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Uncertainty assessment of deterministic water quality model for a combined sewer system with the GLUE method

Wei Zhang, Tian Li*, Meihong Dai

State Key Laboratory of Pollution Control and Resource Reuse, Tongji University, 200092 Shanghai, China, Tel./Fax: +86 21 65987355; email: weizhang021@163.com (W. Zhang), Tel./Fax: +86 21 65988421; email: tianli@tongji.edu.cn (T. Li), Tel./Fax: +86 21 65987355; email: meihongdai2012@126.com (M. Dai)

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ABSTRACT

Water quality modeling of the urban drainage system is critical to the assessment of discharged pollutant loads and development of drainage system management. Here, application of water quality modeling to a combined sewer system on a complex network scale in Shanghai, China is presented. The uncertainty of the water quality parameters used in pollutant buildup, wash-off, and sewer sediment erosion/deposition models was assessed based on a well-calibrated water quantity model using the generalized likelihood uncertainty estimation (GLUE) method. Moreover, the influences of a single objective function and a multi-objective function on identification of water quality parameters within the GLUE method were discussed. The identification of water quality parameters was improved and the prediction uncertainty band was reduced when the multi-objective function approach was used. The multi-objective function approach is an effective alternative method to parameter identification and uncertainty analysis that will be useful to similar studies and applications into water quality modeling of combined sewer systems.

Keywords: Water quality modeling; Combined sewer system; Sewer sediment; Pollutant buildup and wash-off; Uncertainty analysis; Generalized likelihood uncertainty estimation (GLUE)

1. Introduction

Water quality modeling of the urban drainage system is critical to assessment of discharged pollutant loads and development of drainage system management. Pollutant transportation processes in urban drainage systems are complex and dependent on system-specific circumstances. Water quality modeling of separate storm sewer systems has been used for many years [1,2]. However, the large uncertainty of model inputs, parameters, and structures makes generalization of water quality modeling of stormwater systems difficult to implement [3]. Moreover, the processes in combined sewer systems are more complex. Water quality models have been developed to describe the general behavior of a system; however, the actual physical, chemical, and biological processes in different sewer systems cannot be expressed accurately and completely with a universal and simple mathematical model [4].

Most studies of sewer sediment have been conducted using conceptual models, modeling theory, laboratory pilots, and system performance assessments

*Corresponding author.

based on site monitoring [5–8]. Previous studies have provided a basis for improved sewer system water quality modeling while also identifying gaps in knowledge that need to be filled [9]. Some full-scale studies and field experiments of sewer sediment modeling have been reported [10–12]. However, these studies focused on individual sewer sections, trunk sewer sections, or subsystems in a combined sewer system, not a complex sewer network, and the performance of water quality modeling in full-scale sewer networks has rarely been studied.

Several classic sediment erosion/deposition models have been incorporated into popular commercial models such as Infoworks CS/ICM, MOUSE/Mike Urban, MUSIC, and XPSWMM, as well as into some simpler conceptual models as proposed in previous studies [13,14]. The sewer sediment modules in the commercial models are usually modified and improved with the development of knowledge of sewer sediment. These deterministic hydraulic models coupled with the sewer sediment models provide an easily implementable or alternative approach to assess the water quality performance of urban drainage systems. However, the reliability of prediction and performance of these deterministic models needs to be discussed.

As reported in previous studies, the water quality modeling of a sewer system is dependent on site-specific conditions and generally produces results with low confidence [15]. Each model established by this approach must be adapted to site-specific conditions based on calibration of the measurement data. However, parameter identification is not easy to accomplish when there are larger numbers or correlations among the parameters [16]. Given the lack of confidence in the current prediction, it would be useful to provide sewer system operators with methods for predicting water quality, as well as estimating the levels of uncertainty associated with the prediction [17]. Uncertainty analysis of the deterministic water quality model with the Bayesian or non-Bayesian approach, which is also known as the "probabilistic shell" [17], provides an alternative method by which to accomplish this process.

