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Parameter uncertainty analysis in watershed total phosphorus modeling using the GLUE methodology

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ABSTRACT

Deterministic watershed models are frequently used for agricultural non-point source (NPS) pollution simulations. However, parameter uncertainty should be analyzed before the modeling results are used to make decisions regarding watershed NPS pollution control programs. In this study, the Soil and Water Assessment Tool (SWAT) was used to simulate the total phosphorus (TP) loads caused by NPS pollution in the upper Daning River Watershed in China's Three Gorges Reservoir Area. The Generalized Likelihood Uncertainty Estimation (GLUE) methodology was used to analyze the parameter uncertainty in SWAT modeling. The impacts of three subjective options of GLUE, the parameter ranges, the level of confidence, and the threshold value of the likelihood measure, on the parameter uncertainty analysis results were analyzed. Specifically, we investigated if there was a combination of these factors that was most appropriate for expression of the uncertainty assessment results. The results indicated that the "observed data" may not always lie within the confidence intervals of GLUE, so the confidence interval was not sufficient to represent the uncertainty for the specific requirements of this study. Therefore we suggest there should be alternative measures to express the parameter uncertainty of GLUE.

1. Introduction

Agricultural non-point source (NPS) pollution contributes in a major way to the water quality of aquatic systems in most cases. Excess nutrients (phosphorus and nitrogen) that run off from land into water may cause eutrophication and thus impact aquatic ecology. Accordingly, water pollution control programs are often established to control NPS pollution. To achieve management objectives, the NPS pollution loads should first be assessed to obtain a baseline scenario. Such assessments are conducted using deterministic watershed models, which are practical to examine the impacts of changing agricultural management operations on the NPS pollution.

There are many conceptual and physical parameters in the watershed models. The conceptual parameters are determined by calibration. Some of the physical parameters vary greatly across spatial and temporal scales, and they are constrained by measurement devices and methods; therefore, they may not be feasibly assigned to particular values and hence also have to be determined by calibration. Accordingly, parameter uncertainty is inevitable in modeling and should be assessed before the simulation results are used in the decision making process.

Sensitivity analysis (Van Griensven et al., 2006; Arabi et al., 2007), first-order error analysis (Melching and Yoon, 1996; Shen et al., 2008), the Monte Carlo method (Migliaccio and Chaubey, 2008; Sun et al., 2008), the Bootstrap method (Efron, 1979; Li et al., 2010; Selle and Hannah, 2010), the Bayesian approach (Bayes, 1763; Freni and Mannina, 2010), and the Generalized Likelihood Uncertainty Estimation method (GLUE) (Beven and Binley, 1992; Beven and Freer, 2001; Freni et al., 2008) are commonly used for parameter uncertainty analysis. However, parameters with high sensitivity and low uncertainty may have less influences on the final results of such analyses than parameters with low sensitivity and high uncertainty (Melching and Bauwens, 2001). Hence, advanced uncertainty research should be conducted following sensitivity analysis. The first-order error analysis method assumes that there is a linear relationship between output and input, which makes it unsuitable for complex models with non-linear structures (Melching and Yoon, 1996). The Monte Carlo method is inefficient because it requires a great deal of computational time for repeated model runs. The advantage of the Bootstrap method is its simplicity in implementation, which means it can be applied with the use of existing computer programs (Li et al., 2010). It involves relatively few assumptions while guaranteeing a relevant error distribution that is taken directly from the data (or model residuals) (Selle

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and Hannah, 2010). The Bayesian approach has a rigorous theoretical framework and the possibility of evaluating the impact of new knowledge on model parameter estimates. Nevertheless, the Bayesian approach relies on some hypotheses that have to be carefully analyzed and the selection of prior parameter distributions that are usually not obtained from physical observations may prevent Bayesian approaches from being objective (Freni and Mannina, 2010).

Sensitivity analysis, first-order error analysis, and the Monte Carlo method are generally used to assess the uncertainties associated with individual parameters. However, in the GLUE methodology, the parameter set, and not individual parameters, determines the performance of the model (Beven and Binley, 1992). Additionally, different parameter sets may result in similar predictions in a phenomenon known as equifinality. Based on the concept of equifinality, GLUE focuses on parameter sets rather than on the behavior of individual parameters and their interactions. The parameter interactions and non-linearities can be handled implicitly in the GLUE methodology through the likelihood measure (Vázquez et al., 2009). Furthermore, GLUE is a simple concept and is relatively easy to implement. Therefore, GLUE is used in this study for parameter uncertainty analysis.

