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# Uncertainty in flow and water quality measurement data: A case study in the Daning River watershed in the Three Gorges Reservoir region, China

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ABSTRACT

Measurement data are used to calibrate and validate the effect of models. In this study, four types of uncertainty categories covering flow measurement, sample collection, sample preservation/storage and laboratory analysis were quantified for flow, sediment and water quality measurement data under best-, typical- and worst-case scenarios. The root mean square error propagation method was used to calculate the overall uncertainty. A case study was conducted in the Daning River with the Soil and Water Assessment Tool. Based on the results, the probable error range values of flow were lower than those of sediment and nutrients, indicating greater uncertainty in the sediment and total phosphorus results. It is also indicated that the uncertainty was smaller when the model outputs had a normal distribution. This research provides scientific data of measurement uncertainty in China, which can assist modelers in evaluating model performance by quantifying the "quality" of the response data.

*Keywords:* Uncertainty; Measurement data; SWAT model; Daning River watershed; Flow; Water quality

## 1. Introduction

Watershed models are widely used to support sound practices in hydrology and water quality management [1]. The response data, including measured flow, sediment and pollution date, are always used to calibrate and validate watershed models [2–4]. However, uncertainties during the process of sample collection and measurement are important and cannot be ignored [5,6]. Hence, the uncertainty of measured water quality data and its effect on modeling have become an important research subject in the field of water pollution [7].

Four procedural categories—flow measurement, sample collection, sample preservation/storage and laboratory analysis—will introduce uncertainties into measured water quality data [8]. Previous studies have provided valuable knowledge of the uncertainty

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related to sampling and chemical analysis procedures. The Guide to the Expression of Uncertainty in Measurement [9], from the international organization for standardization (ISO), is the standard for the evaluation of measurement uncertainty in metrology. Compatible with the ISO Guide for the expression of uncertainty in measurement, data on fuzzy uncertainty propagation in measurement have been available thanks to fuzzy arithmetic, which is a generalization of interval analysis, yielding both worst-case results and best estimates simultaneously [10]. The Bayesian approach to uncertainty evaluation is put into effect by employing numerical integration techniques [11]. Gerd et al. [12] evaluated measurement uncertainty on the basis of probability density functions (PDFs) using a Monte Carlo method. Chew Gina and Walczyk Thomas [13] also developed a guide to express the uncertainty in measurement by using both the partial derivative approach and the Monte Carlo approach. The Robust analysis of variance is applied [14] to estimate the total measurement uncertainty and to quantify the contributions to the uncertainty that arise from the processes of primary sampling and chemical analysis.

However, few complete error propagation analyses, including all error sources, have been conducted for measured water quality data. The scientific community has not gained an adequate understanding of the uncertainty of measured flow water quality data and has not adequately described the effects of uncertainty on water quality management. Thus, describing the effects of measured water quality data uncertainty on water quality management is particularly important.

The aims of this study were: (1) to evaluate the error of measured flow and water quality data and (2) to evaluate the uncertainty caused by measurement data in the Soil and Water Assessment Tool (SWAT) model.

## 2. Materials and methods

### 2.1. The study site and available data

The upper Daning River watershed, covers an area of 2,027 $km^2$, is located in Wuxi County in the Three Gorges Reservoir Region of China (Fig. 1). The watershed is characterized by a northern subtropical monsoon climate and has an annual mean precipitation of 1,182 mm and an annual mean temperature of 16.6℃. The altitude of the region ranges from 200 to 2,588 m. The primary land uses in the watershed include 12.5% grassland, 25.3% cropland and 61.8% forest. The crops consist of corn, wheat, rice and potatoes. The primary soil types include yellow brown soil, yellow cinnamon soil and purple soil.

Due the lack of measured flow and water quality data in China, only flow, sediment and TP data in the study area were available. Monthly stream flow data from the Wuxi gauge for 2000–2007 and monthly sediment yield data from the Wuxi gauge for 2000–2007 were obtained from the Changjiang Water Resource Commission, China. Monthly TP concentration data from the Wuxi gauge for 2000–2007 were obtained from the Wuxi County Environment Protection Agency.

