# Quantifying input uncertainty in the calibration of water quality models: reordering errors via the secant method

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**Abstract.** Uncertainty in inputs can significantly impair parameter estimation in water quality modeling, necessitating accurate quantification of input errors. However, decomposing input error from model residual error is still challenging. This study develops a new algorithm, referred to as Bayesian error analysis with reordering (BEAR), to address this problem. The basic approach requires sampling errors from a pre-estimated error distribution and then reordering them with their inferred ranks via the secant method. This approach is demonstrated in the case of total suspended solids (TSS) simulation via a conceptual water quality model. Based on case studies using synthetic data, the BEAR method successfully improves the identification of the input errors in the model calibration. The results of a real case study demonstrate that even with the presence of model structural error and output data error, the BEAR method can approximate the true input and bring a better model fit through an effective input modification. However, its effectiveness is limited by the accuracy and selection of the input error model. The application of the BEAR method in TSS simulation can be extended to other water quality models.

## 1 Introduction

For robust water management, uncertainty analysis is of growing importance in water quality modeling (Refsgaard et al., 2007). It can provide knowledge of error propagation and the magnitude of uncertainty impacts in model simulations to guide improved predictive performance (Radwan et al., 2004). However, the implementation of uncertainty analysis in water quality models (WQMs) is still challenging due to complex interactions among sources of multiple errors, generally caused by a simplified model structure (structural uncertainty), imperfect observed data (input uncertainty and observation uncertainty in calibration data) and limited parameter identifiability (parametric uncertainty) (Refsgaard et al., 2007).

Among them, input uncertainty is expected to be particularly significant in a WQM, interpreted here as the observation uncertainty of any input data. Observation uncertainty is different from other sources of uncertainty in modeling since these uncertainties arise independently of the WQM itself, thus, their properties (e.g. probability distribution family and distribution parameters) can, at least in principle, be estimated prior to the model calibration and simulation by analysis of the data acquisition instruments and procedures (McMillan et al., 2012). Rode and Suhr (2007) and Harmel et al. (2006) reviewed the uncertainty associated with selected water quality variables based on the empirical quality of observations. The general

methodology developed in their studies can be extended to the analysis of other water quality variables. Besides the error coming from the measurement process, the error from surrogated data is another major source of input uncertainty (McMillan et al., 2012). Measurements of water quality variables often lack desirable temporal and spatial resolutions, thus, the use of surrogate or proxy data is necessary for improved inference of water quality parameters (Evans et al., 1997, Stubblefield et al., 2007). For the surrogate error, its probability distribution is easy to estimate from the residuals between the measurements and proxy values. In this process, the measurement errors are ignored given the errors introduced from the surrogate process are commonly much more than the measurement errors (McMillan et al., 2012). These estimated error distributions are "prior knowledge" of input uncertainty before any model calibration and can serve as the a-priori uncertainty estimation in the modeling process.

Input uncertainty can lead to bias in parameter estimation in water quality modeling (Chaudhary and Hantush, 2017, Kleidorfer et al., 2009, Willems, 2008). Improved model calibration requires isolating the input uncertainty from the total uncertainty. However, the precise quantification of time-varying input errors is still challenging when other types of uncertainties are propagated through to the model results. In hydrological modeling, several approaches have been developed to characterize time-varying input errors, and these may hold promise for application in WQMs. The Bayesian total error analysis (BATEA) method provides a framework that has been widely used (Kavetski et al., 2006). Time-varying input errors are defined as multipliers on the input time series and inferred along with the model parameters in a Bayesian calibration scheme. This leads to a high-dimensionality problem, which cannot be avoided (Renard et al., 2009) and restricts the application of this approach to the assumption of event-based multipliers (the same multiplier applied to one storm event). In the Integrated Bayesian Uncertainty Estimator (IBUNE) (Ajami et al., 2007) approach, multipliers are not jointly inferred with the model parameters, but sampled from the assumed distribution and then filtered by the constraints of simulation fitting. This approach reduces the dimensionality significantly and can be applied in the assumption of data-based multiplier (one multiplier for one input data) (Ajami et al., 2007). However, this approach is less effective because the probability of co-occurrence of all optimal error/parameter values is very low, resulting in an underestimation of the multiplier variance and misidentification of the uncertainty sources (Renard et al., 2009). From the above, a new strategy should be developed to avoid high dimensional computation and ensure the accuracy of error identification.

To complete this goal, this study develops a new algorithm – Bayesian error analysis with reordering (BEAR). The derivation and details of the BEAR algorithm in quantifying input errors are described in Sect. 2. Section 3 introduces the build-up/wash-off model (BwMod) to illustrate this approach. Its model input, streamflow, often suffers from observational errors from a rating curve. By comparing the results with other calibration frameworks, the ability of the BEAR method is explored in two synthetic cases and a real case. In this way, the new algorithm is tested in a controlled situation (with the knowledge of the true error and data value) and in a realistic situation (with the interference of multiple error sources) respectively. Section 4 evaluates the BEAR method and its implementation. Finally, Section 5 outlines the main conclusions and recommendations for this work.

## 2 Methodology

### 2.1 Basic theory of identifying the input error in model calibration

A WQM in the ideal situation without any error can be described as

$$\boldsymbol{Y}^* = M(\boldsymbol{X}^* \mid \boldsymbol{\theta}^*) \tag{1}$$

where the asterisk $^*$ implies the true value without error, and the true output $\boldsymbol{Y}^*$ is simulated by the perfect model *M* with the true input $\boldsymbol{X}^*$ and the true model parameter $\boldsymbol{\theta}^*$. Here and in the following contents, a capital bold letter (e.g. $\boldsymbol{X}, \boldsymbol{Y}$) represents a vector and a lower case (e.g. $x, y$) represents a scalar.

In reality, the model input $\boldsymbol{X}^o$ (typically the rainfall or streamflow in a WQM) inevitably suffers from input error $\boldsymbol{\varepsilon}_X$. This will result in a calibrated model parameter $\boldsymbol{\theta}^c$ biased from the true value $\boldsymbol{\theta}^*$ (Kleidorfer et al., 2009). Thus, under the assumption that the output data and model structure are generally without errors and the input errors are additive to the true input data $\boldsymbol{X}^*$, the model residual $\boldsymbol{\varepsilon}$ in a traditional calibration can be described by

$$\boldsymbol{\varepsilon} = \boldsymbol{Y}^o - \boldsymbol{Y}^s = \boldsymbol{Y}^o - M(\boldsymbol{X}^o \mid \boldsymbol{\theta}^c) = \boldsymbol{Y}^* - M(\boldsymbol{X}^* + \boldsymbol{\varepsilon}_X \mid \boldsymbol{\theta}^c) \tag{2}$$

where $\boldsymbol{Y}^s$ is the output simulated from the model *M* corresponding to the observed input $\boldsymbol{X}^o$ and model parameter $\boldsymbol{\theta}^c$, and the observed output $\boldsymbol{Y}^o$ is assumed without observational errors in the derivation, thus can be denoted as $\boldsymbol{Y}^*$.

It should be noted that the derivation of the BEAR method is based on the assumption that the model only suffers from input error and parameter error, but other sources of error (i.e. model structural error and output observational error) can also impair the estimation of the model parameters and are inevitable in the WQM. Considering this realistic situation, the ability of the BEAR method will be tested in a case study where the interference of other sources of error has been considered.

To counter the influence of input errors in a traditional calibration, an appealing approach is to subtract estimated errors $\boldsymbol{\varepsilon}_X^p$ from the observed input $\boldsymbol{X}^o$. This is illustrated as the "proposed" approach and the superscript *p* represents the values in this "proposed" approach. The residual $\boldsymbol{\varepsilon}^p$ will change to

$$\boldsymbol{\varepsilon}^P = \boldsymbol{Y}^o - \boldsymbol{Y}^P = \boldsymbol{Y}^* - M(\boldsymbol{X}^P \mid \boldsymbol{\theta}^P) = \boldsymbol{Y}^* - M(\boldsymbol{X}^* + \boldsymbol{\varepsilon}_X - \boldsymbol{\varepsilon}_X^p \mid \boldsymbol{\theta}^P) \tag{3}$$

If the equivalence between $\boldsymbol{\varepsilon}_X$ and $\boldsymbol{\varepsilon}_X^p$ can be ensured for each data point, the modified input $\boldsymbol{X}^P$ then becomes the same as the true value $\boldsymbol{X}^*$. The proposed calibration (Eq. (3)) will turn into an ideal calibration where the optimal parameters $\boldsymbol{\theta}^P$ will lead to the same simulation corresponding to the true values $\boldsymbol{\theta}^*$ and the model residual $\boldsymbol{\varepsilon}^P$ will decrease to zero. If the inverse

problem (from the zero residual to find the optimal parameter) is not unique, the calibrated parameter $\theta^p$ may not converge to the true parameter $\theta^*$, but lead to the same simulation as the true parameter. In this study, these parameters are also denoted as $\theta^*$ and called ideal model parameters. Besides, if the identified input error and the model parameter can compensate each other, multiple combinations of model parameter and input error may yield zero residual and their estimates will be biased from the ideal values. A possible way to weaken this compensation effect will be explored in Sect. 4.2. Although the aforementioned problems cannot be avoided, selecting the optimal input error series according to the model residual error is the basic theory of not only this study but also current methods identifying the input errors (i.e. BATEA (Kavetski et al., 2006). and IBUNE (Ajami et al., 2007)).

The above approach does not improve the input error model itself but improves the WQM specification to have parameters closer to what would be achieved under no error conditions. Then the model can be more effectively used for scenario analysis (where we may know the hydrologic regime of a catchment in a hypothetical future), for forecasting under the assumption of perfect inputs (where the driving hydrologic forecast is independently obtained via a numerical weather prediction and a hydrologic model) or for regionalization of the WQM (where the model is transferred to a catchment without data). In all of these cases, an ideal model should have unbiased parameter estimates. This is our goal in identifying the optimal input errors, not to use the model for predictions with input data suffering the same errors.

### 2.2 The introduction of the secant method

Considering the limitations of BATEA and IBUNE framework discussed in the introduction, an improved strategy should be explored to avoid the high dimension challenge and meanwhile promote the error estimation accuracy. This study attempts to transform the input error quantification into the rank domain to realize it. Here, the rank is defined as the order of any individual value relative to the other sampled values, and determines the relative magnitude of each error in all data errors. For example, in the 1$^{st}$ iteration in Table A 1, the error at 15$^{th}$ time step, -0.29, is the smallest value among all the sampled errors, therefore, its rank is 1. In current methods, an assumption of input error model is necessary to set, which provides an overall distribution for the estimated input errors. If there is knowledge of the error distribution (i.e. cumulative distribution function (CDF) of input errors), the error value only depends on its rank in this distribution. Therefore, under the condition of a certain input error model, the rank estimation will bring similar results as the direct value estimation. Besides, the rank estimation has a few advantages over the direct value estimation. The discussion on this is stated in Sect. 4.1.

In the rank domain, the challenge turns to find a way to effectively adjust the input error rank to minimize the residual error. The secant method can be applied to address this problem. It is an iterative process to produce better approximations to the roots of a real-valued equation (Ralston and Jennrich, 1978). Here, the root is the optimal rank of each input error and the equation is the corresponding model residual equal to zero. The secant method (Ralston and Jennrich, 1978) can be repeated as

$$k_{i,q} = k_{i,q-1} - \varepsilon^{p}_{i,q-1} \frac{k_{i,q-1} - k_{i,q-2}}{\varepsilon^{p}_{i,q-1} - \varepsilon^{p}_{i,q-2}} \tag{4}$$

until a sufficiently accurate target value is reached. In this study, the target value is a residual of zero ( $\varepsilon^{p}_{i,q} = 0$ ), indicating a perfect model fit with input errors estimated exactly. Here, $k_{i,q}$ and $\varepsilon^{p}_{i,q}$ represents the estimated rank of input error and the model residual at *i*th time step and *q*th iteration respectively. The error rank of each data point is updated respectively via Eq.(4), where *i* =1,…*n*. *n* is the data length and also the number of the estimated errors as these errors are data-based.