However, there are a few subjective options in an application of the GLUE methodology, such as the parameter ranges, the level of confidence, and the threshold value of the likelihood measure (Blasone et al., 2008; Jin et al., 2010); and these have impacts on the parameter uncertainty analysis results. Moreover, the observed data may not always lie within the confidence intervals of GLUE (Montanari, 2005; Beven, 2006; Xiong and O'Connor, 2008), which results in the confidence interval not being able to represent all the uncertainty of specific variables. Accordingly, this study was conducted to assess the parameter uncertainty in watershed total phosphorus (TP) modeling using the GLUE methodology while analyzing the influences of the three aforementioned subjective options and the uncertainty expression of GLUE.

2. Materials and methods

2.1. Study area and data

Previously we conducted NPS pollution modeling work and individual parameter uncertainty analysis for the drainage area controlled by the Wuxi hydrological gauge (WX) on the Daning River (Shen et al., 2008). In the present study, a larger area in the Daning River Watershed defined by the boundary of Wuxi County and its downriver county was selected (Fig. 1). This area is located in Wuxi County in the Three Gorges Reservoir Area of China and covers an area of 2421 km^2. The area is characterized by the north subtropical monsoon climate and has an annual mean precipitation of 1182 mm. The altitude of this region ranges from 200 to 2605 m and the primary land uses in the watershed include forest, arable land, and pasture. The primary soil types are yellow brown soil, yellow cinnamon soil and purple soil.

Because phosphorus has been identified as the limiting factor of eutrophication in most tributaries of the Three Gorges Reservoir Area, TP was evaluated in this study. Monthly stream flow data from the Ningqiao (NQ) gauge for 2000–2004, the Ningchang (NC) gauge for 2000–2007, and the Wuxi (WX) gauge for 2000–2007, as well as monthly sediment yield data for the WX gauge for 2000–2007, were collected from Changjiang Water Resources Commission, China. Monthly TP concentration data from the WX gauge and the confluence point of Daning and Baiyang Rivers (CF) for 2000–2007 were collected from Wuxi County Environmental Protection Agency.

Table 1
The observed data used in calibration and validation.

Variable	Gauge	Calibration	Validation	Time step
Stream flow	NQ	2004–2005	2000–2003	Monthly
	NC	2004–2007	2000–2003	Monthly
	WX	2004–2007	2000–2003	Monthly
Sediment	WX	2004–2007	2000–2003	Monthly
TP	WX	2004–2007	–	Monthly
	CF	–	2001–2007	Monthly

2.2. Watershed model and calibration technique

The Soil and Water Assessment Tool (SWAT, version ArcSWAT 2.1.1 beta) was used in this study. SWAT is a process-based distributed-parameter simulation model that operates on a daily step that was developed to predict the impact of land management practices on water, sediment and agricultural chemical yields in large complex watersheds with varying land uses, soil types and management conditions over long periods (Arnold et al., 1998; Neitsch et al., 2005).

Since the study area was different from the one in our earlier study, the SWAT model was re-calibrated and validated using the highly efficient Sequential Uncertainty Fitting version-2 (SUFI-2) procedure (Abbaspour et al., 2007). This calibration method is an inverse optimization approach that uses the Latin hypercube sampling procedure along with a global search algorithm to examine the behavior of objective functions. Parameterization is applied to a parameter set rather than to individual parameters. The initial parameter ranges can be updated for every iteration, and the recommended new parameter ranges are always centered on the current best estimate (Abbaspour et al., 2004). The procedure has been incorporated into the SWAT-CUP software, which can be downloaded for free from the Eawag website (Abbaspour, 2009).

The Nash–Sutcliffe efficiency values (E_{NS}) was used to assess the SWAT performances. E_{NS} is expressed as (Nash and Sutcliffe, 1970):

$$E_{NS} = 1 - \frac{\sum_{i=1}^{n}(O_i - P_i)^2}{\sum_{i=1}^{n}(O_i - \bar{O})^2} \quad (1)$$

where O_i and P_i are the observed and simulated values for the ith pair, $\bar{O}$ is the mean of the observed values, and n is the total number of paired values. The range of the E_{NS} value is from ∞ to 1, with 1 indicating a perfect fit.

SWAT outputs were summarized on a monthly step in this study. The observed monthly data available for calibration and validation are listed in Table 1. Because there were relatively more TP data for 2004–2007, this period was used for calibration for all variables.

2.3. GLUE analysis

The GLUE methodology (Beven and Binley, 1992) was used for uncertainty assessment in the present study. The GLUE framework is not a parameter optimization tool since it is based on the use of multiple acceptable models for estimation of the prediction uncertainties generated from Monte Carlo simulations using different parameter sets (Dean et al., 2009). This methodology is grounded on a conception that conflicts with the model calibration procedures, such as the one applied in this study, that strives to derive a single best optimal parameter set to satisfy a user-defined fitness function. However, the goal of parameter calibration and validation was to obtain a parameter set that could yield relatively acceptable stream flow, sediment and TP loads information. The parameter set was used as the base-case parameters for the uncertainty analysis.

For application of the GLUE methodology, the model was implemented by randomly sampled parameter sets throughout the