A balanced calibration of water quantity and quality by multi-objective optimization for integrated water system model

Yongyong Zhang^{a,*}, Quanxi Shao^{b,*}, John A. Taylor^c

^a Key Laboratory of Water Cycle and Related Land Surface Processes, Institute of Geographic Sciences and Natural Resources Research, Chinese Academy of Sciences, Beijing 100101, China

^b CSIRO Digital Productivity Flagship, Leeuwin Centre, 65 Brockway Road, Floreat Park, WA 6014, Australia

^c CSIRO Digital Productivity Flagship, GPO Box 664, Canberra, ACT 2601, Australia

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SUMMARY

Due to the high interactions among multiple processes in integrated water system models, it is extremely difficult, if not impossible, to achieve reasonable solutions for all objectives by using the traditional step-by-step calibration. In many cases, water quantity and quality are equally important but their objectives in model calibration usually conflict with each other, so it is not a good practice to calibrate one after another. In this study, a combined auto-calibration multi-process approach was proposed for the integrated water system model (HEQM) using a multi-objective evolutionary algorithm. This ensures that the model performance among inseparable or interactive processes could be balanced by users based on the Pareto front. The Huai River Basin, a highly regulated and heavily polluted region of China, was selected as a case study. The hydrological and water quality parameters of HEQM were calibrated simultaneously based on the observed series of runoff and ammonia-nitrogen ($\text{NH}_4\text{-N}$) concentrations. The results were compared with those of the step-by-step calibration to demonstrate the rationality and feasibility of the multi-objective approach. The results showed that a Pareto optimal front was formed and could be divided into three clear sections based on the elastic coefficient of model performance between $\text{NH}_4\text{-N}$ and runoff, i.e., the dominated section for $\text{NH}_4\text{-N}$ improvement, the trade-off section between $\text{NH}_4\text{-N}$ and runoff, and the dominated section for runoff improvement. The trade-off of model performance between runoff and $\text{NH}_4\text{-N}$ concentration was clear. The results of the step-by-step calibration fell in the dominated section for $\text{NH}_4\text{-N}$ improvement, where just the optimum of the runoff simulation was achieved with a large potential to improve $\text{NH}_4\text{-N}$ simulation without a significant degradation of the runoff simulation. The overall optimal solutions for all the simulations appeared in the trade-off section. Therefore, the Pareto front provided different satisfactory solutions for users to choose according to their specific objectives. This study is expected to promote the application of multi-objective calibration in water system modeling, and provide scientific and technological supports for the implementation of integrated river basin management.

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1. Introduction

Integrated water system modeling is a popular practice in water related sciences nowadays due to the availability of high-performance computing facilities, more data sources and intensive exchange of interdisciplinary knowledge (Kirchner, 2006). Such water system models can be divided into two major categories based on their original purposes. Hydrological models are formulated to simulate the dominant runoff process, as well as

its corresponding water quality and ecological processes (such as SWAT (Arnold et al., 1998), HSPF (Bicknell et al., 1993) and SHE (Refsgaard and Storm, 1995)), while biogeochemical models focus on pollutant transportation and transformation processes and vegetation physiological processes with water flows being just as one of the major constraints (such as EPIC (Sharpley and Williams, 1990), DNDC (Li et al., 1992; Deng et al., 2011) and APSIM (McCown et al., 1996)). Integrated water system models play a significant role in many aspects of river basin management such as flood forecasting, water resources allocation, pollution control, environmental flow assessment and climate change impact evaluation.

* Corresponding authors. Tel.: +61 (8) 9333 6613; fax: +61 (8) 93336121.

E-mail addresses: Zhangyy003@igsnr.ac.cn (Y.Y. Zhang), Quanxi.shao@csiro.au (Q.X. Shao).

However, parameter calibration is always one of the key issues in model applications, especially for the complicated integrated models mainly due to over-parameterization. Such issues restricted their usefulness and effectiveness to real resources management and decision making. Currently, manual trial-and-error or automatic calibration are the most pervasive approaches to obtain the estimates of parameter values (Boyle et al., 2000; Vrugt et al., 2003; Tang et al., 2006; Afshar and Hamideh, 2012; Huang, 2014). However, manual trial-and-error is a crude and inefficient method because it always depends on subjective justification of the optimal estimates (Afshar and Hamideh, 2012; Huang, 2014). Along with the increasing computing efficiency, the automatic calibration approach has become more popular, together with the development of optimization algorithms.