After calculating Eq.(4) , it is possible that the rank $k_{i,q}$ is out of the rank range (for example, less than 1 or more than n), or not an integer. Sorting $k_{i,q}$ in all the ranks $k_{i,q}(i = 1,...,n)$ can address this problem by effectively assigning to each of them a new integer rank based on its position in the sorted list. Thus, in Eq.(4), $k_{i,q}$ should be changed to $K_{i,q}$ , representing the pre-rank. After sorting $K_{i,q}$ for all the errors, the post-rank $k_{i,q}$ will then belong to reasonable values. The specific calculation of the error rank is demonstrated in the 7th and 8th row in Table A 1.

From the above, estimating the rank of input errors via the secant method can be described as the following two equations:

Update the rank of each input error $K_{i,q}$ via the secant method respectively for $i = 1,...,n$ :

$$K_{i,q} = k_{i,q-1} - \varepsilon^{p}_{i,q-1} \frac{k_{i,q-1} - k_{i,q-2}}{\varepsilon^{p}_{i,q-1} - \varepsilon^{p}_{i,q-2}} \tag{5}$$

Sorting $K_{i,q}$ $(i = 1,...,n)$ in all the error pre-ranks $\boldsymbol{K_q}$ to obtain a reasonable rank:

$$k_{i,q} = k(K_{i,q}) \tag{6}$$

where *k( )* means calculating its rank.

Thus, the procedure of input error quantification has been developed via the following key steps: 1) Sample the errors from the assumed error distribution to maintain the overall statistical characteristics of the input errors; 2) Update the input error ranks to minimize the model residual via the secant method (Eq. (5) and (6)); 3) Reorder these sampled errors according to the updated error ranks; 4) Repeat 2) and 3) for a few iterations until a defined target is achieved. This new algorithm is referred to as Bayesian error analysis with reordering (BEAR). An example to illustrate how the BEAR method works is presented in Appendix A.

### 2.3 Integrating the BEAR method into the Sequential Monte Carlo approach

The core strategy of the BEAR method is to identify the input errors by estimating their ranks, which can be easily integrated into formal Bayesian inference schemes (for example, Markov chain Monte Carlo (MCMC, (Marshall et al., 2004)) and Sequential Monte Carlo (SMC, (Jeremiah et al., 2011, Del Moral et al., 2006))) and other calibration schemes (for example, the generalized likelihood uncertainty estimation (GLUE, (Beven and Binley, 1992))). Based on the traditional calibration approach, the BEAR method works by replacing the observed input with a modified input that is obtained through the estimated input error rank via the secant method. This study applies the SMC sampler and derives the BEAR method from a Bayesian theoretical foundation in Appendix B. In the SMC approach, the model parameter is first sampled from a prior distribution and then propagated through a sequence of intermediate populations by repeatedly implementing the reweighting, mutation and resampling processes, until the desired posterior distribution is achieved (Del Moral et al., 2006). The details of the SMC algorithm can be found in the study of Jeremiah et al. (2011).

Figure 1 demonstrates the integration of the BEAR method into the SMC sampler. In the SMC scheme, $s$ refers to the number of sequential populations. A population means a group of parameter vectors (particles) that is updated in each iteration. The maximum number of the population $S$ is set as 200 in this study. In each sequential population, $N$ particles of model parameters are calibrated. $N$ is set as 100 in this study. For each particle of the model parameters, the corresponding input error ranks are updated over $q$ iterations, where $q$ increases until the acceptance probability is larger than a number randomly sampled from 0 to 1. It should be noted that if the model parameters are far away from the true values, especially in the initial population, iterative updating of the error ranks will have little effect in reducing the model residual. Therefore, the maximum number of iterations should be set, referred to as $Q$. $Q$ is set as 20 in this study. If $q$ exceeds $Q$, the algorithm returns to the mutation step in Fig. 1.

### 2.4 Comparison with other methods

The application of the BATEA framework is limited by high dimension computation (Renard et al., 2009). It probably becomes impractical in quantifying the data-varying errors (rather than the event-varying errors in the study of BATEA (Kavetski et al., 2006)), where the dimension easily exceeds 1000 (Haario et al., 2005). Therefore, the BATEA method is not considered in the comparison. In this study, three methods, including the "Traditional" method, "IBUNE" method and "BEAR" method, are compared to evaluate the ability of the BEAR method in estimating the model parameters and quantifying input errors. "Traditional" method regards the observed input as error-free without identifying input errors (i.e. Eq. (2)), while the other two methods employ a latent variable to counteract the impact of input error and build the modified input (i.e. Eq.(3)). In the "IBUNE" method, potential input errors are randomly sampled from the assumed error distribution and filtered by the maximization of the likelihood function (Ajami et al., 2007). Although the comprehensive IBUNE framework additionally deals with the model structural uncertainty via the Bayesian Model Averaging (BMA) method, this study only compares the

capacity of its input error identification approach. The "BEAR" method adds a reordering process into the "IBUNE" method to improve the accuracy of input error quantification.

## 3 Case studies

### 3.1 Water quality model: the build-up/wash-off model (BwMod)

This study tests the BEAR algorithm in the context of the build-up/wash-off model (BwMod), which is a group of models to simulate two processes in sediment dynamics, including the build-up of sediments during dry periods and the wash-off process during wet periods. The two formulations were developed in a small-scale experiment (Sartor and Boyd, 1972), while in applications at the catchment scale, the conceptualized parameters largely abandon their physical meanings and the formulations can be considered a "black-box" (Bonhomme and Petrucci, 2017). This study chooses Eq. (7) to describe the build-up process and Eq. (8) to express the wash-off of sediments, representing the non-linear relationship between the wash-off load (output) and the runoff-rate (input). These two equations were applied in the research of Sikorska et al. (2015) and in this study are integrated with the BEAR method. This study will test the BEAR algorithm in a case of simulating the daily sediment dynamics of one catchment, thus, the time scale is typically set as daily and the spatial scale is set as the catchment. This version of BwMod has four parameters (Table 1). The model input is streamflow, which typically comes from the observation of a rating curve. As discussed in the introduction, the error distribution can be estimated prior to the model calibration via a rating curve analysis. The output of the BwMod is the concentration of total suspended solids (TSS), whose transport can be efficiently simulated by the conceptualization of the build-up/wash-off process (Bonhomme and Petrucci, 2017, Sikorska et al., 2015). Although BwMod is relatively simple compared with process-based WQMs, its nonlinearity and the use of surrogates for the input data can make it a typical WQM scenario to test the BEAR algorithm.

The overall BwMod equations are:

$$\frac{dS_{a,t}}{dt} = \kappa \cdot \left( S_{max} - S_{a,t} \right) - s\left( S_{a,t} \right) \tag{7}$$

where the descriptions of $\kappa$ and *Smax* are shown in Table 1, $S_{a,t}$ (kg) is the sediment amount available on the catchment surface to be washed-off at time *t*; $s\left( S_{a,t} \right)$ (kg/s) is the amount of sediment in the stream at time *t*, described by the function

$$s(S_{a,t}) = a \cdot (Q_t)^b \cdot S_{a,t} \tag{8}$$

where the descriptions of *a* and *b* are shown in Table 1, and $Q_t$ is the streamflow at the catchment outlet at time *t*.

The output TSS concentration $C_{TSS,t}$ ($kg/m^3$) is derived via:

$$C_{TSS,t} = \frac{s\left(S_{a,t}\right)}{Q_t} \tag{9}$$

### 3.2 Case study 1: Synthetic data suffering from input errors and parameter errors

To test the capability of the secant method in identifying the input error ranks in the process of the model parameter estimation, the BEAR method is first implemented in a controlled situation with synthetic data, where the model is affected only by input errors and parameter errors. The true input $\boldsymbol{X}^*$ is set as the daily streamflow data of the catchment in the real case (USGS ID: 04087030), covering 1095 days from 2009/10/01 to 2012/09/29. The true output $\boldsymbol{Y}^*$ is the simulated TSS concentration via BwMod corresponding to the true input $\boldsymbol{X}^*$ and model parameters set as the reference values in Table 1. In case study 1, the observed output $\boldsymbol{Y}^o$ is assumed to be the same as the true simulation $\boldsymbol{Y}^*$, i.e. without error. The observed input $\boldsymbol{X}^o$ is generated based on two types of input error models: an additive formulation and a multiplicative formulation, and the errors are assumed to follow a normal distribution with mean $\mu$ as 0.2 and standard deviation (SD) $\sigma$ as 0.5. If the input errors are estimated based on a rating curve, like the procedure in the following real case, the mean of input error should be 0. But in order to test the ability of the BEAR method in wider applications, a systematic bias 0.2 has been considered in the synthetic case even though this is unlikely to manifest in real situations. An additive formulation (denoted as '*add*' in Table 2) is suitable to illustrate the error generation in measurements, while the multiplicative formulation (denoted as '*mul*' in Table 2) is specifically applied for errors induced from a log-log regression procedure, which is common for water quality proxy processes (Rode and Suhr, 2007). In the additive formulation, the generated input may be negative. If so, the negative input should be truncated to a positive value. In the multiplicative formulation, the generated input will stay positive. Given the description in the introduction, the input error model can be pre-estimated independent of calibration by analysing the input data in some studies. While in other cases, the input error model cannot be estimated or its accuracy is in question. Therefore, two scenarios about the prior information of $\sigma$ have been considered: one is fixed as the reference values (denoted as '*fixed*' in Table 2), the other one is estimated as the hyperparameters with the model parameters (denoted as '*inferred*' in Table 2). Therefore, Synthetic case 1 considers four scenarios, including two sets of input data generating from two input error models and two types of prior information about the error parameter $\sigma$ (the details are shown in Table 2).

Each scenario is calibrated via the traditional method, the IBUNE method and the BEAR method respectively. Their algorithms are described in Sect. 2.4. Considering the unknown initial sediment loads in real applications, the calibration sets 90 days as a warm-up period to remove the influence of antecedent conditions. To compare the ability of different methods in estimating the input error and model parameter, this study selects the following statistical characteristics. The SD of the estimated input errors represents the accuracy of the input error distribution (0.5 is the reference value). The correlation between the estimated

input error and the true input error evaluates the capability of the method in catching the temporal dynamics of input error. The Nash-Sutcliffe efficiency (NSE) of the modified input vs true input measures the precision of the input data after removing the estimated input errors. In the calibration part, the simulated output corresponds to the modified input and estimated model parameters, and its NSE compared to the true output measures the goodness-of-fit. In the validation part, the simulated output corresponds to the true input and estimated model parameters, and its NSE compared to the true output can assess the accuracy of the model parameter estimation. These statistical characteristics are calculated as the weighted-average values considering the weights of each estimation in the posterior distribution and compared in Fig. 2. Figure C 1 in Appendix C demonstrates the temporal dynamics of input estimations and model simulations of synthetic case 1. In Fig. C1, "Reliability" is the ratio of observations caught by the confidence interval of 2.5%-97.5%, and the average width of this interval band is referred to as "Sharpness" (Yadav et al., 2007, Smith et al., 2010).