### 2.2. Uncertainty expression

#### 2.2.1. Error of measured data

Error in the measured data can be introduced in each step of the measurement process. Bed scour/deposition, bank erosion, vegetation changes and deposition changes in channel dimensions are the major sources of uncertainty in measured flow for natural channels. Despite whether manual or automated sampling is used, ignorance of the spatial and temporal variability in constituent concentrations will introduce substantial uncertainties in point sampling at random times and/or locations during flow events. Numerous factors, such as the container's characteristics, the storage environment, chemical preservatives and the filtration methodology, will all influence these physical, chemical and biological processes during the interval between sample collection and analysis. The main potential sources of uncertainty in the laboratory are associated with sample handling, chemical preparation, analytical method and equipment, personal expertise, calibration standards and reference materials.

#### 2.2.2. Root mean square error propagation

The root mean square error propagation method [15] shown in Eq. (1), designed to combine all potential errors and to produce realistic estimates of cumulative uncertainty, was used to estimate the cumulative probable uncertainty for the overall resulting flow and water quality data in this study.

$$\mathrm{PER} = \sqrt{\sum_{i=1}^{n}(E_1^2 + E_2^2 + E_3^2 + \ldots + E_n^2)} \qquad (1)$$

where PER is the probable error range (±%), $n$ is the number of potential error sources, and $E_1, E_2, E_3 \ldots E_n$ is the uncertainty associated with each potential error source (±%).

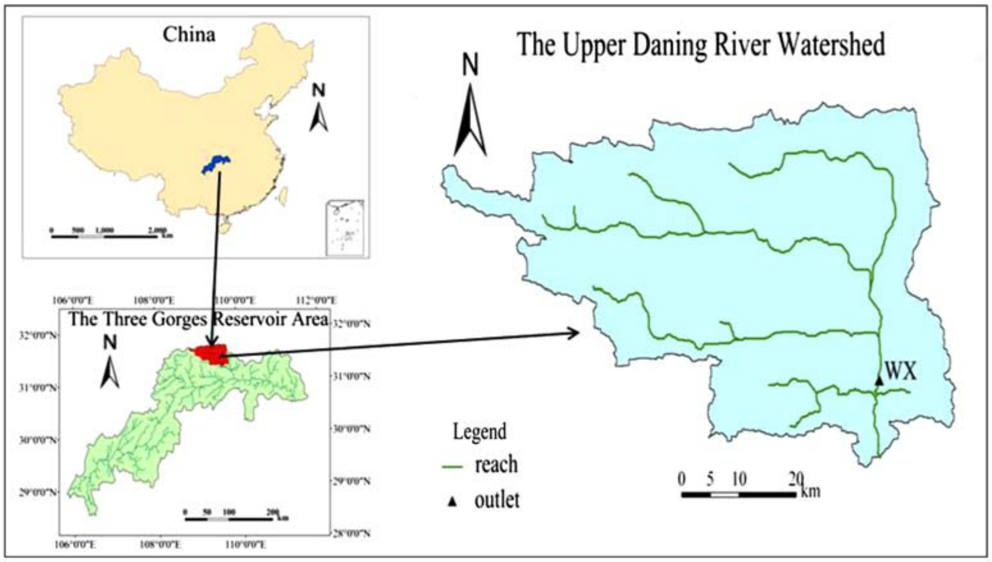


Fig. 1. Location of the Upper Daning River Watershed.

### 2.3. The effect of measurement uncertainty on model evaluation

#### 2.3.1. Effect on output deviations

To more appropriately calculate the deviation between each pair of measured and predicted values based on the measured uncertainty, modification deviations [16] were made to calculate the difference between each pair of measured and modeled values. The modifications are shown in Eq. (2).

$$eu2_i = \frac{CF_i}{0.5} \times (O_i - P_i) \tag{2}$$

where $eu2_i$ is the modified deviation between measured and predicted data, $CF_i$ is the correction factor based on the probability distribution, $O_i$ is the measured data, and $P_i$ is the modeled data.