In practice, the commonly used calibration approaches are single objective or weighted average of multiple objectives in model calibration. Both of these approaches are logically clear, feasible and effective for calibrating individual water related components (e.g. high flow, low flow, water quality variables) (Gupta et al., 1999; Sincok et al., 2003). Although these approaches are also applied to water related systems in which multiple objectives are considered, it is a great challenge to obtain the optimal solution among different objectives because of the degree of interaction among the many processes involved, the complexity of model structures and model uncertainty. For example, at least water quantity and quality need to be considered in river basin management, but they are interrelated (Zhang et al., 2016).

Multi-objective optimization (MOO) is an efficient and effective way to solve the issues mentioned above. This approach has become increasingly popular in water related sciences over the past 15 years (Yapo et al., 1998; Vrugt et al., 2003; Efstratiadis and Koutsoyiannis, 2010), and the applications focus on the multi-objective auto-calibration of flow components and water quality variables, respectively. The calibration strategies are divided into three categories according to the different objectives formed by (a) considering different flow components (e.g. low flow, high flow, total water volume, groundwater table, peak timing) (Liong et al., 2001; Madsen, 2003; Vrugt et al., 2003; Tang et al., 2006; Khu and Madsen, 2005; Schoups et al., 2005; Fenicia et al., 2007; Parajka et al., 2007; Shafii and De Smedt, 2009) or water quality variables (e.g. water temperature, sediment, dissolved oxygen: DO, biological oxygen demand: BOD, total phosphorus or nitrogen and chlorophyll a) (Afshar and Hamideh, 2012); (b) using different evaluation criteria (e.g. bias, mean absolute or relative errors, root mean square errors, coefficient of determination, correlation coefficient, Nash–Sutcliffe efficiency) (Gupta et al., 1998; Yapo et al., 1998; Boyle et al., 2000; Madsen, 2000; Cheng et al., 2002; Khu and Madsen, 2005; Krause et al., 2012; Zhou et al., 2014); and (c) considering observed series from multiple sites (Bekele and Nicklow, 2007; Moussa et al., 2007; Li et al., 2010b). The popular algorithms are non-dominated evolutionary algorithms such as MOCOM-UA (Duan et al., 1992; Yapo et al., 1998), SPEA 2 (Zitzler and Thiele, 1999), MOCSEM-UA (Vrugt et al., 2003), NSGA-II (Deb et al., 2002; Kollat and Reed, 2006, MA) (Liu et al., 2012, 2014).

For the calibration of water quantity and quality, most existing cases calibrate flow components and water quality variables by multi-stage single objective optimization (i.e., step-by-step calibration). That is the flow components are calibrated first in order to provide hydrological boundaries for water quality calibration (Francos et al., 2001; Sincok et al., 2003; Bekele and Nicklow, 2007; Engel et al., 2007; Moriasi et al., 2007; Hesse et al., 2008; Paredes-Arquiola et al., 2010; Pisinaras et al., 2010; Wang et al., 2013). The main historic reason for separating the calibration was that the water quality characteristics are assumed not to affect the water flows, that is, water flows affect water quality but not

vice versa. As a result, the two systems are not completely coupled during the calibration. However, due to the uncertainties of in-situ runoff data (Yen et al., 2014), the simulation errors from the calibrated hydrological components could also distort the subsequent water quality calibration and, as a result, directly affect the performance of the water quality simulation. Several studies reported that the simulations of water quality variables were usually unsatisfactory although the runoff simulation performance was acceptable due to the error accumulation caused by the uncertainties in the in-situ runoff and water quality data (Santhi et al., 2001; White and Chaubey, 2005; Kang et al., 2006; Bekele and Nicklow, 2007; Moriasi et al., 2007; Zhang et al., 2011, 2013). Moreover, due to the uncertainties in the model structure and calibrated parameter values, it is more reasonable to think that the water quality samples also infer some uncertainties in the hydrological processes (e.g. the contributions of river flow into groundwater, interflow, surface flow, low flow regimes and flood pattern) (Mroczkowski et al., 1997; Meixner et al., 2002; van Griensven and Bauwens, 2003; Aubert et al., 2013). Given that the module for water quality process is reasonable, the unacceptable simulation of water quality processes would also be caused by the uncertainty in the hydrological parameters equifinality, even if the hydrological processes are well-simulated. Nevertheless, the sources of observed information are only used to calibrate their corresponding processes and are ignored in the calibration of the other related processes. In reality, the hydrological and water quality processes take place simultaneously and inseparably, and the water quantity and quality objective functions are obviously conflicting in optimization. For example, overland flows (surface runoff, interflow and baseflow) determine both water volume and nonpoint source pollutant load into rivers (Tesoriero et al., 2009; Zhang et al., 2016). The transportation and transformation processes of pollutants occur with flow routing. Furthermore, the nutrient losses by water erosion directly disturb the soil nutrient balance, probably restrict crop growth, and then influence the transpiration of plants in the hydrological processes especially in the nutrient-limited regions. Therefore, it might be more logical and scientifically sound to calibrate all the components or modules simultaneously in the integrated water system models.