Evaluating the model simulation, the BEAR method always produces the best output fit in all scenarios, supported by the highest green bars in Fig. 2(4). Although its correlations with the true error series are much higher than the IBUNE method (red bars) in all scenarios (in Fig. 2(2)), the BEAR method cannot ensure a better input estimation (in Fig. 2(3)) and its ability depends on the prior information of the input error parameter. When the error parameters are fixed at the reference values (in the scenarios *add-fixed* and *mul-fixed*), the BEAR method always outperforms the other two methods in the input modification and model parameter estimation, as its NSE is the highest (green bars in Fig. 2(3) and (5)). Without the reordering strategy, the IBUNE method even gives worse input modification, model simulation and parameter estimation than the traditional method, demonstrated by the lower red bars than blue bars in Fig. 2(3), (4) and (5). When the error parameters are inferred (in the scenarios of *add-inferred* and *mul-inferred*), the IBUNE method can improve the input data and the model parameter estimation compared with the traditional method (in Fig. 2(3) and (5)) although the estimations of $\sigma$ via the IBUNE method are always smaller than the reference value (in Fig. 2(1)). This result has also been reported in the study of Renard et al. (2009), which indicates that the randomness of the likelihood function leads to an underestimation of $\sigma$ of input errors. Unlike the IBUNE method, the performance of the BEAR method depends on the setting of the input error model. In the *add-inferred* scenario, the BEAR method is still better than other methods, having a bigger NSE (in Fig. 2(3), (4) and (5)) and the closer $\sigma$ estimation to reference value (in Fig. 2(1)). While in the *mul-inferred* scenario, the modified inputs and estimated parameters via the BEAR method are worse than the IBUNE method (in Fig. 2(3) and (5)).

### 3.3 Case study 2: Synthetic data suffering from input errors, parameter errors and output observation errors

Case study 1 is an ideal situation that is used to test the effectiveness of the BEAR method in isolating the input error and the model parameter error. However, in real-life cases, other sources of errors (i.e. model structural error and output data error) will impact this effectiveness. To explore the ability of the BEAR method with the interference of other sources of errors, the output observational errors with the increasing standard deviations are considered to build the synthetic data based on the scenario 3 and 4 in the case study 1 (the details has been shown in Table 2).

Figure 3 demonstrates in the *mul-fixed* scenario where the prior information of standard deviation of input errors is accurate, the BEAR method always brings a better input modification than other methods, although its ability is impaired by the impact of the output observational errors as the NSEs reduces with the increasing SD of the output observational error. The IBUNE method leads to an even worse modified input than the input data without modification in the Traditional method. In the *mul-inferred* scenario where the standard deviation of input errors cannot pre-estimated accurately and given in a wide range, the BEAR method brings worse input data while the IBUNE method can modify the input data.

### 3.4 Case study 3: Real data

To explore the ability of the BEAR method in real-life applications, a real case of one catchment located in southeast Wisconsin, USA is demonstrated. Table 3 is a description of the test catchment and data (Baldwin et al., 2013). The daily TSS concentration and streamflow data are collected from the USGS database on National Real-Time Water Quality (https://nrtwq.usgs.gov/). The daily streamflow data in the USGS database comes from a stage-streamflow rating curve, where the stage and streamflow form a log-log linear relationship and the streamflow proxy errors follow a normal distribution with $\mu$ as 0 and $\sigma$ as 0.103. This prior information is used in the real calibration, denoted as *O-fixed* scenario in Table 2, where "*O*" represents the input data that comes from the observations of the rating curve. According to the results of Figure 3 and the assumption of the methodology derivation, the BEAR method works better when the input uncertainty is more significant, so another input data source with more significant data uncertainty, a streamflow simulation from a hydrological model, has been considered. This study selects GR4J (Perrin et al., 2003) as the hydrological model and calibrates its parameters with the USGS streamflow data as calibration data. If the USGS streamflow data is regarded as the true input data, the residual error after the model calibration can approximate the data error of GR4J simulation, which follows a normal distribution in log space with $\mu$ as 0 and $\sigma$ as 0.764. The BwMod calibration using this input data source and the prior information on data error is denoted as *S-fixed* scenario in Table 2, where "*S*" represents the input data that comes from the simulations of GR4J model. To explore the ability of the BEAR method in other situations where the prior information about the input error is not sufficient, two scenarios with a wider range of the error parameters has also been considered, denoted as *O-inferred* and *S-inferred* in Table 2. The real case is also calibrated via three methods (i.e. the traditional method, the IBUNE method and the BEAR method) and adopts the same setting of the calibration algorithm as the synthetic case.

Figure 4(2) demonstrates the BEAR method always produces a better fit to the output data than the IBUNE method, consistent with the synthetic case shown in Fig. 2(4). In Fig.4(3), except for the *O-fixed* scenario, the results of the BEAR method (in green) show much smaller sharpness than the traditional method (in blue) and the IBUNE method (in red) with almost the same reliability. According to the results of the traditional method in Fig. C2, the simulations from the "*O*" streamflow (in (a1)) catch the dynamics of observed TSS concentration better than the simulations from the "*S*" streamflow (in (a3)). Thus, compared with the simulated streamflow via GR4J ("*S*" streamflow), the observed streamflow from the rating curve ("*O*" streamflow) should be closer to the true input data. In Fig. C2, the modified inputs via the BEAR method are closer to the "*O*"

streamflow (blue dots) than the "*S*" streamflow (pink dots), even in (c3) and (c4) where the original input data comes from the "*S*" streamflow. However, the modified input via the IBUNE method is always centred on the original input data it uses. Given being always closer to the "*O*" streamflow, the modified inputs via the BEAR method are more reasonable than the IBUNE method.

## 4 Discussion

### 4.1 The effectiveness of rank estimation

The novelty of the BEAR method lies in transforming a direct error value estimation to an error rank estimation. In a continuous sequence of data, the potential error values have an infinite number of combinations, while the error rank has limited combinations, dependent on the data length. For example, in Table A1, the estimated error at the 1st time step could be any value. Even under a constrain of the range from the minimized to the maximized sampled errors (i.e. [-0.29,0.16] in the 1st iteration), its value estimation still has infinite possibilities due to the continuous nature of the error. In contrast, the rank is discrete, having only 20 possibilities (i.e. the integrity in [1,20]). From this point of view, it is more efficient to estimate the error rank than estimate the error value,

However, the rank estimation will suffer from the sampling bias problem. The sampling bias problem is that even corresponding to the same rank, the error sampled at different times could be largely different, especially for a small sample size (depending on the data length) or a large $\sigma$ of the assumed error distribution. This problem can be addressed by selecting the optimal solution from multiple sampling according to the maximum of likelihood function. In three cases of this study, the sample size is larger than 1000, where the sampling bias problem can be neglected and one error sampling is enough. But in some cases where the sample size is small (i.e. around 10), multiple sampling should be undertaken.

Besides, to avoid the high-dimension calculation, modifying each input error according to its corresponding residual error only works in the rank domain. In the value domain, if there is no constraint on the estimated input errors, they will fully compensate for the residual error to maximize the likelihood function and subsequently be overfitted. There are two ways to impose restrictions. One is to regard errors and model parameters as a whole in calibration, like the BATEA framework (Kavetski et al., 2006), resulting in a high dimensional computation. The other is to sample error randomly from the assumed error model, like the IBUNE framework (Ajami et al., 2007), whose precision cannot be guaranteed due to the error randomness. However, in the BEAR method, the inference focuses on the error rank where the value range of the sampled errors can be effectively limited by the assumed error model. Additionally, adjusting the order of the sampled errors according to the inferred error rank can reduce the randomness in the IBUNE framework (Ajami et al., 2007), which significantly improves the accuracy of the error estimation (as demonstrated by much higher NSEs than the IBUNE method in Fig. 2). The reordering step is implemented when the model parameter has been updated and aims to find the optimal input error series corresponding to the minimized residual error. After the reordering step, the optimal input error is a deterministic function of the model parameter. Thus, unlike

formal Bayesian inference, the BEAR method does not update the posterior distribution of the input errors, but identifies the input error through the deterministic relationship between the input error and model parameter.

### 4.2 The impacts of prior information of input error model

The IBUNE method takes advantage of stochastic error samples to modify the input observations (Ajami et al., 2007). Figure C 5 demonstrates compared with *O-fixed* and *O-inferred* scenarios, *S-fixed* and *S-inferred* scenarios uses simulated streamflow whose input error is more significant, and the resultant simulations (black line) via the IBUNE method are further away from the observed outputs (red dots). As per the findings in the previous study of Renard et al. (2010), if the $\sigma$ of input errors is inferred with the model parameters, the IBUNE method will underestimate $\sigma$ (in Fig. 2(1) and Fig. 4(1)). If $\sigma$ is fixed via prior information, the input modification and model simulation cannot be improved, especially in the scenarios with large intrinsic $\sigma$ of input errors (in Fig. 2 and Fig. 3). From the above, the ability of the IBUNE method depends on the input data quality and the improvement of the input data and model simulation only happens when the $\sigma$ of the estimated input error is small. The availability of prior information is insignificant for the IBUNE method, especially when the intrinsic $\sigma$ of the input error is large.

However, the findings in the BEAR method are quite different. Accurate prior information about the input error model is important in the BEAR method. Figure 3 demonstrates *fixed* scenarios calibrated via the BEAR method always produce a higher NSE of the modified input than *inferred* scenarios. This is likely because the prior information can constrain the input error distribution and reduce the impacts of other sources of errors. The availability of prior information of the input error relies on studies about benchmarking observational errors of water quality and hydrologic data, and the selection of a proper input error model is important. Comparing the results in Figure 2, when the input error model is an additive formulation, the BEAR method consistently brings the best performance regardless of the prior information of the error $\sigma$. When the input error model is a multiplicative formulation, the BEAR method cannot improve the input data if the prior information of the error $\sigma$ is not accurate. This illustrates that the compensating effect between the input error and parameter error is weaker in the additive form of the input error. This is probably related to the specific model structure, as the exponent parameter $b$ in BwMod has a stronger interaction with the multiplicative errors than the additive errors. Thus, more comprehensive comparisons should be undertaken to explore the capacity of different input error models in different model applications.

To sum up, the ability of the BEAR method depends on the accuracy of prior information of the input error parameter and the selection of the input error model. The IBUNE method can modify the input data when the standard deviation of the estimated input error is much smaller than the true value. It is most likely to make use of the stochastic errors to improve the original input data, but not effectively identify the input error.

### 4.3 The extension to other modeling scenarios

In this study, the BEAR method was developed in the calibration of BwMod at the daily time scale, whose input and output can be regarded as the correspondence at each time step. Therefore, in Eq.(5), the model residual $\varepsilon^{p}_{i,q-1}$ and input error rank $k_{i,q-1}$ are at the same time step *i*. If the water quality system exhibits delayed response, the time lag between the forcing data and the response (described as *lag*) should be considered in the algorithm and Eq. (5) needs to be modified as Eq. (10).

$$K_{i,q} = k_{i,q-1} - \varepsilon^{p}_{i+lag,q-1} \frac{k_{i,q-1} - k_{i,q-2}}{\varepsilon^{p}_{i+lag,q-1} - \varepsilon^{p}_{i+lag,q-2}} \tag{10}$$

If the response caused by an input is not instantaneous but exhibits persistence (i.e. occurs over several time steps), the autocorrelation in the output should be addressed to ensure the independence assumption of the rank updating is satisfied. Current ways to deal with this problem in hydrologic modelling can provide a reference to the potential modification of the BEAR method. Autocorrelation in the residual errors can be represented by an autoregressive moving average (ARMA) model (Kuczera, 1983) or autoregressive (AR) (Schaefli et al., 2007, Bates and Campbell, 2001). The correlated part of the error is removed from the residual error and the remaining part will be only impacted by the input error. Thus, the correspondence between the input error and the residual error part is ensured and the latter process will be the same as the application of the BEAR method in this study. Following this idea, the autoregressive (AR) model has been integrated with the BEAR method in the study of Wu et al. (2021) to deal with the autocorrelation of residual errors in a hydrologic model. The results prove this integration is effective to improve the input error estimation.

However, this treatment may not guarantee the improvement of the input error estimation in this study where the sediment concentrate is simulated at the daily time scale (Figure D 1). At this time scale, one input (streamflow) may not impact the response (sediment concentration) for multiple time steps and autocorrelation may not be well represented via a simple autocorrelation function. When the temporal resolution of the data is high (i.e. minute) and one model output is affected by many inputs, the memory effect may be addressed effectively via the AR model. Therefore, the specific representation of the autocorrelation in the residual error needs further discussion through comparisons in different time scales or with different characteristics in the memory effect.