The Bayesian method is a common approach used in uncertainty analysis of environmental models [18–22]. The generalized likelihood uncertainty estimation (GLUE) methodology based on the theory of equifinality [23] has been shown to be effective at quantitative evaluation of uncertainty in urban drainage models [20,24]. Equifinality here means that multiple parameter sets may lead to equally acceptable simulation results. The uncertainty estimation of stormwater quality and quantity models with the GLUE method has been thoroughly investigated [14,20,24–29]. In these studies, stormwater quality models were analyzed independently, as well as discussed as components of an integrated urban water quality model. Although the GLUE method has been applied to water quality modeling of combined sewer systems, most water quality models used in these studies were simple models [13,30,31]. The high computing cost needed for simulation of dry weather periods is one of obstacles to implementing uncertainty assessments of detailed deterministic water quality models for combined sewer systems [15].

Because of the large computing cost required to implement the probabilistic method, a response database method is used in sewer sediment modeling [15,17]. The computing cost of this method is lower than that of the GLUE method; however, there are some drawbacks to the response data method, such as the linear assumption of the function between any two values in the response database [17].

Different uncertainty techniques in urban stormwater quantity and quality modeling were compared by Dotto et al. [14], who found that identification of the most appropriate method for uncertainty estimation is a trade-off between the need for a strong theory-based description of uncertainty, simplicity, and computing cost [14]. Although there is some degree of subjectivity involved in the GLUE method, it is advantageous in that it is able to assess the uncertainty associated with complex models, such as water quality models of combined sewer systems. This is because prior knowledge is not needed for this method. For these reasons, the GLUE method was adopted for uncertainty analysis in this study.

We applied Infoworks CS to a combined sewer system located in a highly urbanized catchment in Shanghai, China. Uncertainty of the water quality modeling was assessed by the GLUE method based on a well-calibrated water quantity model. A comprehensive monitoring campaign was carried out from April through October for both 2012 and 2013. The study objectives were to: (1) estimate the uncertainty associated with water quality prediction of a combined sewer system by a deterministic model on a complex network scale and (2) gather insight into parameter identification of a water quality model of a combined sewer system. Overall, the results presented herein provide a basis for future research and application to water quality modeling of combined sewer systems.

2. Materials and methods

2.1. Experimental sites

This study was applied to the Anshan combined sewer system, which is located in a highly urbanized residential district in the downtown area of Shanghai. The combined sewer network is independent from the surrounding sewer systems. The climatology of Shanghai is characterized by an average annual rainfall of 1,180 mm, most of which occurs during the period from May to October.

The catchment area is 130 ha, and the sewer system serves 48,100 inhabitants. The sewer is characterized by circular and oval pipes with maximum dimensions of 2,400 mm. The monitored Anshan system is a pump lifting combined sewer system. The pump station has four stormwater lifting pumps and four interception pumps. The nameplate flow of the two stormwater lifting pumps is 2.8 m^3/s, while that of the other two is 2.3 m^3/s. The nameplate flow of the two interception pumps is 0.41 m^3/s, while that of the other two is 0.28 m^3/s.

2.2. Field sampling and testing

Rainfall was monitored using a 0.1-mm tipping bucket rain gauge located in the Anshan catchment. The dry/wet weather flow and water level data were obtained from the supervisory control and data acquisition system of the pump station.

Water samples were collected continuously with an automated sampler (ISCO 6,712, ISCO Inc., NE, USA) at the outlet of the combined sewer system. The automatic sampler was programmed to collect a 1,000 ml sample at a time interval of 15–20 min during wet weather flow, as well as a 1,000 ml sample at a time interval of 120 min during dry weather flow. All samples were transported to the laboratory for analysis of total suspended solids (TSS) using standard methods [32].

Field sampling was performed from April to October in both 2012 and 2013, and 14 rainfall events were monitored for water quality and quantity [33]. Table 1 presents the characteristics of the monitored events.

To help determine appropriate sewer sediment parameters, a measurement campaign was carried out in this catchment in May 2012. During the campaign, sewer sediment was collected from 10 sites throughout the catchment. Sediment characteristics such as sediment surface level, grain size distribution, and grain density were collected and analyzed. The monitoring campaign of the water quality and quantity for dry/wet weather flow and the sewer sediment was used for model calibration and uncertainty analysis.

2.3. Model and water quality parameters

The Infoworks CS software package (v11.0 Wallingford software, UK), which is one of most popular deterministic commercial models for water quality and quantity modeling of urban drainage systems, was used in this study. The build up of sediment in the network and movement of sediment and pollutants through the drainage system during a rainfall event could be implemented by water quality modeling in Infoworks CS. The water quality model involves a separate calculation process that effectively occurs in parallel with the hydraulic modeling calculations. In fact, the hydraulic calculations are made before the water quality calculations at each time step.