Earlier works by van Griensven and Bauwens (2003) and van Griensven and Meixner (2007) also recognized the inseparable relationship of water quantity and quality processes, and proposed a single objective auto-calibration method (a weighted average method) to aggregate the criteria of flow components and water quality variables into one single criterion. They also pointed out that the final distribution of objective functions in their global optimization criterion could be affected by an initial random sampling, and the quantity and reliability of observed data. Although this method was commonly-used in multi-site, multi-criteria or multi-period calibrations (Li et al., 2010b; Zhang et al., 2011; Ahmadi et al., 2014), the weights also need to be pre-defined and, in fact, the resulted parameter estimation was only one of many possible Pareto optimal solutions. As a generalization, we promote the simultaneous calibration of water quantity and quality by multi-objective Pareto-optimization.

The objective of this study is to explore a balanced calibration of water quantity and quality that effectively considers the interaction of different processes. We will demonstrate how to obtain the Pareto front of the sub-optimal solutions of conflicting objectives by taking full advantages of multiple observation sources. The hydrological and water quality processes are regarded as individual entities, and their observations are used for simultaneous calibration. The method is applied in the Shaying River, which is the largest and heavily polluted tributary of Huai River Basin in China. The proposed method is compared with the traditional step-by-step single objective calibration to demonstrate its

efficiency and effectiveness in integrated water quantity and quality simulation.

2. Study area and data processing

Shaying River Catchment ($112^{\circ}45' \sim 113^{\circ}15'E$, $34^{\circ}20' \sim 34^{\circ}34'N$), the largest catchment of the Huai River Basin, China, is selected as the study area. It is an agriculturally dominated region with a drainage area of 36,651 km² and its major landuse is dryland agriculture, accounting for over 80% of total area. Water shortage, floods and heavy pollution are the major water issues, which have significantly restricted the regional sustainable development. Fuyang Station is a key monitoring station downstream of Shaying River and controls over 90% of the whole drainage area.

The GIS, meteorological, socio-economic and agricultural management data were collated for model development, including a Digital Elevation Model (DEM), soil, landuse and crop types, daily precipitation, daily minimum and maximum air temperature, populations, fertilization (amount and timing), point source pollutant load. The observed daily runoff and intermittent observations of NH₄-N concentrations at Fuyang Station were collected from 2003 to 2007. The first three year's data (from 2003 to 2005) with the mean runoff of 167.13 m³/s and mean NH₄-N concentration of 3.55 mg/L were used for model calibration, and the last two year's data (from 2006 to 2007) with the mean runoff of 139.19 m³/s and mean NH₄-N concentration of 3.00 mg/L were used for model validation.

Forty-six sub-basins were created using the Arc GIS platform according to the spatial distributions of landuse and geographical

positions of dams, sluices and gauges (Fig. 1). The weather data series (daily precipitation, maximum and minimum air temperature) and socio-economic data (populations in urban and rural area, breeding stock of large animals and livestock, chemical fertilizer amounts) were interpolated to each sub-basin and used as the driving factors of the model. The detailed data processing procedures were presented in Zhang et al. (2016).

3. Models and methodology

3.1. Integrated water system model (HEQM)

HEQM is an integrated water system model developed by Zhang et al. (2016) for the simultaneous simulation of water related processes at basin scale, including hydrological, soil biogeochemical and water quality processes. The current version contains seven major modules (i.e. hydrological cycle module, soil biochemical module, crop growth module, soil erosion module, overland water quality module, water quality module of water bodies and dam regulation module) and a parameter analysis tool. The model framework was presented in Fig. 2. The proposed model can simulate several key water related components in a river network, such as runoff and water quality variables.