## 5 Conclusion

Taking advantage of the prior information of an input error model, a new method, Bayesian error analysis with reordering (BEAR), is proposed to approach the time-varying input errors in WQM inference. It contains two main processes: sampling the errors from an assumed error distribution and reordering them with the inferred ranks via the secant method. Through the investigation of synthetic data and real data, this method is shown to be effective but its ability is limited by the accuracy and selection of the input error model. The novelties of this algorithm are: (1) The estimation focuses on the error rank rather than

the error value, which enhances the constraints of the input error model on the estimated errors and avoids the high dimensionality problem resulting from calibrating all the errors along with the model parameter as a whole. (2) The introduction of the secant method realizes updating the error rank of each input data according to its corresponding residual and tackles the nonlinearity challenge in the WQM transformation.

However, the work in this study still identifies a few areas needing to be explored. Firstly, the availability of prior knowledge of the input error model is important. When this information is not reliable or even cannot be estimated, a significant issue is the selection of a suitable error assumption. Thus, a general measure should be found to judge whether an error model is appropriate, especially in real cases where the "true" information is limited. Secondly, extensions of the BEAR method to other water quality modeling scenarios are subject to problems such as delayed and autocorrelated responses. Related studies in hydrologic modeling to deal with the delay and persistency of responses could be references in the modification of the BEAR method. Thirdly, if the sampling and reordering strategy is developed within a more comprehensive framework to quantify multiple sources of error, the interactions amongst these error sources might be well-identified and the quantification of individual errors might be improved. This study provides a starting point for developing the rank estimation via the secant method to identify input error. Further study is necessary to modify the algorithm and improve confidence in extended case studies or model scenarios.

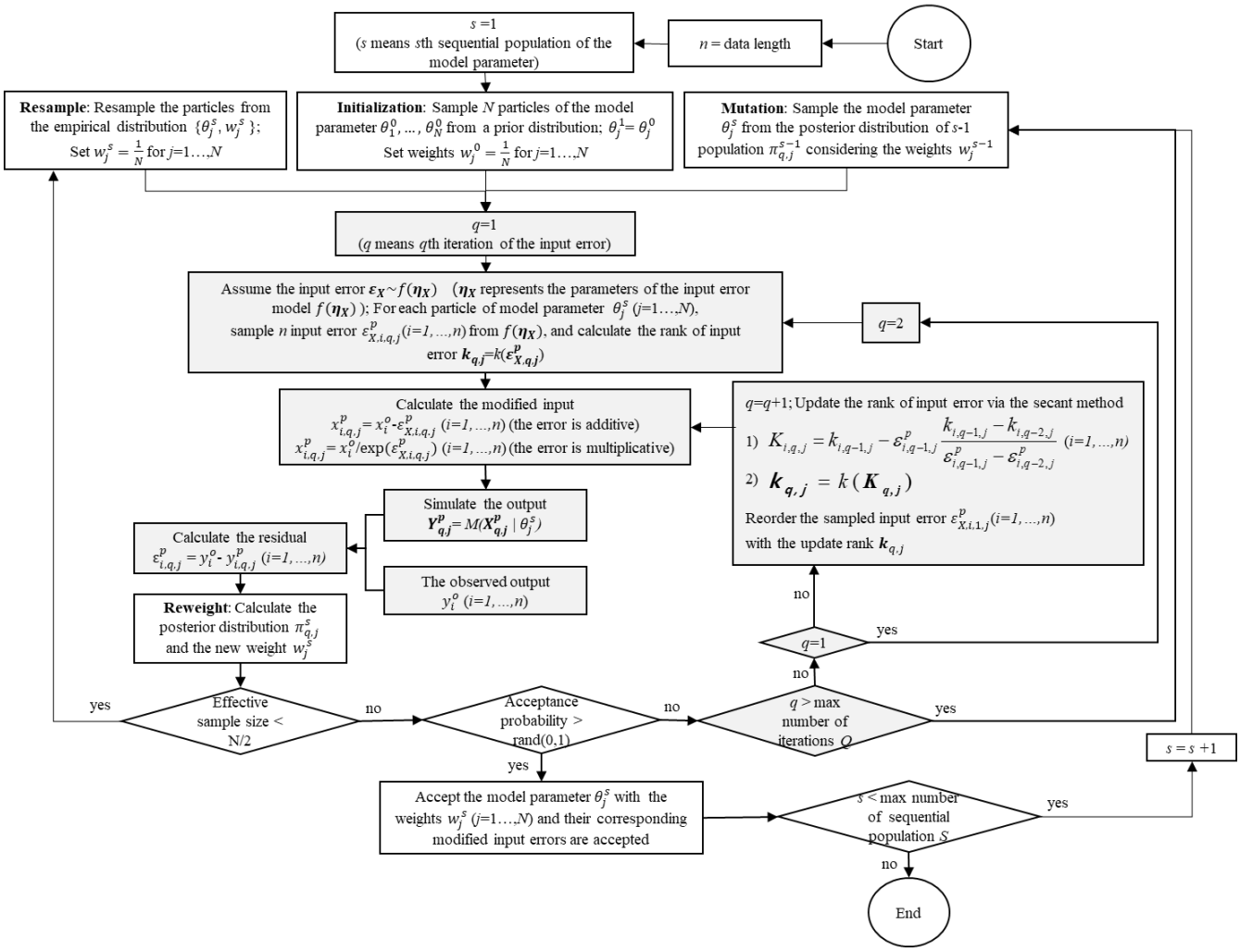


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**Figure 1 Flowchart of the algorithm to quantify the input errors via Bayesian error analysis with reordering (BEAR) method in the SMC calibration scheme (The grey charts demonstrate the BEAR method while the white charts demonstrate the SMC algorithm. The details of the BEAR method can refer to Appendix A. The details of the SMC algorithm can refer to the study of Jeremiah et al. (2011), including the Mutation step, the Reweight step and calculating the acceptance probability. rand(0,1) means a number**
400 **randomly sampled from 0 to 1.)**

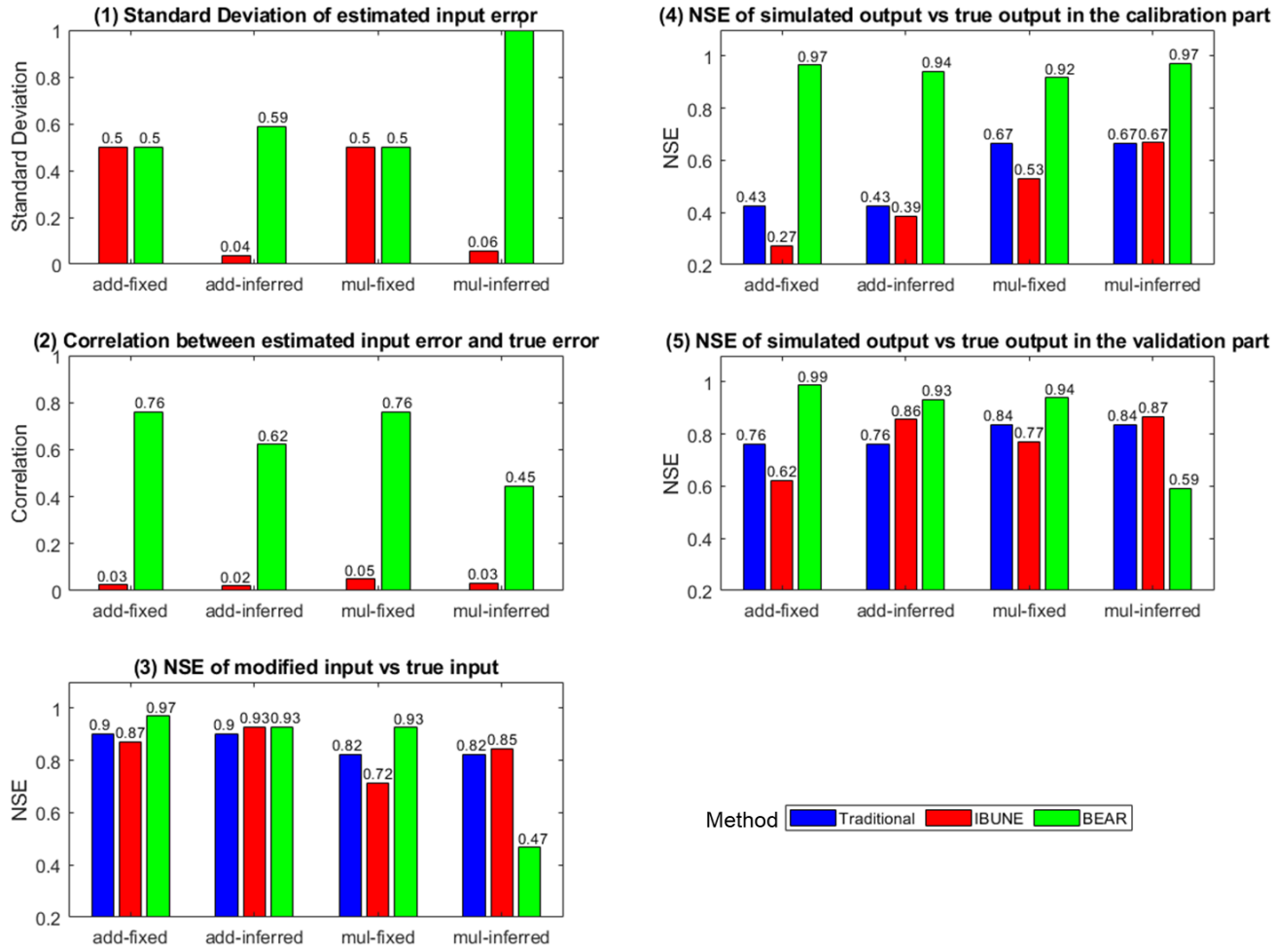


**Figure 2: Comparison of statistical characteristics of four calibration scenarios in the synthetic case 1 (including *add-fixed*, *add-inferred*, *mul-fixed* and *mul-inferred*; notations are given in Table 2) via three calibration methods (including the traditional method, the IBUNE method and the BEAR method, their algorithms are explained in Sect. 2.4)**

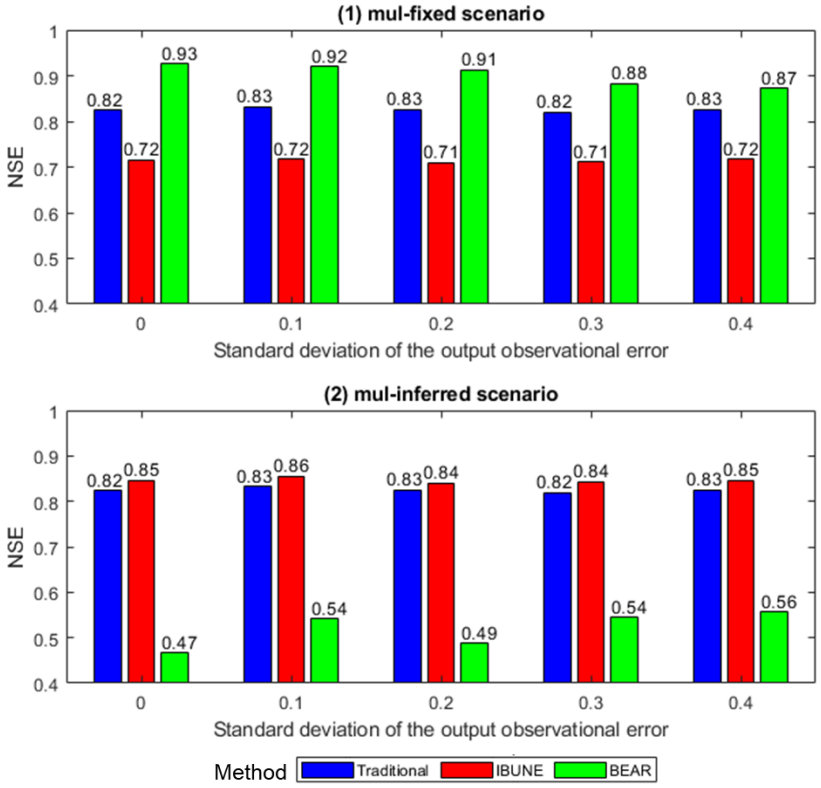


**Figure 3 Comparison of Nash-Sutcliffe efficiency (NSE) of the modified input v.s true input under the interference of the output observational errors with the increasing standard deviations in two calibration scenarios in the synthetic case 2 (including *mul-fixed* and *mul-inferred*; notations are given in Table 2) via three calibration methods (including the traditional method, the IBUNE method and the BEAR method, their algorithms are explained in Sect. 2.4)**