The uncertainty range of the modeled results can be obtained based on Eq. (2), as Eq. (3) shown. When the modeled result is a uniform distribution, the mean of the modeled results is the observed data, and the uncertainty range is $(O_i - e_i, O_i + e_i)$. For normal distribution modeled results, the confidence range is $(\mu - 3\sigma, \mu + 3\sigma)$ and the confidence level is 0.997.

$$P_i = O_i \pm e_i \tag{3}$$

#### 2.3.2. Effect on error deviation

The SWAT model was calibrated by using the highly efficient Sequential Uncertainty Fitting version-2 (SUFI-2) procedure [17]. The calibration data covered 2004–2007, and data of 2000–2003 were used in the validation period. Two goodness-of-fit indicator values (*Ens* and $R^2$) for the calibration and validation periods are listed in Table 1. The values are all above the suggested lower *Ens* limit of 0.5 [18], which indicates the satisfactory performance of the model.

The Monte Carlo method was selected to provide approximate solutions to a variety of mathematical problems by performing statistical sampling experiments on a computer. Because too many dates needed to be sampled, a Latin Hypercube method was used to obtain 10,000 random samples in the modified uncertainty range of the modeled flow and the sediment and TP results to improve sampling efficiency. Then, the mean simulated value (*M*), standard deviation (SD), 90% confident interval and coefficient of variation (CV) were calculated based on the random sampling in the uncertainty range of the modeled results, which was based on the Monte Carlo

Table 1
The good-of-fit indicator values for calibration and validation period

| Period | Variable | $R^2$ | $E_{NS}$ |
|---|---|---|---|
| Calibration | Flow | 0.79 | 0.66 |
| | Sediment | 0.83 | 0.73 |
| | TP | 0.86 | 0.76 |
| Validation | Flow | 0.95 | 0.89 |
| | Sediment | 0.83 | 0.67 |
| | TP | 0.81 | 0.51 |

method, to characterize the uncertainty of the modeled results.

## 3. Results and discussion

### 3.1. The probable error range of measured flow and water quality data

Due to the limitations of the measured data types in the studied watershed, only the measurement uncertainty intervals of flow, sediment and TP data were calculated in this study. Various "data quality" scenarios (best, typical and worst case) were created for each step in measuring the water quality loads. The classification of scenarios (best, typical and worst) was based on a quality assurance/quality control effort constrained by financial and personal resources and hydrologic conditions. The classification of individual steps in these data quality scenarios was based on professional experience and judgment [19]. Based on the conditions in China, the uncertainty range of the measured water quality data was calculated as the basis of the uncertainty analysis using the SWAT model. Cumulative uncertainties introduced by different sources of error in the best, typical and worst measurement conditions of flow, sediment and TP are shown in Table 2.

For flow, the worst-case scenario involved flow estimation with Manning's equation with a stage-discharge relationship for an unstable, mobile bed and a shifting channel. The typical scenario involved a range of individual run-off measurement techniques, channel types, and channel conditions. The best-case scenario included flow measurement under ideal hydrologic conditions, specifically a pre-calibrated flow control structure (stable bed and channel) and a stilling well for stage measurement. Under these three conditions, the calculated cumulative probable uncertainty (±%) errors were 2, 9 and 36%, respectively.

For sediment and TP, the worst-case scenario involved liberal estimates of error associated with sample collection at a single point, infrequent time-interval sampling at a high minimum flow threshold, and disregard of conditions outside the sampling period. Also involved was unpreserved, unrefrigerated sample storage for 144 h and then refrigerated storage for 48 h prior, with liberal estimates of error for constituents present in very low concentrations to analysis. The typical-case scenario involved moderate errors associated with frequent flow- or time-interval sample collection at a single point and estimation of conditions outside a high flow threshold during sampling. Also involved was refrigerated sample storage for 54 h prior, with moderate error estimates for low constituent concentrations to analysis. The best-case scenario involved conservative error estimates associated with frequent flow- or time-interval sample collection at a single point and estimation of conditions outside a low flow threshold during sampling. Also involved was iced sample storage for 6 h prior, with conservative error estimates for constituents present in moderate concentrations during the analysis period. Under the three conditions, the calculated cumulative probable uncertainty (±%) errors were 2, 16 and 102% for sediment and 2, 26 and 221% for TP, respectively.