To implement the water quality modeling of a combined sewer system, an initialization stage simulation, which is a dry weather flow simulation for reaching a steady state of the network, was conducted.

The surface buildup equation determines the mass of sediment buildup on the surface of the catchment after the buildup period at the start of a simulation or at the end of each time step [34].

$$M_0 = M_d e^{-K_1 NJ} + \frac{P_s}{K_1}(1 - e^{-K_1 NJ}) \quad (1)$$

where M_0 is the mass of sediment after the buildup period, or the projected mass of sediment at the end of the time step (kg/ha); M_d is the initial mass of sediment (kg/ha); K_1 is the buildup decay factor (d^{-1}); NJ (d) is the time step length, or the buildup period at the start of the simulation; P_s is the surface buildup factor (kg/ha d).

The surface wash-off equation determines the sediment deposits left on the catchment surface and washed off into the drainage system during a simulation.

$$\frac{dM_e}{dt} = K_a M(t) - f(t) \quad (2)$$

$$M_e(t) = Kf(t) \quad (3)$$

$$K_a(t) = C_1 i(t)^{C_2} - C_3 i(t) \quad (4)$$

where $M(t)$ is the mass of surface-deposit pollution (kg/ha); K_a is the erosion/dissolution factor related to rainfall intensity (1/s); $M_e(t)$is the mass of pollutant dissolved or in suspension (kg/ha); $f(t)$ is the pollutant flow (kg/(ha·s)); K is the linear reservoir coefficient (s); $K_a(t)$ is the rainfall erosion coefficient; $i(t)$ is the effective rainfall in m/s; C_1, C_2 and C_3 are rainfall erosion calibration coefficients; and t is time.

The Ackers–White Model [35,36], which is one of most common sewer sediment erosion and deposition models [37–39], was used for water quality modeling of sewer sediment erosion and deposition in this study.

Table 1
Characteristics of rainfall events monitored during 2012–2013 (n = 14)

Name (unit)	Depth (mm)	Duration (min)	Mean intensity (mm/h)	Max. intensity (mm/h)	ADP[a] (d)
Minimum	15.6	50.0	2.2	28.8	2.0
Median	37.9	302.5	8.3	66.6	5.5
Maximum	140.4	1,635.0	30.8	129.6	21.0
Mean	46.6	493.2	9.8	74.2	7.7
Standard Deviation	34.4	491.5	7.7	29.9	6.5

[a]Antecedent dry period.

2.4. GLUE methodology

This study employed the GLUE methodology to assess the uncertainty of water quality parameters in the Infoworks CS. This method is popular because it does not require detailed distribution functions for the observed variables or errors when the explicative models provided are complex or highly parameterized [14,25]. For urban drainage system modeling, 20–40% of the total uncertainty in prediction was due to the uncertainty in flow quantity modeling, including the rainfall input uncertainty, whereas 80–60% was due to the uncertainty associated with the water quality sub-model [15]. Dotto et al. reported that the uncertainty associated with the sewer water quality model was one order of magnitude higher than that of the quantity model [14]. In the present study, the uncertainty associated with the water quantity model was ignored. The water quantity parameters of the combined sewer system model were calibrated and validated based on 14 rainfall events with variable characteristics (Table 1). The results showed that the goodness of fit between the simulated outputs and observed values met the general requirements of urban drainage hydraulic modeling. The calibrated model was used in the uncertainty analysis of water quality parameters.

The sensitivity for all water quality parameters of pollutant buildup, wash-off, and sewer sediment erosion/deposition sub-models was analyzed, and seven water quality parameters were selected for use in the uncertainty analysis (Table 2). Furthermore, a primary manual calibration of these parameters was carried out to determine a relatively appropriate variation range (Table 2). The primary analysis would be conductive to obtaining a better result of uncertainty analysis with a relatively low-computing cost. However, too narrow a variation range should be avoided because it may not contain the possible optimal parameter sets, and the observed data may fall outside the uncertainty band obtained by uncertainty analysis.