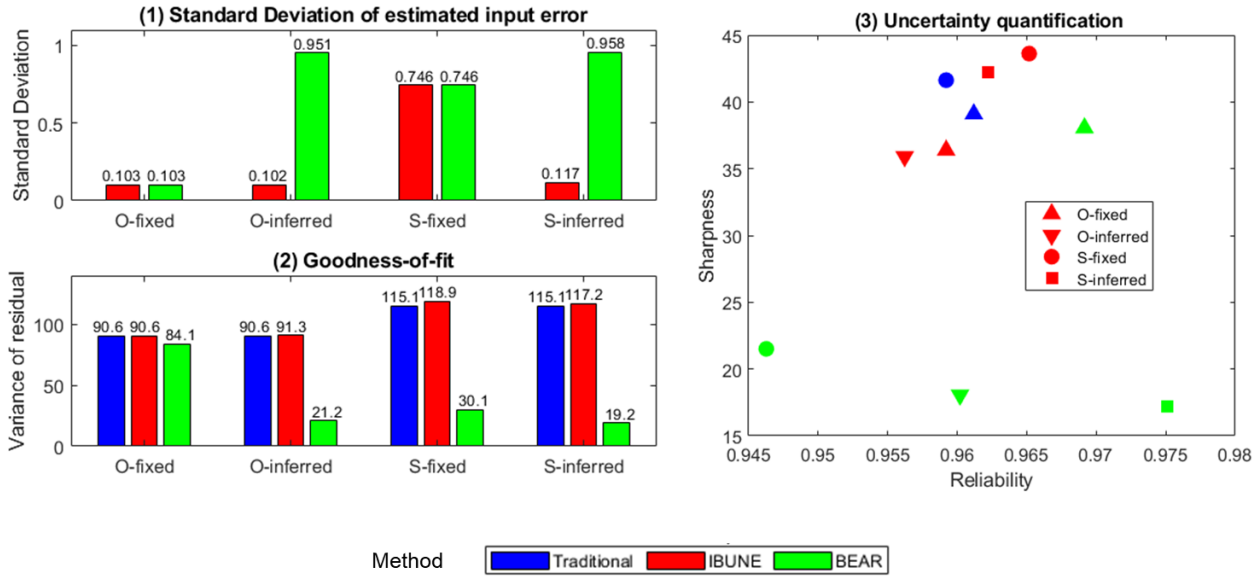


**Figure 4: Comparison of statistical characteristics of four calibration scenarios in the real case (including *O-fixed*, *O-inferred*, *S-fixed* and *S-inferred*, their notations are given in Table 2) via three calibration methods (including the traditional method, the IBUNE method and the BEAR method, their algorithms are explained in Sect. 2.4)**

**Table 1 Descriptions of BwMod parameters**

| Model | Parameter | Description | Unit | Reference value in the synthetic case | Prior range in the case study |
|---|---|---|---|---|---|
| BwMod | *a* | wash-off coefficient | - | 0.04 | (0, 2) |
| | *b* | wash-off exponent | - | 1.6 | (0, 3) |
| | $\kappa$ | sediment accumulate rate | - | 0.1 | (0, 1) |
| | *Smax* | maximum amount of sediment possible to be accumulated | kg | 7000 | (0, 15000) |

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**Table 2 Summary of the calibration scenarios in case studies**

| Scenario in the synthetic case 1 | Notation | Input error model in the synthetic input generation | Prior information of input error model in calibration |
|---|---|---|---|
| 1 | *add-fixed* | $\boldsymbol{X}^o = \boldsymbol{X}^* + \boldsymbol{\varepsilon}, \boldsymbol{\varepsilon} \sim N(0.2, 0.5^2)$ | $\boldsymbol{X}^o = \boldsymbol{X}^* + \boldsymbol{\varepsilon}, \boldsymbol{\varepsilon} \sim N(0.2, 0.5^2)$ |
| 2 | *add-inferred* | | $\boldsymbol{X}^o = \boldsymbol{X}^* + \boldsymbol{\varepsilon}, \boldsymbol{\varepsilon} \sim N(\mu, \sigma^2), \mu$=0.2, $\sigma \in (0,1)$ |
| 3 | *mul-fixed* | $\boldsymbol{X}^o = \boldsymbol{X}^* \exp(\boldsymbol{\varepsilon}), \boldsymbol{\varepsilon} \sim N(0.2, 0.5^2)$ | $\boldsymbol{X}^o = \boldsymbol{X}^* \exp(\boldsymbol{\varepsilon}), \boldsymbol{\varepsilon} \sim N(0.2, 0.5^2)$ |
| 4 | *mul-inferred* | | $\boldsymbol{X}^o = \boldsymbol{X}^* \exp(\boldsymbol{\varepsilon}), \boldsymbol{\varepsilon} \sim N(\mu, \sigma^2), \mu$=0.2, $\sigma \in (0,1)$ |
| Scenario in the synthetic case 2 | Notation | Observational error model in the synthetic output generation | Prior information of input error model in calibration |
| 1 | *mul-fixed* | $\boldsymbol{Y}^o = \boldsymbol{Y}^* \exp(\boldsymbol{\varepsilon}), \boldsymbol{\varepsilon} \sim N(0, \sigma_Y^2)$ | $\boldsymbol{X}^o = \boldsymbol{X}^* \exp(\boldsymbol{\varepsilon}), \boldsymbol{\varepsilon} \sim N(0.2, 0.5^2)$ |
| 2 | *mul-inferred* | $\sigma_Y^2$=0, 0.1, 0.2, 0.3, 0.4 | $\boldsymbol{X}^o = \boldsymbol{X}^* \exp(\boldsymbol{\varepsilon}), \boldsymbol{\varepsilon} \sim N(\mu, \sigma^2), \mu$=0.2, $\sigma \in (0,1)$ |
| Scenario in the real case | Notation | Input data source in the real case | Prior information of input error model in calibration |
| 1 | *O-fixed* | Observations from the rating curve (USGS database) | $\boldsymbol{X}^o = \boldsymbol{X}^* \exp(\boldsymbol{\varepsilon}), \boldsymbol{\varepsilon} \sim N(0, \sigma^2), \sigma$=0.103 |
| 2 | *O-inferred* | | $\boldsymbol{X}^o = \boldsymbol{X}^* \exp(\boldsymbol{\varepsilon}), \boldsymbol{\varepsilon} \sim N(0, \sigma^2), \sigma \in (0,1)$ |
| 3 | *S-fixed* | Simulations from a hydrological model | $\boldsymbol{X}^o = \boldsymbol{X}^* \exp(\boldsymbol{\varepsilon}), \boldsymbol{\varepsilon} \sim N(0, \sigma^2), \sigma$=0.764 |
| 4 | *S-inferred* | | $\boldsymbol{X}^o = \boldsymbol{X}^* \exp(\boldsymbol{\varepsilon}), \boldsymbol{\varepsilon} \sim N(0, \sigma^2), \sigma \in (0,1)$ |

425 **Table 3 Characteristics of the study catchments and calibration data**

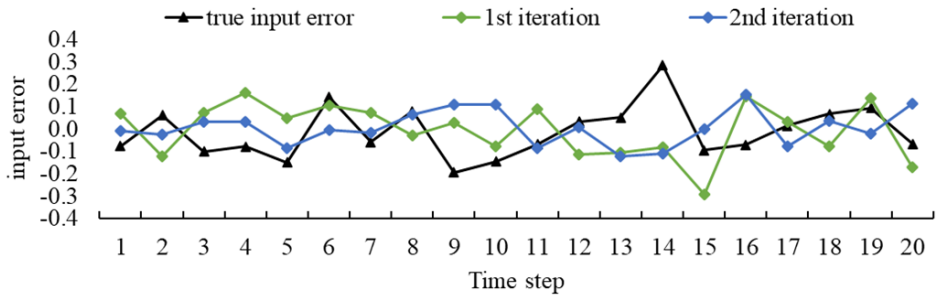
| USGS station number | location | | State | Drainage area ($km^2$) |
|---|---|---|---|---|
| 04087030 | Menomonee River at Menomonee Fall | | Wisconsin, USA | 89.83 |
| | land use | | | |
| Urban (percent) | Agricultural (percent) | Natural (percent) | Period of Data | Number of Data (days) |
| 35 | 38 | 27 | 2009/10/01 - 2012/09/29 | 1095 |

## Appendix A: The illustration of the BEAR method

**Table A 1 An example illustrating the BEAR method**

| row | time step | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **1st iteration (the input errors are randomly sampled)** | | | | | | | | | | | | | | | | | | | | | |
| 1 | sampled input error | 0.07 | -0.12 | 0.07 | 0.16 | 0.05 | .0.07 | 0.07 | -0.03 | 0.03 | -0.08 | 0.09 | -0.11 | -0.11 | -0.08 | -0.29 | 0.14 | 0.03 | -0.08 | 0.14 | -0.17 |
| 2 | input error rank | 13 | 3 | 14 | 20 | 12 | 17 | 15 | 9 | 10 | 7 | 16 | 4 | 5 | 6 | 1 | 19 | 11 | 8 | 18 | 2 |
| 3 | model residual error | -0.29 | 0.49 | -0.58 | -0.98 | -0.78 | 0.29 | -0.66 | 0.59 | -1.31 | -0.31 | -0.87 | 0.76 | 0.46 | 0.54 | 0.25 | -0.80 | -0.07 | 0.56 | -0.23 | 0.40 |
| | MSE | 0.40 | | | | | | | | | | | | | | | | | | | |
| **2nd iteration (the input errors are randomly sampled)** | | | | | | | | | | | | | | | | | | | | | |
| 4 | sampled input error | -0.01 | -0.02 | 0.03 | 0.03 | -0.09 | 0.00 | -0.02 | 0.06 | 0.11 | 0.11 | -0.09 | 0.01 | -0.12 | -0.11 | 0.00 | 0.15 | -0.08 | 0.04 | -0.02 | 0.11 |
| 5 | input error rank | 9 | 6 | 14 | 13 | 3 | 10 | 8 | 16 | 17 | 18 | 4 | 12 | 1 | 2 | 11 | 20 | 5 | 15 | 7 | 19 |
| 6 | model residual error | -0.13 | 0.23 | -0.43 | -0.41 | -0.21 | 0.70 | -0.23 | 0.09 | -1.88 | -1.52 | 0.20 | 0.17 | 0.53 | 0.60 | -0.43 | -0.72 | 0.36 | 0.12 | 0.47 | -0.82 |
| | MSE | 0.47 | | | | | | | | | | | | | | | | | | | |
| **3rd iteration (the error ranks are updated via the secant method)** | | | | | | | | | | | | | | | | | | | | | |
| 7 | calculated pre-rank | 5.8 | 8.7 | 14.0 | 8.0 | -0.3 | 22.0 | 4.3 | 17.3 | -6.1 | 4.2 | 6.2 | 14.3 | 31.3 | 42.0 | 4.7 | 29.0 | 10.0 | 16.9 | 14.4 | 7.6 |
| 8 | ranked rank (post rank) | 6 | 10 | 12 | 9 | 2 | 17 | 4 | 16 | 1 | 3 | 7 | 14 | 19 | 20 | 5 | 18 | 11 | 15 | 13 | 8 |
| **3rd iteration (the input errors are reordered with the updated error ranks)** | | | | | | | | | | | | | | | | | | | | | |
| 9 | reordered input error | -0.02 | 0.00 | 0.01 | -0.01 | -0.11 | 0.11 | -0.09 | 0.06 | -0.12 | -0.09 | -0.02 | 0.03 | 0.11 | 0.15 | -0.08 | 0.11 | 0.00 | 0.04 | 0.03 | -0.02 |
| 10 | model residual error | -0.23 | 0.20 | -0.34 | -0.24 | -0.12 | 0.19 | 0.14 | 0.08 | -0.40 | -0.31 | -0.22 | 0.03 | -0.17 | 0.26 | -0.09 | -0.55 | 0.11 | 0.14 | 0.27 | -0.23 |
| 11 | MSE | 0.06 | | | | | | | | | | | | | | | | | | | |