Overall, the PER values of flow were the smallest, while TP had the largest PER values, indicating that the reliability of measured flow was much higher than that of the measured pollutants load. The large uncertainty of sediment and nutrient load may be due to the errors of sediment and nutrients coming from both flow measurement and other steps, including sample collection, sample storage and laboratory analysis. The measurement uncertainty of the sediment was lower than that of nutrition because the sediment was more stable than the nutrient loading (especially dissolved nitrogen and phosphorus) without the effect of storage time and storage conditions.

Proceeding from China's actual conditions, there were insufficient funds to obtain the best instruments and professional staff at any monitoring station, so it was difficult to obtain measured data with the best "quality". However, the reliability and accuracy are the baseline of the measurement. If the data quality is out of demand, it is better to do nothing than obtain a set of wrong data. The results of this study indicated a large gap between the typical- and worst-case scenarios, but there was less difference between the typical- and best-case scenarios. Thus, for important stations, such as those for drinking water resources and certain rivers, the best monitoring conditions would be most acceptable; for other sites, if there are insufficient funds, a typical monitoring condition might also be feasible.

Table 2
Cumulative uncertainty, represented by PER, for run-off, sediment and TP for best case, typical case and worst scenarios (±%)

| Scenarios | Run-off | Sediment | Total P |
|---|---|---|---|
| Worst case scenario | 36 | 102 | 221 |
| Typical scenario maximum | 16 | 48 | 95 |
| Typical scenario average | 9 | 16 | 26 |
| Typical scenario minimum | 4 | 5 | 7 |
| Best case scenario | 2 | 2 | 2 |

### 3.2. Effect on SWAT modeling

#### 3.2.1. The modified deviation of measured data

As Eq. (3) shows, the uncertainty interval $(O_i - e_i, O_i + e_i)$ of the model results is available when the observation and correction errors $eu2_i$ are known. Because most of the measured data were normally distributed [16], this study focused on measuring the modified deviation $eu2_i$ of normally distributed measurement data (Fig. 2). The results show that the difference between the modified measurement data and the model results decreased gradually as the PER values increased. The average modified deviation of flow was 18.74, 18.45 and 11.17 $m^3/s$ when the PER was 2, 9 and 36%, respectively, which indicates a better modification effect in the SWAT model for the simulation results of flow.

Because there were less data of measured sediment and TP, only the average results of annual sediment and TP were given (Table 3). The modified deviation change tendency of sediment and TP were the same as flow: all decreased as the PER value increased, indicating that after considering the measurement uncertainty, the model effect improved. Considering China's national conditions and the most common distribution patterns of measured data, the PER values under the typical case (i.e. 9% for flow, 16% for sediment, and 26% for TP) were selected. The modified deviation $eu2_i$ of the measurement data under the normal distribution conditions was selected as the error to calculate the uncertainty values.

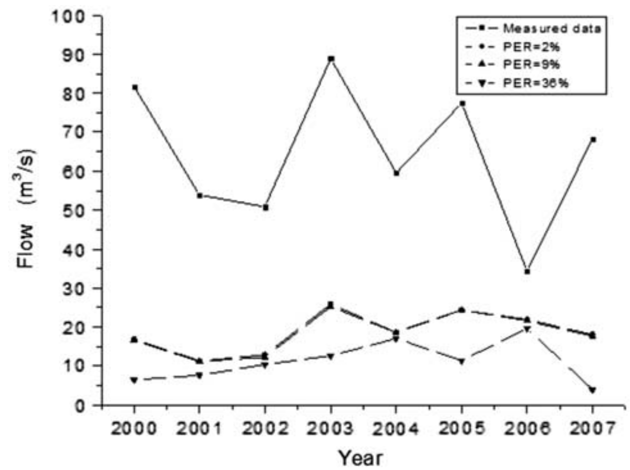

Fig. 2. Modified $eu2_i$ of measured flow.