Uncertainty analysis of the water quality parameters was performed in strict accordance with the GLUE framework provided by Beven and Binley [23]. Three single objective functions (*NS* efficiency index, percent bias (*BIAS*), and root mean square error (*RMSE*)) and a multi-objective function that combined the first three functions and corresponding acceptability thresholds were applied separately within the GLUE methodology. These three single objective functions are shown in Eqs. (5)–(7). A threshold level of 0.0 was determined for the *NS* efficiency index; the best 10% rule was used for the *RMSE*; and a relative error <20% was used for *BIAS*. The acceptability thresholds were applied in both the single objective and multi-objective functions. A multi-objective function combining three single functions and the corresponding acceptability thresholds defined as $\{P(NS) \mid NS > 0.0\} \cap \{P(BIAS\%) \mid -20\% < BIAS\% < 20\%\} \cap \{P(RMSE) \mid RMSE \in \text{the best } 10\%\}$, and $P(NS)$, $P(BIAS\%)$ and $P(RMSE)$ are posterior parameter sets observed from objective function *NS*, *BIAS* and *RMSE*.

$$NS = 1 - \frac{\sum_{t=1}^{n} (L_{obs}^t - L_{sim}^t)^2}{\sum_{t=1}^{n} (L_{obs}^t - \overline{L_{obs}})^2} \tag{5}$$

$$BIAS\% = \frac{\sum_{t=1}^{n} (L_{obs}^t - L_{sim}^t)}{\sum_{t=1}^{n} L_{obs}^t} \tag{6}$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{t=1}^{n} (L_{sim}^t - L_{obs}^t)^2} \tag{7}$$

where L_{sim}^t is the simulated value at time t, L_{obs}^t is the observed value at time t, n is the total number of time steps, and $\overline{L_{obs}}$ is the mean of the observed value.

Taking the objective function *NS* as an example, the *NS* of each simulation with parameter sets obtained by Monte Carlo sampling from the parameter range with uniform distribution was calculated. If this value is higher than the acceptability threshold ($NS = 0.0$), the model simulation is regarded as "behavioral" and used for subsequent analysis, otherwise, it is regarded as "non-behavioral" and rejected. Furthermore, the cumulative likelihood distributions of water

Table 2
Parameter variation ranges used in uncertainty analysis

	Parameter	Symbol	Unit	Range
Build-up model	Build-up decay factor	K_1	d^{-1}	0.01–0.15
	Buildup Factor	P_s	kg/ha d	5–40
Wash-off model	Rainfall erosion coefficient 1	C_1	–	5×10^7–5×10^8
	Rainfall erosion coefficient 2	C_2	–	1.9–2.1
	Rainfall erosion coefficient 3	C_3	–	15–60
Sediment erosion/deposition	Sediment D50	D_{50}	mm	0.01–0.08
	Specific gravity	Sg	1	1.1–2.2

quality parameters and the uncertainty band of model outputs can be obtained based on these behavioral simulations.

3. Results and discussion

A rainfall event on September 13, 2013, was selected as an example for the uncertainty analysis of water quality parameters. Selection of the particular rainfall event for this analysis was made based on the characteristics of the combined sewer overflow; specifically, the event overflow duration, event overflow volume, event mean flow rate, and event maximum flow rate. The characteristics of the rainfall event selected were similar to the average values of the 14 rainfall events monitored. The depth of the selected rainfall event was 86.9 mm over 585 min, and the antecedent dry period (ADP) was approximately 16 d. The following discussion is based on the September 13 event, although similar trends were observed for other rainfall events.

To discuss the uncertainty of the water quality parameters, the normal objective function (the *NS* efficiency index) was used within the GLUE framework with an acceptability threshold of $NS = 0.0$ [20,40]. The results indicated that the proportion of behavioral simulation was relatively low. When a higher acceptability threshold was used, e.g. $NS = 0.3$, the model did not return a sufficient number of behavioral parameter sets (<1% behavioral). Additionally, the average *NS* value of these behavioral simulations was around 0.2, which was generally lower than the *NS* values in stormwater quality models [14,26,40]. This is because the water quality model of the combined sewer system is more complicated than the stormwater quality model owing to the influence of sewer sediment and dry weather flow.

According to the GLUE approach, 5 and 95% cumulative likelihood distributions were calculated. The cumulative likelihood distributions of the water quality parameters K_1, P_s, C_1, C_2, C_3, D_{50}, and Sg obtained by the GLUE methodology are shown in Fig. 1.

As shown in Fig. 1, none of the water quality parameters, except the pollutant buildup parameter P_s, were identified well by the GLUE method with the objective function of $NS = 0.0$. When a single objective function (e.g. the *NS* efficiency index) was used, some parameters could not be easily identified within the GLUE methodology. The objective function selection could be an important factor that influences the results of an uncertainty analysis [41]. This is because a single objective function could emphasize only certain characteristics of an observed time series.