The construction of HEQM is based on the hypothesis that the cycles of water and nutrients (N, P and C) are inseparable and act as the critical linkages among all the modules (Fig. 3). In this study, we only calibrate for water quantity and quality objectives. These are grouped into the “yield” and “migration” processes. The yield

Fig. 1. The research area and sub-basin delineation.

Fig. 2. The framework of HEQM and its interactions among modules.

Fig. 3. The interaction of hydrological and environmental processes in HEQM.

processes of overland runoff and nonpoint pollutant load are briefly described as

$$\begin{cases} R = P(R) - E(R) - I(R) - VS(R) \\ M = M_{in} + M_{org} \\ = F(M) + P(M) - E(M) - I(M) - VS(M) - D_{yield}(M) \\ D_{yield}(M) = f_{d_yield}(SW, ST, SP) \end{cases} \quad (1)$$

where R is runoff; M is the pollutant including inorganic matter (M_{in}) and organic matter (M_{org}), respectively; $F(M)$ is agricultural fertilizing processes; $P(\cdot)$, $E(\cdot)$ and $I(\cdot)$ are the processes of precipitation, evapotranspiration and infiltration, respectively; $VS(\cdot)$ is the variation of water and matter in the soil layer; $D_{yield}(\cdot)$ is the matter degradation in the soil layer, which has a complicated nonlinear relation $f_{d_yield}(\cdot)$ with the soil related factors, such as soil water (SW), soil temperature (ST) and soil properties (SP) (Xia et al., 2005).

The overland or instream migration processes of runoff and nonpoint pollutant load are briefly described as

$$\begin{cases} R' = f_{mig}^R(R) \\ M' = f_{mig}^{in}(M_{in}, R) + f_{mig}^{org}(M_{org}, Sed) - D_{mig}(M) + PL(M) \\ D_{mig}(M) = f_{d_mig}(R, LUCC, OS, OL, WT, SL) \end{cases} \quad (2)$$

where R and M are the runoff and pollutant after migration, respectively; Sed is the sediment yield; $f_{mig}^R(\cdot)$ is the runoff routing process, which has an exponential relationship with the migration time; $f_{mig}^{in}(\cdot)$ and $f_{mig}^{org}(\cdot)$ are the migration processes of M_{in} and M_{org} , respectively, and have linear relationships with the runoff routing; $D_{mig}(\cdot)$ is the pollutant degradation and loss during the overland or instream processes, which has a complicated nonlinear relation $f_{d_mig}(\cdot)$ with runoff, water temperature (WT), landuse type ($LUCC$),

overland slope (OS) and length (OL), as well as stream length (SL) (Zhang et al., 2016).

3.2. Multi-objective auto-calibration algorithm

Nondominated sorting genetic algorithm II (NSGA-II), an improved version of NSGA (Srinivas and Deb, 1994), was proposed by Deb et al. (2002) to effectively solve the conflicts among different objectives and obtain a set of trade-off optimal solutions (Pareto front solution). This algorithm contains a fast non dominated procedure in an elitist-preserving approach and crowded comparison parameterless niching operator. It alleviates the criticism of computational complexity, lack of elitism and the need for specifying a sharing parameter in other multi-objective evolutionary algorithms.

Currently, NSGA-II has been considered as a landmark in the field of evolutionary multi-objective optimization (Coello, 2006) and widely applied in economic and finance (Tapia and Coello, 2007), electric power dispatch (Abido, 2006), engineering shape design (Deb and Goel, 2001), water resources and environmental management (Suen and Eheart, 2006; Maringanti et al., 2009), numerical model auto-calibration like hydrological model (Khu and Madsen, 2005; Tang et al., 2006; Fenicia et al., 2007; Shaffi and De Smedt, 2009), water quality model (Bekele and Nicklow, 2007), and so on.

3.3. Integration between HEQM and NSGA-II

3.3.1. Integration procedures

The source code of NSGA-II was downloaded from the website of Kanpur Genetic Algorithms Laboratory (<http://www.iitk.ac.in/>)

[kangal/index.shtml](#)) and was coupled with HEQM by interchanging the parameter value sets and their corresponding function values, respectively. The framework is shown in Fig. 4 and the procedures are presented below.