#### 3.2.2. Expression of measurement uncertainty

The statistical results of the 10,000 samples under the uniform and normal distribution conditions were calculated (Fig. 3). The average range of flow was from 34.36 (2006) to 89.22 $m^3/s$ (2003) under the uniform distribution condition and was from 34.42 (2006) to 89.28 $m^3/s$ (2003) under the normal distribution. There was little difference between the average simulated flow data of different distribution patterns. However, when the data were normally distributed, the standard deviation and CV values were 6.10 $m^3/s$ and 0.101, respectively, both lower than those under the uniform distribution, which was 10.68 $m^3/s$ and 0.178, respectively. This result indicates that the uncertainty of the normally distributed data was less than that of the uniformly distributed data.

To characterize the uncertainty range of the flow model results, the 5th percentile of the 10,000 samples of flow data was selected as the lower limit of the 90% confidence interval, and the 95th percentile was the upper limit (Table 4). There was a narrower uncertainty range of the normally distributed simulated flow data than the uniformly distributed data. The confidence interval width was closely related to the flow values. The largest confidence interval width was from 2003, which also had the largest simulated flow, with 44.68 $m^3/s$ under the uniform distribution condition and 27.14 $m^3/s$ under the normal distribution condition. In 2001, the flow was the smallest and the confidence interval was the narrowest, at 20.39 $m^3/s$ under the uniform distribution condition and 11.90 $m^3/s$ under the normal distribution condition.

The statistical results (mean value, standard deviation, CV values, and 90% confidence interval) of the 10,000 samples for sediment and TP under the uniform distribution and normal distribution conditions were calculated (Table 5). There was no large difference of average sediment values between the uniform distribution and normal distribution, at 283.65 and 280.34 Kt, respectively. However, the standard deviation value (50.70 tons) and CV value (0.181) under the normal distribution were both less than under the uniform distribution condition, at 85.34 tons and 0.301, respectively. In addition, the mean value, standard deviation, CV value and confidence interval of the TP had the same change tendency as the flow and sediment. The main reason for this result is that there was a larger confidence interval in the normally distributed data than in the uniformly distributed data. When the modified deviation was used to calculate the difference of deviation between the measured and modeled data, the difference was less for the normally distributed data, resulting in narrower CV, mean and standard deviation values.

Overall, the average CV value of the sediment was the largest, followed by TP. The CV value of flow was

