different sources of uncertainty

The proposed framework to incorporate uncertainty from parameterization, input data, model structure, and observation data used for calibration is provided in Fig. 1 where it is compared with typical watershed modeling.

2.1.1. Input data uncertainty

Input data such as rainfall, temperature, soils, and land use/cover are critical drivers for watershed simulation. For simplicity in this study only the uncertainty from rainfall was considered. The integrated Bayesian uncertainty estimator (IBUNE) (Ajami et al., 2007) was used to account for uncertainty contributed by rainfall data through an input error model as shown in Eq. (1), which assumed a random Gaussian error as a multiplier for every input observation (Ajami et al., 2007).

$$R_{a\_t} = kR_t; \quad k \sim N\left(m, \sigma_m^2\right) \tag{1}$$

where R_{a_t} and R_t are the adjusted and observed rainfall depth at time step t (e.g., the given day t), respectively, k is the normally distributed random noise with mean m, $m \in [0.9,1.1]$ and variance σ_m^2, $\sigma_m^2 \in [1e-5, 1e-3]$ as defined by (Ajami et al., 2007).

For each SWAT simulation run, the two variables (m and σ_m^2) from this input error model were added as two unknown parameters to the system and a random multiplier (k) to each time step was drawn from the normal distribution $N(m, \sigma_m^2)$. A parameter estimation technique, dynamically dimensioned search (DDS) (Tolson and Shoemaker, 2007) (see Section 2.1.3.) was used to search the SWAT model parameters and the input error model parameters (m and σ_m^2) simultaneously. Through SWAT simulation, the uncertainty associated with the input error model parameters and the SWAT model parameters were propagated through the system.

2.1.2. Model structure uncertainty

Uncertainty is also contributed by the inability of the model structure to perfectly mimic watershed processes. Different models have different degrees of complexity and different algorithms to mimic natural processes. Even within a given modeling system, alternative methods may be offered. Uncertainty due to model structure can significantly impact the accuracy of model outputs. Although researchers have included a set of mutually exclusive models in analyzing model structural uncertainty (e.g., Abrahart and See, 2002; Georgakakos et al., 2004; Ajami et al., 2007), there are potentially many alternative ways to formulate the analysis by combining different models considering there are many hydrologic and water quality models out there. In this study, we only considered the widely used SWAT model. SWAT offers two options to calculate the curve number retention parameter, s. The first one is the traditional method which allows s to vary with soil profile water content (SCSI). An alternative method (SCSII) allows s to vary with accumulated plant evapotranspiration. These two methods were considered in this study for model structural uncertainty.

SWAT is a continuous-time and semi-distributed parameter model, which is developed to simulate/predict hydrologic and water quality processes at the large watershed scale (Arnold et al., 1993, 1998) and it is widely applied for assessing water resource and nonpoint-source pollution problems (e.g., Du et al., 2005; Jayakrishnan et al., 2005; Green et al., 2006; Moriasi et al., 2009; Arnold et al., 2010; Chiang et al., 2010; Douglas-Mankin et al., 2010; Ghebremichael et al., 2010; Kim et al., 2010; Meng et al., 2010; Srinivasan et al., 2010). Comprehensive descriptions of SWAT are presented in Gassman et al. (2007) and Arnold et al. (2012).

The Bayesian Model Averaging (BMA) was used in this study for account for model structural uncertainty. BMA is a probabilistic scheme for model combination (Raftery et al., 2005; Ajami et al., 2007; Wöhling and Vrugt, 2008). The posterior distribution of the BMA prediction, y_{BMA}, under the two SWAT model options of M_1 = SCSI and M_2 = SCSII is given as:

$$p\left(y_{\mathrm{BMA}}\middle|M_1, M_2, \tilde{X}, \tilde{y}\right) = \sum_{k=1}^{2} p\left(M_k\middle|\tilde{X}, \tilde{y}\right) \times p_k\left(y_k\middle|M_k, \tilde{X}, \tilde{y}\right) \tag{2}$$

where $\tilde{X}$ is the SWAT model input forcing data, $\tilde{y}$ is SWAT output variables of interests (here streamflow and water quality NO_3–N), $p(M_k|.\tilde{X}, \tilde{y})$ is the posterior probability of model M_k, $p_k(y_k|.M_k, \tilde{X}, \tilde{y})$ is the forecast posterior distribution of y_k given prediction quantities from model M_k with input data $\tilde{X}$ and corresponding prediction $\tilde{y}$. The$p_k(y_k|.M_k, \tilde{X}, \tilde{y})$ is represented by the normal distribution with mean equal to the output of model M_k and standard deviation σ_k. The term $p(M_k|.\tilde{X}, \tilde{y})$ is also known as the likelihood of model M_k being the correct model, or BMA weight, which should be summed to one.

$$\sum_{k=1}^{2} p\left(M_k\middle|\tilde{X}, \tilde{y}\right) = 1 \tag{3}$$