**(a) at the 1st and 2nd iteration where the input errors are randomly sampled**




**(b) at the 3rd iteration where the input errors are reordered according to the updated error ranks**

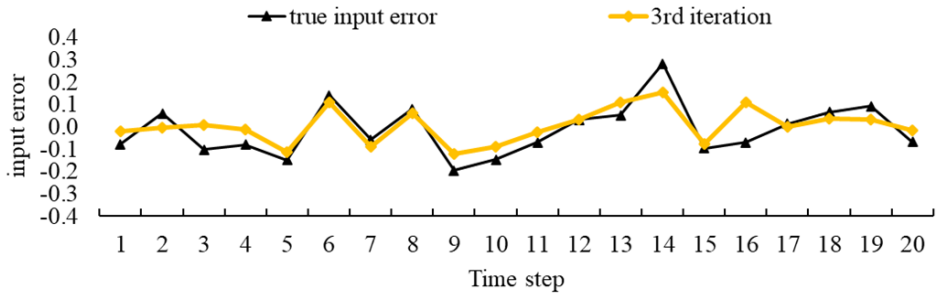



**Figure A 1 Demonstration of the input error estimated in Table A.1**

The BEAR method for identifying the input errors is implemented after generating the model parameters and contains two main parts: sampling the errors from an assumed error distribution and reordering them with the inferred ranks via the secant method. An example is illustrated in Table A 1 and the explanation about the specific steps is presented in the following contents.

(1) In the 1st iteration ($q$=1), the errors are randomly sampled from the assumed error distribution (row 1), and then are sorted to get their ranks (row 2). This error series is employed to modify the input data, which leads to a new model simulation and model residual (row 3).

(2) Repeat step (1) in the 2nd iteration ($q$=2) as two sets of samples are prerequisites for the updating via the secant method. The results are shown in row 4, 5 and 6. Figure A 1(a) demonstrates that the ranges of the error distribution are the same between the true input errors (black line) and the sampled errors (blue and green lines) as they come from the same error distribution under the condition that prior knowledge of the input error distribution is correct. However, the values at each time step cannot match due to the randomness of the sampling.

(3) At the 1st time step in the 3rd iteration ($i$=1, $q$=3 in Eq. (4)), the pre-rank $K_{1,3}$ is calculated via the secant method (illustrated as the following Eq. (4)). The details are demonstrated in solid boxes in Table A.1.

$$K_{1,3} = k_{1,2} - \varepsilon_{1,2}^{p} \frac{k_{1,2} - k_{1,1}}{\varepsilon_{1,2}^{p} - \varepsilon_{1,1}^{p}} = 9\text{-}(\text{-}0.13)\frac{9-13}{-0.13-(-0.29)} = 5.8$$

(4) Repeat step (3) for all the time steps. The calculated pre-ranks are shown in row 7.

(5) Sort all the pre-ranks to get the integral error rank (row 8).

(6) According to the updated error ranks (row 8), the sampled errors in the 2nd iteration (row 4) are reordered. The example for the 1st time step is demonstrated in dotted boxes in Table A.1. The error rank at the 1st time step is updated as 6, and the rank 6 corresponds to the error value -0.02 in the 2nd iteration. Therefore, -0.02 is the input error at the 1st time step in the 3rd iteration. Following this example, the sampled errors at all the time steps are reordered. The results are shown in row 9. Figure A 1 (b) demonstrates that after reordering the errors with the inferred ranks, the estimated errors are much closer to the true input error, and the mean square error (MSE) of the model residual reduces in Table A 1.

(7) The reordered input error will lead to a new input data, a new model simulation and a new model residual. The residual result and its MSE statistic are shown in row 10 and 11 respectively.

(8) Check the convergence: If the objective function or likelihood function meets the convergence criterion, stop and the input error estimation is accepted. Otherwise, $q$=$q$+1, repeat step (3)~(8) until $q$ is larger than the maximum numbers of iteration $Q$.

**Appendix B: Theoretical foundation of the BEAR method**

(1) Basic notation

In general, a model *M*() simulates the output $\boldsymbol{Y}^{s}$ given the observed input $\boldsymbol{X}^{o}$ and model parameters $\boldsymbol{\theta}$, as follows:

$$\boldsymbol{Y}^{s} = M(\boldsymbol{X}^{o}, \boldsymbol{\theta}) \tag{1}$$

Here and in the following, $^{s}$ represents the simulated value, $^{o}$ represents the observed value, and $^{*}$ represents the true value.

(2) Input errors

The input errors $\boldsymbol{\varepsilon}_X$ are assumed to be represented by input multipliers, which are sampled from an uncorrelated lognormal distribution, and the observed input $\boldsymbol{X}^{o}$ can then be related to the true input $\boldsymbol{X}^{*}$ by the following equation:

$$\boldsymbol{X}^{o} = \boldsymbol{X}^{*} \exp(\boldsymbol{\varepsilon}_X), \boldsymbol{\varepsilon}_X \sim N(\mu_X, \sigma_X^2) \tag{2}$$

where $\boldsymbol{\varepsilon}_X$ are assumed to follow a Gaussian distribution with mean $\mu_X$ and variance $\sigma_X^2$.

(3) Output observational errors and model structural errors

In the derivation, these two parts are assumed to be error-free, therefore,

$$\boldsymbol{Y}^{o} = \boldsymbol{Y}^{*} \tag{3}$$

$$M() = M^{*}() \tag{4}$$

(4) Remnant errors

Based on the previous assumptions, the observed output equals the true output, and the difference between the simulated output and the observed output, $\boldsymbol{\varepsilon}$, will be equal to the difference between the simulated output and the true output, as follows:

$$\boldsymbol{Y}^{s} = \boldsymbol{Y}^{o} + \boldsymbol{\varepsilon} = \boldsymbol{Y}^{*} + \boldsymbol{\varepsilon}, \boldsymbol{\varepsilon} \sim (0, \sigma^2) \tag{5}$$

where the remnant errors $\boldsymbol{\varepsilon}$ are assumed to follow a Gaussian distribution with mean 0 and variance $\sigma^2$.

(5) Bayesian inference

According to the study of Renard et al. (2010), the posterior distribution of all inferred quantities is given by Bayes' theorem, as follows:

$$p(\boldsymbol{\theta},\boldsymbol{\varepsilon}_X,\mu_X,\sigma_X,\sigma\,|\,\boldsymbol{Y}^o,\boldsymbol{X}^o)\propto$$
$$p(\boldsymbol{Y}^o\,|\,\boldsymbol{\theta},\boldsymbol{\varepsilon}_X,\boldsymbol{X}^o)\,p(\boldsymbol{\varepsilon}_X\,|\,\mu_X,\sigma_X)\,p(\boldsymbol{\theta},\mu_X,\sigma_X,\sigma) \quad (6)$$

The full posterior distribution comprises the following three parts: the likelihood of the observed output $p(\boldsymbol{Y}^o\,|\,\boldsymbol{\theta},\boldsymbol{\varepsilon}_X,\boldsymbol{X}^o)$, the hierarchical parts of the input multiplier $p(\boldsymbol{\varepsilon}_X\,|\,\mu_X,\sigma_X)$ and the prior distribution of deterministic parameters and hyperparameters $p(\boldsymbol{\theta},\mu_X,\sigma_X,\sigma)$.

Renard et al. (2009) argue that in the IBUNE method, $\boldsymbol{\varepsilon}_X$ are randomly sampled in each evaluation of the likelihood function and their different values at different evaluations will lead to the nondeterministic nature of the likelihood function (Equation (6)). In Bayesian inference, the likelihood function should return a fixed value for a given set of arguments. However, the randomness of the likelihood function in the IBUNE method breaks this theoretical foundation. Conversely, in the BEAR method, the secant method is applied to find a deterministic relationship between the rank of each input error and its corresponding model residual error. The residual errors depend on the model parameters $\boldsymbol{\theta}$. The magnitude of the whole input errors (i.e. their cumulative distribution function (CDF)) is related to the hyperparameters of the multipliers $\mu_X,\sigma_X$. Given the value of each input error is determined by the CDF of the whole input errors and its relative rank among them, $\boldsymbol{\varepsilon}_X$ depends on $\mu_X,\sigma_X$ and $\boldsymbol{\theta}$, as follows:

$$\boldsymbol{\varepsilon}_X = f(\boldsymbol{\theta},\mu_X,\sigma_X) \quad (7)$$

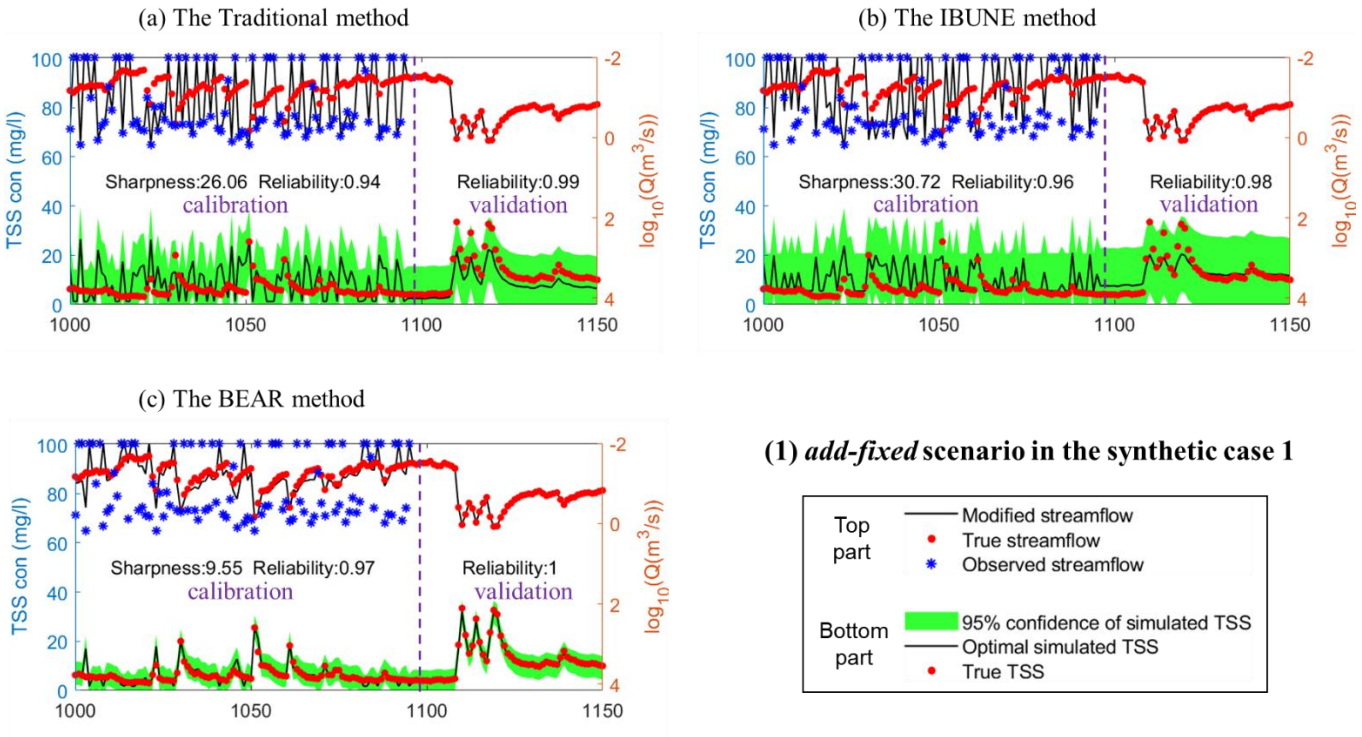
Considering $\boldsymbol{\varepsilon}_X$ are sampled from $N(\mu_X,\sigma_X^2)$, $p(\boldsymbol{\varepsilon}_X\,|\,\mu_X,\sigma_X)$ is fixed when $\mu_X,\sigma_X$ are determined and do not need to be considered in Equation (6). Therefore, the posterior distribution of all inferred parameters (Equation (6)) in the BEAR method will turn into:

$$p(\boldsymbol{\theta},\boldsymbol{\varepsilon}_X,\mu_X,\sigma_X,\sigma\,|\,\boldsymbol{Y}^o,\boldsymbol{X}^o)\propto$$
$$p(\boldsymbol{Y}^o\,|\,\boldsymbol{\theta},\mu_X,\sigma_X,\boldsymbol{X}^o)\,p(\boldsymbol{\theta},\mu_X,\sigma_X,\sigma) \quad (8)$$