- (1) Pre-determine the hydrological and water quality parameters of HEQM to be estimated as well as their value ranges by, for example, sensitivity analysis;
- (2) Randomly generate a large number of parameter sets (parent population with size of N) of HEQM by NSGA-II.
- (3) Simulate the runoff and water quality processes by HEQM for each parameter set and calculate the values of their objective functions.
- (4) Sort the nondomination ranks of the objective values and their corresponding parameter sets by the fast nondominated sorting procedure of NSGA-II.
- (5) Generate the child population (size: N) by the critical processes of genetic algorithm (i.e. selection, crossover, mutation) and calculate the values of their objective functions of the child population by HEQM.
- (6) Sort the nondomination ranks of the objective values and their corresponding parameter sets and combine with the parent population (size: $2N$).
- (7) Estimate the crowded distance of each objective value and compare between different objective values for the elitism of a new parent population (size: N) and a uniformly spread out Pareto front.
- (8) Check the convergence statistics and the iterations. If the convergence criteria or maximum iterations are satisfied, output the parameter sets and Pareto front solution; otherwise, return to step 5.

There are seven main control parameters in NSGA-II, i.e., the number of objectives, the number of parameters to be estimated,

the number of constraints, the population size, the maximum number of iterations, the cross-over probability and its type (1: simple point or 2: uniform), the mutation probability. The numbers of objectives, parameters and constraints were determined by users while the default values of other parameters are set as 100, 200, 0.90, 1 and 1.0, respectively. In this paper, two objectives were set because runoff and water quality processes were calibrated simultaneously, and the estimated parameters and constraints were the selected sensitive parameters of HEQM and their ranges, respectively.

For ease of discussion, the Pareto fronts were divided into three sections according to the elastic coefficient (ECQ) of model performance between water quantity and quality, defined as

$$ECQ = \frac{\Delta P_C}{P_C} / \frac{\Delta P_Q}{P_Q} \quad (3)$$

where P_Q and P_C are the evaluated index values of model performance of water quantity and quality, respectively; ΔP_Q and ΔP_C are the variation ranges of simulation performance of water quantity and quality, respectively. The ECQ should be always negative because of a tradeoff between the simulation performance of water quantity and quality in the Pareto front, causing the opposite signs of ΔP_Q and ΔP_C .

The dominated section for water quality simulation improvement was the segment with large negative ECQ , the trade-off section between water quantity and quality simulation improvement was the segment with moderate ECQ , and the dominated section for water quantity improvement was the segment with small negative ECQ .

As a comparison, NSGA-II was also applied to the parameter calibration of hydrological and water quality separately by the step-by-step approach, that is, the hydrological parameters were calibrated first and the water quality related parameters were

Fig. 4. The flow chart of NSGA-II for the simultaneous calibration of water quantity and quality.

calibrated conditionally on the values of the optimal calibrated hydrological parameter. The step-by-step procedure was traditional and widely-used in the water quantity and quality calibration of distributed watershed models.

3.3.2. The objective functions for calibration

The objective of model calibration is to make the simulations best match the observations where the overall agreement is quantified by model evaluation criteria. The root mean square error (RMSE) is straightforward and widely used to assess the model performance of runoff, water quality variables and others. The objective function is formulated as

$$RMSE = \sqrt{\sum_{i=1}^N (O_i - S_i)^2 / N} \quad (4)$$

where N is the number of the series, O_i and S_i are the i th observed and simulated values, respectively. For the single objective calibration, the aim is to find the optimal parameter values which minimize the RMSE value.

For the multiple objective functions (i.e., the RMSEs of runoff and water quality series), the aim was to find so-called Pareto optimal in which none of the objective functions can be improved in value without worsening some of the other objective values. In our case study, the objective function was expressed as

$$f_{multi-ob} = \text{minimize}\{RMSE_Q, RMSE_C\} \\ \text{subject to } par(Q, C)_{\min} \leq par(Q, C) \leq par(Q, C)_{\max} \quad (5)$$

where $f_{multi-ob}$ is the multi-objective function; $RMSE_Q$ and $RMSE_C$ are the RMSE of simulated runoff and water quality indicators, respectively. $par(Q, C)$, $par(Q, C)_{\min}$ and $par(Q, C)_{\max}$ are the parameter lists of water quantity and quality, their maximum and minimum limits, respectively.