In this study, the GLUE approach was also applied using different single objective functions with corresponding acceptability thresholds, including *RMSE* and *BIAS*. The cumulative likelihood distributions of water quality parameters obtained by the GLUE with objective functions *RMSE* and *BIAS* are shown in Fig. 1. The results indicated that, with the exception of parameter D_{50}, identification of the water quality parameters was not significantly improved when different single objective function was used. This is because the objective function *RMSE* and *BIAS* emphasizes certain characteristics of the observed time series, while ignoring other characteristics that the objective function *NS* emphasizes [42,43].

To improve identification of water quality parameters, a multi-objective function that was a combination of three objective functions, *NS*, *RMSE* and *BIAS*, with corresponding acceptability thresholds was applied. The results are also illustrated in Fig. 1. When the multi-objective function was used, most of the water quality parameters were easily identified by the GLUE method. Moreover, identification of parameters was significantly improved, and was much better than identification of each individual objective function. Additionally, the computing cost was not obviously increased when the multi-objective function was usedbecause the acceptability thresholds of each

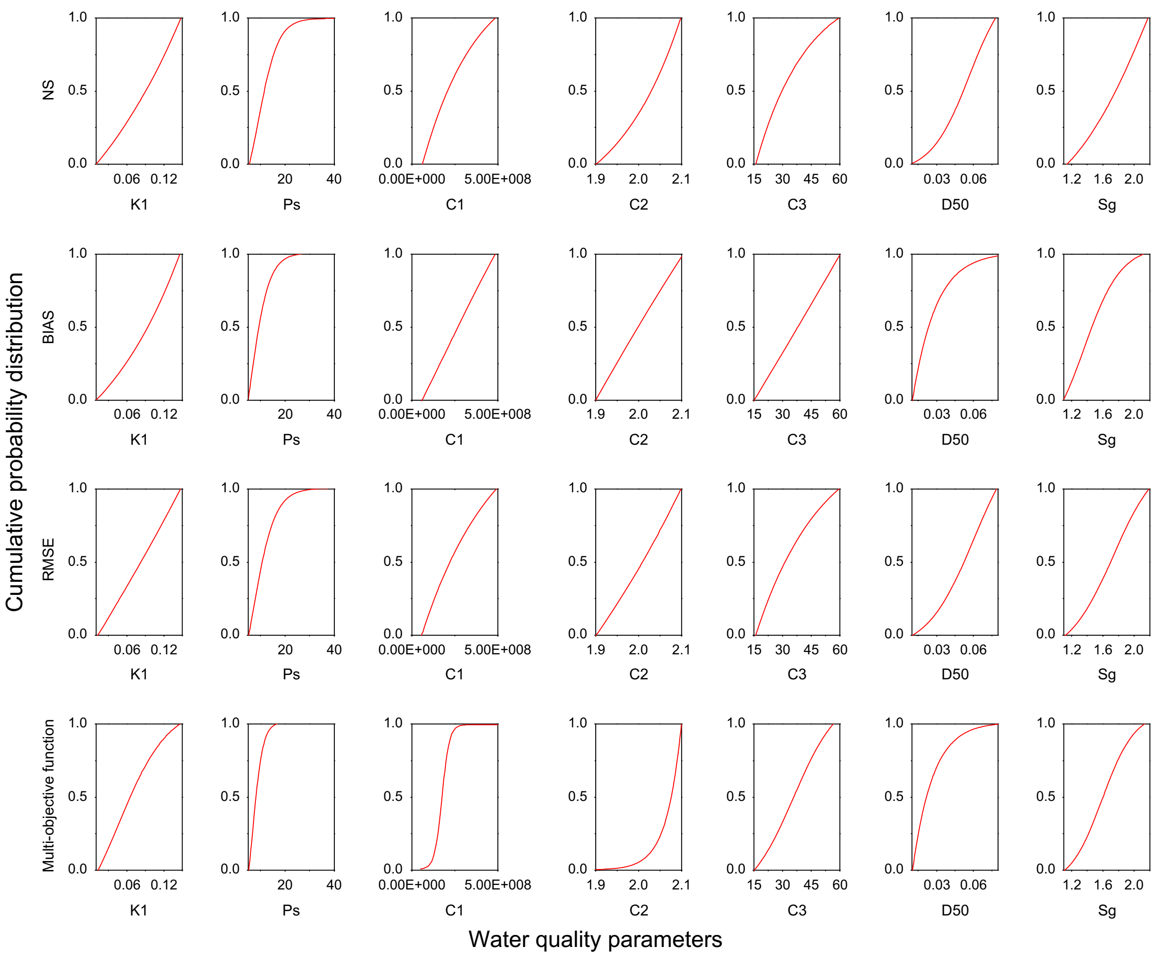

Fig. 1. Cumulative probability distributions of water quality parameters with different single objective functions and the multi-objective function.