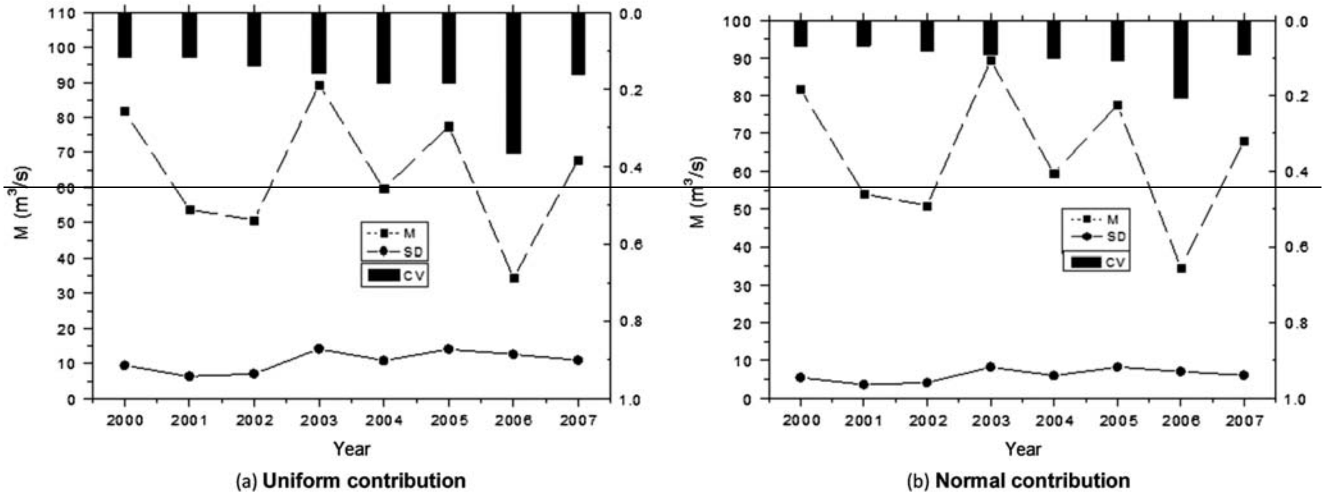


Fig. 3. CV value, Mean, and SD values of uncertainty analysis for flow data.

Table 3
Modified $eu2_i$ of measured sediment and TP

| Sediment ($10^3$ t) | | | | TP (t) | | | |
|---|---|---|---|---|---|---|---|
| Measured data | PER | | | Measured data | PER | | |
| | 2% | 16% | 102% | | 2% | 26% | 221% |
| 281.64 | 153.46 | 150.35 | 146.44 | 22.39 | 11.13 | 10.88 | 8.23 |

Table 4
90% confidence interval of runoff

| Time | Uniform distribution | | Normal distribution | |
|---|---|---|---|---|
| | 5% percentile | 95% percentile | 5% percentile | 95% percentile |
| 2000 | 66.96 | 96.51 | 73.05 | 90.78 |
| 2001 | 43.59 | 63.98 | 48.12 | 60.02 |
| 2002 | 39.88 | 61.97 | 44.10 | 57.54 |
| 2003 | 66.96 | 111.64 | 75.52 | 102.66 |
| 2004 | 42.61 | 76.18 | 49.49 | 68.95 |
| 2005 | 55.12 | 99.50 | 64.65 | 90.71 |
| 2006 | 14.45 | 53.56 | 22.40 | 46.52 |
| 2007 | 50.83 | 85.74 | 57.66 | 77.82 |
| Average | 47.55 | 81.13 | 54.37 | 74.37 |

Table 5
Uncertainty analysis for sediment and TP data

| | Distribution | *M* | SD | CV | 90% confidence interval | |
|---|---|---|---|---|---|---|
| | | | | | 5% lower limit | 95% upper limit |
| Sediment | Uniform | 283.65 | 85.34 | 0.301 | 149.12 | 416.63 |
| ($10^3$t) | Normal | 280.34 | 50.70 | 0.181 | 194.79 | 364.15 |
| TP | Uniform | 22.24 | 6.31 | 0.284 | 12.58 | 32.29 |
| (t) | Normal | 22.41 | 3.60 | 0.161 | 16.55 | 28.45 |

the smallest, indicating that the measurement uncertainty of the sediment had the greatest effect on the simulation result, followed by TP. The measurement uncertainty of flow had the least impact on the simulation result.

## 4. Conclusions

This study found that the PER values of flow were the smallest, while TP had the largest PER values. The simulated results with a normal distribution had less uncertainty under the same PER condition. When the PER values were under the average typical-scenario, the modified deviation values were $18.45\,m^3/s$ for flow, $150.35\times10^3$ t for sediment, and 10.88 t for TP. The CV values of the multiple sampling results within the uncertainty range were 0.101 for flow, 0.181 for sediment, and 0.161 for TP. When the monitoring data fell within a uniform distribution, the simulated results of M, MD and CV values for sediment and TP were both larger than the date, which fell into the normal distribution.

Overall, this article studied the impacts of uncertainty on simulated results from measurement errors in SWAT model response data by introducing the PER value. The results showed that the reliability of the measured flow was much higher than that of the measured pollutants load, and uncertainties in the simulated sediment and TP data errors were greater than those of flow. The results presented could assist the water resource community in assessing the uncertainty of measured data for use in water quality management.

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