The above derivation states if the relationship between the input errors and model parameters (Equation (7)) can be determined, the problem of parameter estimation and input error identification (Equation (6)) can then be interpreted as the updating $\boldsymbol{\theta},\mu_X,\sigma_X$ (Equation (8)) in the Bayesian inference. There are two ways to realize this determined relationship: one is to estimate the parameters and input errors together, as the BATEA approach, which will suffer from the high-dimensionality problem (Renard et al., 2010); the other one is to explore the relationship between each input error rank and model parameters

via the secant method first, and then transform the error rank into the error value according to the estimated error parameters $\mu_X, \sigma_X$, as the BEAR approach in this study.

## Appendix C: The time series of results in the case study




515 **Figure C 1(1) Comparison of time series of synthetic data and uncertainty bands estimated via three calibration methods (including the traditional method, the IBUNE method and the BEAR method; algorithms are explained in Sect. 2.4) for a select period of *add-fixed* scenarios in the synthetic case 1(notations are given in Table 2)**

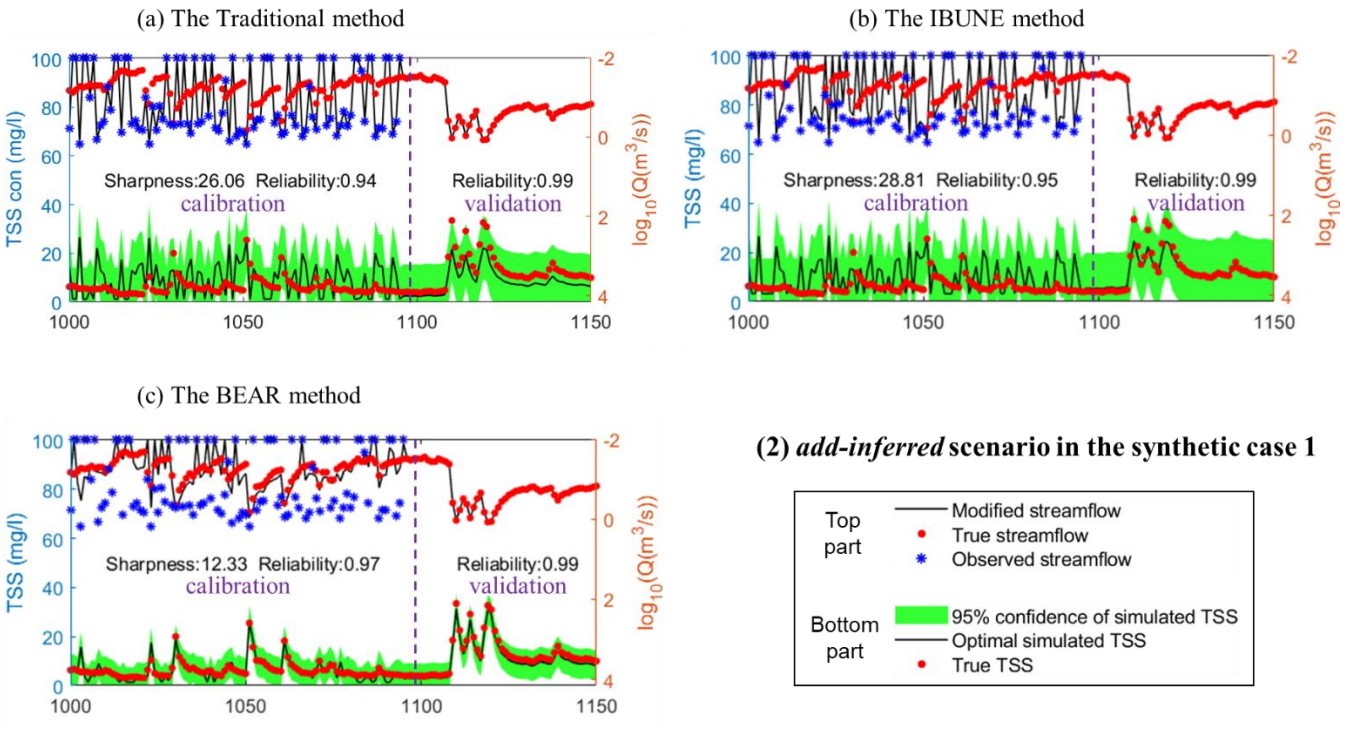



**Figure C 2(2) Comparison of time series of synthetic data and uncertainty bands estimated via three calibration methods (including the traditional method, the IBUNE method and the BEAR method; algorithms are explained in Sect. 2.4) for a select period of *add-inferred* scenarios in the synthetic case 1(notations are given in Table 2)**

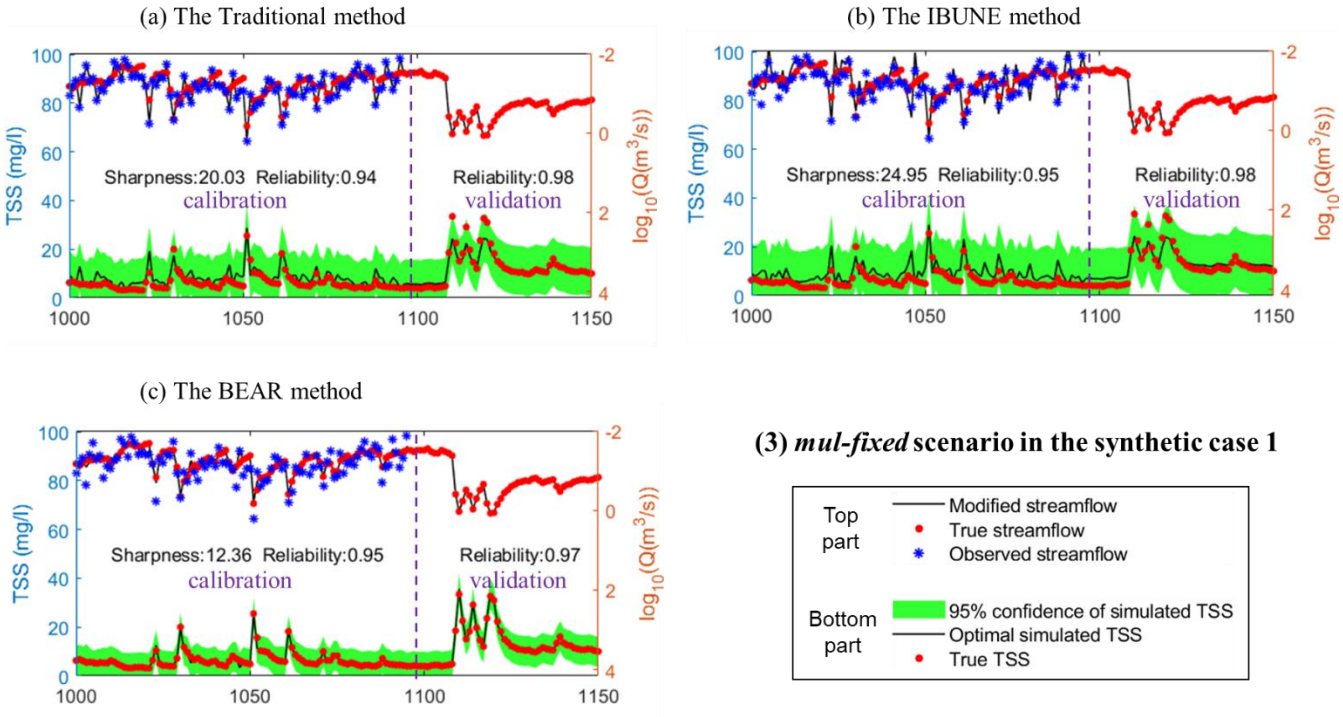



**Figure C 3(3) Comparison of time series of synthetic data and uncertainty bands estimated via three calibration methods (including the traditional method, the IBUNE method and the BEAR method; algorithms are explained in Sect. 2.4) for a select period of *mul-fixed* scenarios in the synthetic case 1(notations are given in Table 2)**

530

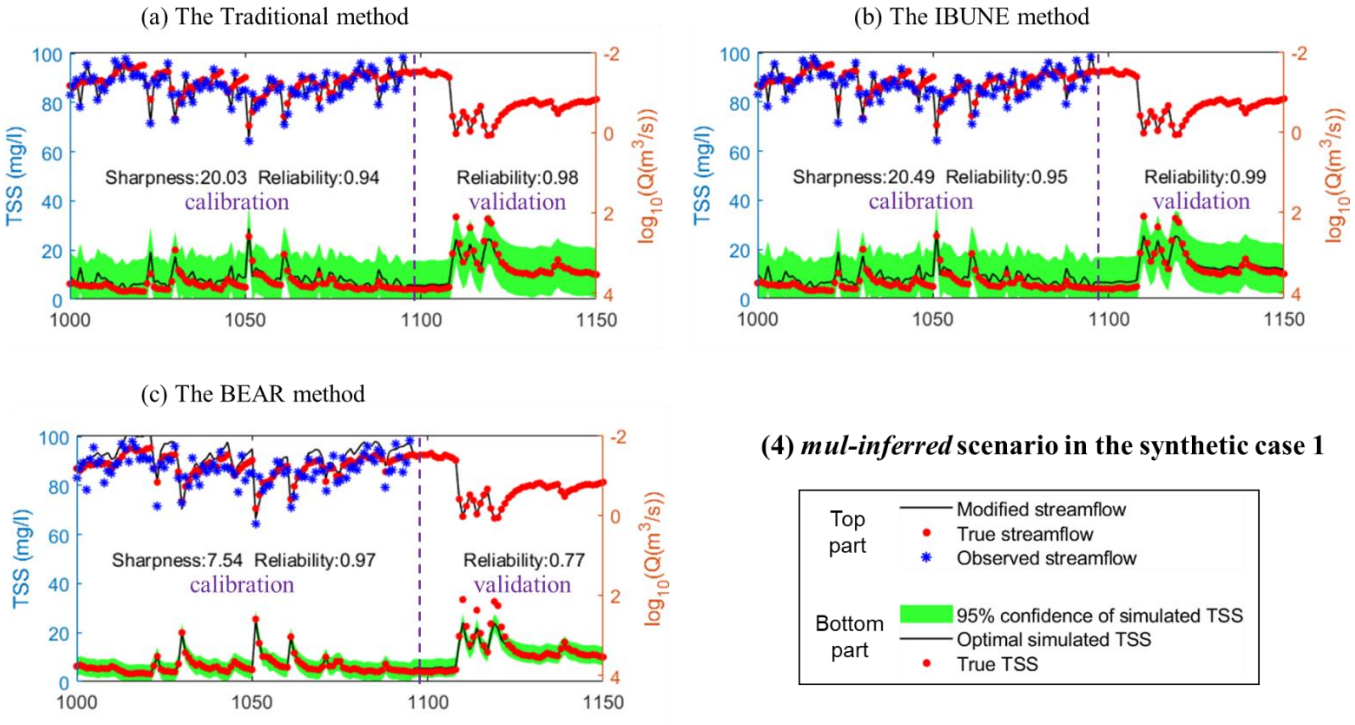



**Figure C 4(4) Comparison of time series of synthetic data and uncertainty bands estimated via three calibration methods (including the traditional method, the IBUNE method and the BEAR method; algorithms are explained in Sect. 2.4) for a select period of *mul-inferred* scenarios in the synthetic case 1(notations are given in Table 2)**