Alternatively, the traditional step-by-step approach for water quantity and quality calibration was as follow.

Step 1: Water quantity parameters were calibrated first using the objective function

$$f_{single-Q} = \text{minimize}\{RMSE_Q\} \\ \text{subject to } par(Q)_{\min} \leq par(Q) \leq par(Q)_{\max} \quad (6)$$

Step 2: Water quality parameters were then calibrated using the objective function

$$f_{single-C} = \text{minimize}\{RMSE_C\} \\ \text{subject to } par(C)_{\min} \leq par(C) \leq par(C)_{\max} \\ \text{with } par(Q) = par(Q)_{opt} \quad (7)$$

with the water quantity parameters fixed at the calibrated values from Step 1, where $f_{single-Q}$ and $f_{single-C}$ are the single objective function of water quantity and quality, respectively; $par(Q)_{opt}$ are the optimal parameter lists of water quantity. The number of objectives in NSGA-II is one for each step and NSGA-II will be performed twice.

3.4. Model evaluation

In addition to the objective RMSE, three more statistics were also used to evaluate the model performance, including normalized bias (Nbias), correlation coefficient (r) and coefficient of efficiency (NS) (Nash and Sutcliffe, 1970) defined as

Normalized bias:

$$Nbias = \frac{\sum_{i=1}^N (O_i - S_i)}{\sum_{i=1}^N O_i} \quad (8)$$

Correlation coefficient:

$$r = \frac{\sum_{i=1}^N (O_i - \bar{O}) \cdot (S_i - \bar{S})}{\sqrt{\sum_{i=1}^N (O_i - \bar{O})^2 \cdot \sum_{i=1}^N (S_i - \bar{S})^2}} \quad (9)$$

Coefficient of efficiency:

$$NS = 1 - \frac{\sum_{i=1}^N (O_i - S_i)^2}{\sum_{i=1}^N (O_i - \bar{O})^2} \quad (10)$$

where O_i and S_i are the i th observed and simulated value, respectively; $\bar{O}$ and $\bar{S}$ are the average observed and simulated value, respectively. The criteria are summarized in Table 1 according to Santhi et al. (2001) and Moriasi et al. (2007). In the situation of conflicting performance ratings among these three indices, the overall model performance is determined conservatively by the worst rating.

4. Results and discussion

4.1. Sensitive parameters selection

There are 182 parameters that control the hydrological, ecological and water quality processes of HEQM (Zhang et al., 2016). The parameter sensitivity analysis was carried out using a global sensitivity analysis tool (LH-OAT: Latin Hypercube One factor At a Time) in order to increase the optimizing efficiency (van Griensven et al., 2006). Nine and twenty-eight distributed sensitive parameters were detected to have close relationships with runoff and $\text{NH}_4\text{-N}$ concentration, respectively (Table 2). The sensitive parameters for runoff simulation were soil related parameters (W_{fc} : 32.73%, W_{sat} : 11.68%, K_r : 9.55% and K_{sat} : 0.33%), surface runoff yield parameters (g_1 : 7.30% and g_2 : 10.54%), baseflow parameters (K_g : 2.91% and T_g : 1.74%) and evapotranspiration parameter (K_{ET} : 23.21%). The sensitive parameters for $\text{NH}_4\text{-N}$ concentration simulation were divided into six hydrological parameters (59.28%), 11 nitrogen parameters (22.46%), five parameters of COD (Chemical Oxygen Demand) (13.00%) and six soil carbon parameters (0.17%).

The key hydrological processes (i.e., soil water, surface runoff and evapotranspiration) explained 26.13%, 22.45% and 10.71% of the variation of $\text{NH}_4\text{-N}$ observations. The related parameters were W_{fc} (11.10%), W_{sat} (11.83%) and K_r (3.20%) for the soil water; g_1 (10.34%) and g_2 (12.11%) for the surface runoff yield and K_{ET} (10.71%) for the evapotranspiration. Specifically, overland flow

Table 1
Model performance criteria for runoff and $\text{NH}_4\text{-N}$ concentration of HEQM.