component (*NS*, *RMSE* and *BIAS*) in this multi-objective function were relatively low.

The sensitivities of parameters to model output (TSS pollutograph) were observed by the cumulative probability distributions (Fig. 1). The results obtained by the multi-objective function were used to discuss the sensitivity of water quality parameters. The pollutant buildup parameter P_s, the pollutant wash-off parameters C_1 and C_2, and the sediment parameter D_{50} were more sensitive to the model outputs than other parameters. Moreover, the uncertainty of parameters in the sediment erosion/deposition model (e.g. grain size parameter, D_{50}) had an obvious influence on the overall uncertainty associated with model outputs of water quality modeling for the combined sewer system.

The uncertainty bands of the TSS-simulated hydrographs at the system outlet were obtained via the GLUE approach. The uncertainty bands (5–95%) obtained from three single objective functions and the multi-objective function are shown in Fig. 2.

As shown in Fig. 2, almost all of the observed data fell within the uncertainty band for the results obtained by the three single objective functions. These findings indicated that the obtained parameter values accurately predicted the rainfall event. Although there were some differences, the three uncertainty bands obtained by the three single objective functions appeared to be similar. When the multi-objective function was used, the uncertainty band was significantly narrower than the bands obtained from three single objective functions. However, some observed data, including the peak value, fell outside the uncertainty band. Accordingly, it is important to check the consistency of the model hypotheses by comparing the observed data to that of an uncertainty band with a confidence level equal to 0.1 when the multi-objective function is used.