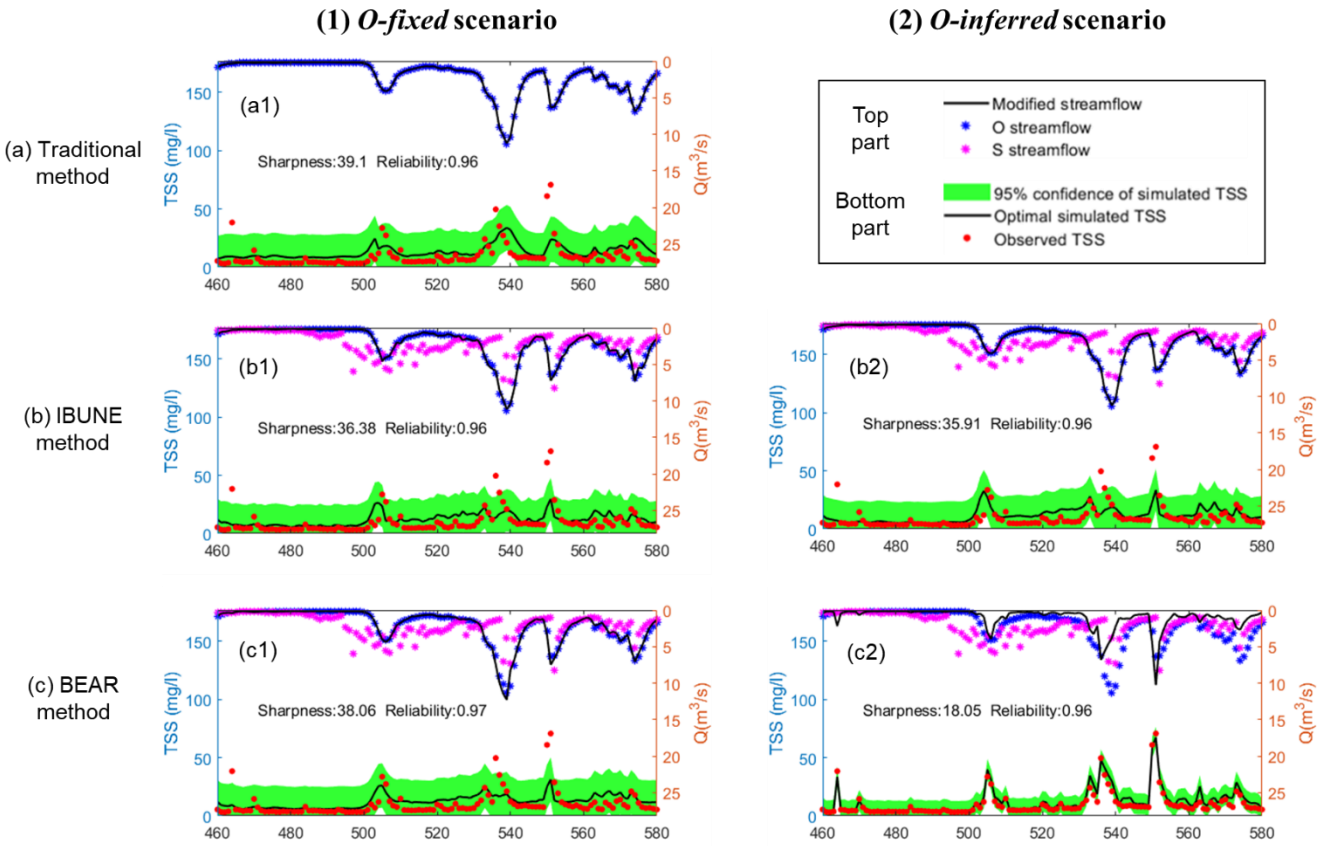



**Figure C 2(1) Comparison of time series of real data and uncertainty bands estimated via three calibration methods (including the traditional method, the IBUNE method and the BEAR method, algorithms are explained in Sect. 2.4) for a select period of *O-fixed*, *O-inferred* scenarios in the real case (notations are given inTable 2)**

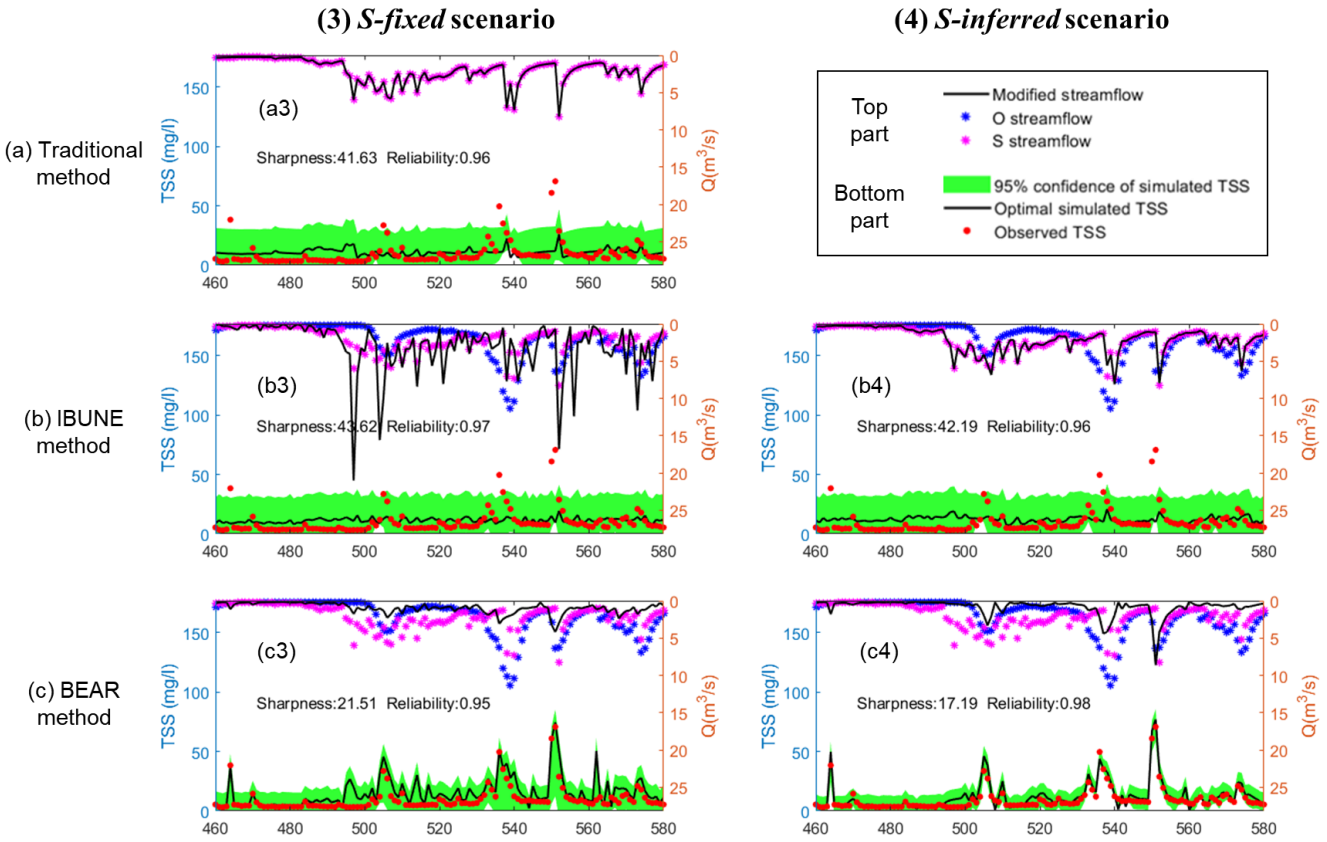



**Figure C 5(2) Comparison of time series of real data and uncertainty bands estimated via three calibration methods (including the traditional method, the IBUNE method and the BEAR method, algorithms are explained in Sect. 2.4) for a select period of *S-fixed* and *S-inferred* scenarios in the real case (notations are given inTable 2)**

**Appendix D: The results after applying the autoregressive (AR) model**

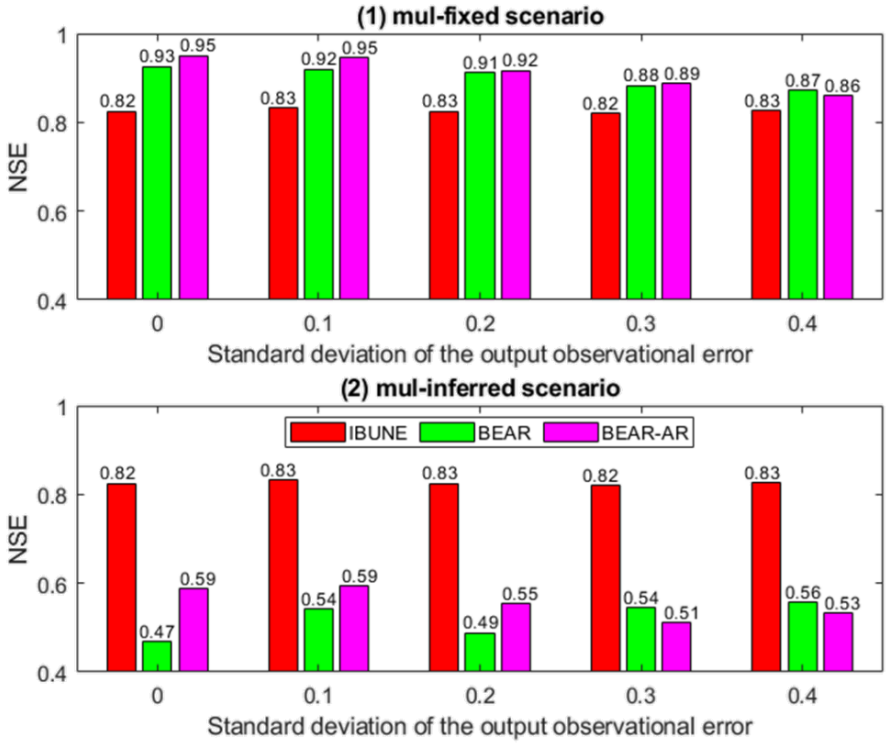



**Figure D 1 Comparison of Nash-Sutcliffe efficiency (NSE) of the modified input v.s true input under the interference of the output observational errors with the increasing standard deviations in two calibration scenarios in synthetic case 2 (including *mul-fixed* and *mul-inferred*; notations are given in Table 2) via three calibration methods (including the IBUNE method and the BEAR method and the BEAR-AR method, the BEAR-AR method is the BEAR method after applying the autoregressive (AR) model to deal with the residual error)**

## Code/Data availability

The daily streamflow and TSS concentration data for real case catchment (ID: USGS 04087030) can be accessed by the National Real-Time Water Quality website of USGS, the link is https://nrtwq.usgs.gov/ .

## Author contribution

Lucy Marshall and Ashish Sharma designed the research. Xia Wu developed the research code, analyzed the results, and prepared the manuscript with contributions from all co-authors.

## Competing interests

The authors declare that they have no conflict of interest.

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