Performance rating	Bias	r	NS
	Runoff		
Very good	[-0.10, 0.10]	[0.85, 1.00]	[0.75, 1.00]
Good	(0.10, 0.15] or [-0.15, -0.10]	(0.15, 0.30] or [-0.30, 0.15]	[0.60, 0.75]
Satisfactory	(0.15, 0.25] or [-0.25, -0.15]	(0.30, 0.50] or [-0.50, -0.30]	[0.50, 0.60]
Unsatisfactory	(0.25, +∞) or (-∞, -0.25)	(0.50, +∞) or (-∞, -0.50)	(-∞, 0.50)

Table 2Sensitive parameters and their ranges, and relative importance for runoff and $\text{NH}_4\text{-N}$ concentration.

Name	Min	Max	Definition	Relative importance for Q	Relative importance for $\text{NH}_4\text{-N}$
W_{fc}	0.20	0.45	Field capacity of soil	32.73	11.0996
W_{sat}	0.45	0.75	Saturation moisture capacity of soil	11.68	11.8310
g_1	0.00	3.00	Basic runoff coefficient	7.30	10.3375
g_2	0.00	3.00	Influence coefficient of soil moisture	10.54	12.1095
K_{ET}	0.00	3.00	Adjustment factor of evapotranspiration	23.21	10.7075
K_r	0.00	1.00	Interflow yield coefficient	9.55	3.1951
T_g	1.00	100.	Delay time for aquifer recharge	1.74	–
K_g	0.00	1.00	Baseflow yield coefficient	2.91	–
K_{sat}	0.00	120.	Steady state infiltration rate of soil	0.33	–
$K_{set}(\text{NH}_4)$	0.00	100.	Settling rate of $\text{NH}_4\text{-N}$ at 20 °C in reservoir	–	14.1678
$R_d(\text{COD})$	0.02	3.40	COD deoxygenation rate at 20 °C in channel	–	6.6208
$K_d(\text{NH}_4)$	0.10	1.00	Bio-oxidation rate of $\text{NH}_4\text{-N}$ at 20 °C in reservoir	–	4.5072
$R_{set}(\text{COD})$	–0.36	0.36	COD settling rate at 20 °C in channel	–	3.5971
$K_d(\text{COD})$	0.02	3.40	COD deoxygenation rate at 20 °C in reservoir	–	2.1214
$R_d(\text{NH}_4)$	0.10	1.00	Bio-oxidation rate of $\text{NH}_4\text{-N}$ at 20 °C in channel	–	1.9710
$K_{set}(\text{COD})$	0.00	269	Settling rate of COD at 20 °C in reservoir	–	0.6128
$K_d(\text{orgN})$	0.20	0.40	Hydrolysis rate of organic N to $\text{NH}_4\text{-N}$ at 20 °C in reservoir	–	0.5609
$R_d(\text{orgN})$	0.20	0.40	Hydrolysis rate of organic N to $\text{NH}_4\text{-N}$ at 20 °C in channel	–	0.5584
$R_{set}(\text{NH}_4)$	–50.0	50	$\text{NH}_4\text{-N}$ settling rate at 20 °C in channel	–	0.2848
$K_{set}(\text{NH}_4)$	0.00	69	Resuspension rate of $\text{NH}_4\text{-N}$ at 20 °C in reservoir	–	0.1951
$R_{set}(\text{orgN})$	0.001	0.10	Organic N settling rate at 20 °C in channel	–	0.0841
$K_d(\text{NO}_2)$	0.20	2.00	Bio-oxidation rate of $\text{NO}_2\text{-N}$ to $\text{NO}_3\text{-N}$ at 20 °C in reservoir	–	0.0627
$K_{set}(\text{COD})$	0.00	269	Resuspension rate of COD 20 °C in reservoir	–	0.0481
μ_{CLAY}	0.01	1.00	Clay content reduction factor	–	0.0408
K_1	0.01	1.00	Decomposition rate of labile C pool	–	0.0377
S	0.01	1.00	Ratio of labile organic C pool in the total biomass	–	0.0371
$R_d(\text{NO}_2)$	0.20	2.00	Bio-oxidation rate of $\text{NO}_2\text{-N}$ to $\text{NO}_3\text{-N}$ at 20 °C in channel	–	0.0332
M_{NO_3}	0.00	1.00	Maintenance coefficient of $\text{NO}_3\text{-N}$ in soil	–	0.0309
km_{sc}	0.01	1.00	Decomposition ratio of stable organic C in microbial biomass pool	–	0.0220
km_{cl}	0.01	1.00	Decomposition ratio of labile organic C pool in microbial biomass pool	–	0.0150
kr_{cvi}	0.01	1.00	Decomposition ratio of very labile organic C pool in residue pool	–	0.0143
Total relative importance				100.00	94.90