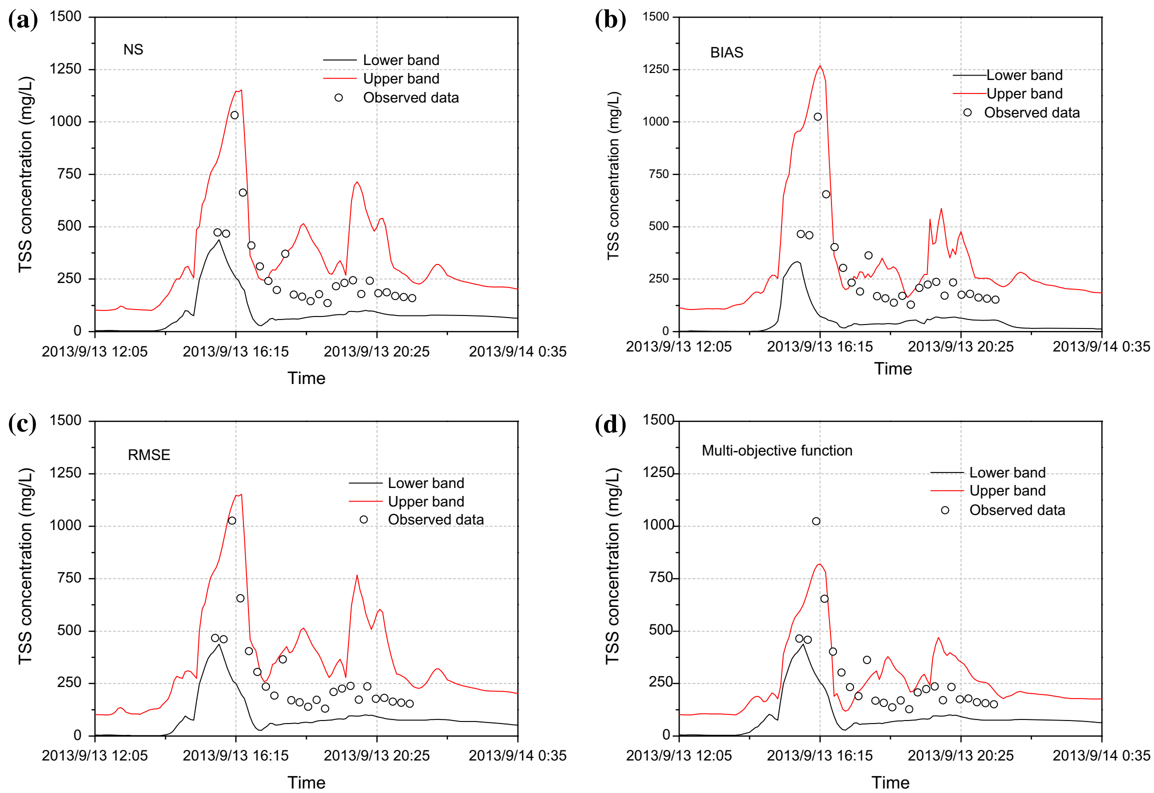

Fig. 2. Uncertainty bands of model outputs for TSS (September 13, 2013) for (a) *NS* > 0.0, (b) −20% < *BIAS* < 20%, (c) Best 10% *RSME*, and (d) Multi-objective function.

Based on uncertainty analysis of the water quality parameters, the accuracy of water quality modeling of a combined sewer system by a deterministic commercial model could be assessed with the GLUE method. However, there are some drawbacks associated with use of the GLUE method for this application. Specifically, there is a large computing cost associated with implementation of the GLUE method. Although computing cost is a common issue for the GLUE method relative to other uncertainty analysis approaches [14], it is higher when the method is applied to water quality models of combined sewer systems. This is because eroded sediments comprise a considerable amount of the pollutants conveyed in sewer systems (e.g. TSS), and an important source contributing to generation of the pollutograph [44,45]. Hence, a long simulation period is needed to reach a state of equilibrium state of sediment deposition during combined sewer system water quality modeling. The maximum initialization stage lasted up to several months, and the simulation time for a complex network on a large scale could be several hours. Moreover, the computing cost for simulation with all of the parameter sets obtained by Monte Carlo sampling was much higher than that associated with water quantity modeling and stormwater quality modeling. Accordingly, uncertainty analysis using the GLUE method may not be feasible in some cases owing to the large computing cost [15]. Another limitation is the subjectivity that exists within the GLUE approach [20]. The selection of the parameter variation range, objective function, and acceptability thresholds may significantly influence the results of uncertainty analysis of the model water quality parameters. The small range will lead to a low uncertainty in model outputs. However, the results will be rejected because the observed data fall outside the uncertainty band. Conversely, a wide parameter range will widen the uncertainty band and reduce the confidence level.

The uncertainty of water quality modeling of the combined sewer system in a complex networks scale was also much higher than that of stormwater quality modeling and water quantity modeling. Although the water quality parameter could be calibrated by the GLUE method for a specific site and rainfall condition, uncertainty analysis with the GLUE and other probabilistic approaches is only feasible for academic exercises, not practical applications. This is because uncertainty analysis is complex and has high computing costs [14]. Accordingly, further studies of water quality models are needed to enable application of water quality modeling to combined sewer systems on a complex network scale.

4. Conclusion

In this study, a water quality model of a combined sewer system in a complex network scale was established using the Infoworks CS. Based on calibration and validation of the water quantity parameters, the uncertainty of the water quality parameters was analyzed using the GLUE methodology.

Several water quality parameters were not identified well by the GLUE method when a single objective function was used, such as $NS = 0.0$. However, identification of parameters was significantly improved when the multi-objective function was used, and the results were much better than those obtained with individual objective functions. Additionally, the uncertainty band obtained by the multi-objective function was narrower than that of individual objective functions. Adoption of the multi-objective function within the GLUE method could improve the parameter identification and reduce the uncertainty band; however, some observed data may fall outside the uncertainty band. Accordingly, it is important to check the consistency of the model hypotheses by comparing the observed data with the uncertainty band when the multi-objective function was used. Assessment of the uncertainty of the water quality parameters of a deterministic commercial model for a combined sewer system in a complex network scale by the GLUE method revealed it was larger than that associated with the stormwater quality model. However, the high-computing cost and subjectivity within the GLUE method may influence implementation of uncertainty analysis by this approach.

The results presented herein are based on a specific case study, and further investigations are needed for generalization. Nevertheless, this study presents the uncertainty analysis of water quality parameters for a complex network-scale combined sewer system, and provides a basis for future research and application into water quality modeling of the combined sewer system.

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