determined the total nonpoint source pollutant loads into rivers, and runoff affected the degradation and settling processes of pollutants in water bodies (van Griensven and Bauwens, 2003). Thus, the observed water quality series also implied useful information about related hydrological processes, which could be used to calibrate related hydrological parameters (i.e., W_{fc} , W_{sat} , K_r , g_1 , g_2 and K_{ET} in our study). In particular, the importance of W_{sat} , g_1 and g_2 parameters for $\text{NH}_4\text{-N}$ concentration simulation was even greater than that for runoff simulation. More information about hydrological processes could be obtained from water quality observations whereas, the step-by-step calibration could not take full advantages of all the calibrated components.

4.2. Pareto fronts of calibration

The final 70 solutions were identified from 20,000 solution sets to form the Pareto front based on the RMSE objectives of runoff and $\text{NH}_4\text{-N}$ concentration (Fig. 5a). The RMSE values of runoff ($RMSE_Q$) were from 159.460 (Q_{min}) to 276.833 m^3/s (Q_{max}), while those of $\text{NH}_4\text{-N}$ concentration ($RMSE_C$) were from 2.359 (C_{min}) to 2.713 mg/L (C_{max}) (Table A1). All of these errors were probably from the uncertainty of model structure. The simulation performances of runoff varied from the unsatisfactory to very good ratings and those of $\text{NH}_4\text{-N}$ were from the satisfactory to good ratings. The $\text{NH}_4\text{-N}$ simulations were not as good as the runoff simulations due to the more complicated yield and migration mechanism of $\text{NH}_4\text{-N}$ and its discontinuous observations. The Pareto front was divided into three sections according to the elastic coefficient (ECQ) of model performance between $\text{NH}_4\text{-N}$ and Q (Fig. 5b), i.e., the dominated section for $\text{NH}_4\text{-N}$ improvement, the trade-off section between $\text{NH}_4\text{-N}$ and Q and the dominated section for Q improvement. The Pareto front provided stakeholders flexibilities to choose the satisfactory solutions based on specific requirements.

Fig. 5. The objective function values, and the elastic coefficients along the Pareto front.

In the dominated section for $\text{NH}_4\text{-N}$ improvement, $RMSE_C$ decreased by 7.60% from 2.713 to 2.507 mg/L , while $RMSE_Q$ increased by only 0.36% from 159.460 to 160.041 m^3/s . The ECQ

values ranged from -352.91 to -20.83 with the mean of -65.64 . For $\text{NH}_4\text{-N}$ simulation, the r and NS values increased slightly from 0.786 to 0.795 and from 0.503 to 0.576 , respectively and all of them were in the satisfactory rating. The $Nbias$ improved obviously from 0.249 (good) to 0.150 (very good) (Fig. 6). For runoff simulation, the evaluation criteria were still in the very good rating and only the $Nbias$ changed from 0.007 to 0.040 . Thus, the small losses of Q simulation performance obviously improved $\text{NH}_4\text{-N}$ simulation, especially for the $Nbias$.

In the trade-off section between $\text{NH}_4\text{-N}$ and Q , $RMSE_C$ decreased by 3.37% from 2.505 to 2.395 mg/L, while $RMSE_Q$ increased by 4.39% from 160.249 to 165.644 m³/s. The ECQ values ranged from -15.51 to -3.02 with the mean of -6.56 . Both $\text{NH}_4\text{-N}$ and runoff simulations changed slightly. For runoff simulation, the values of $Nbias$, r and NS changed from 0.032 to 0.078 , from 0.901 to 0.896 , and from 0.81 to 0.797 , respectively. All of these criteria were still in the very good rating. For $\text{NH}_4\text{-N}$ simulation, the values of $Nbias$, r and NS changed from 0.151 (very good) to 0.056 (very good), from 0.794 (satisfactory) to 0.796 (satisfactory), from 0.576 (satisfactory) to 0.613 (good), respectively. The compromising optimal solution between $\text{NH}_4\text{-N}$ and runoff simulation appeared in this section.

In the dominated section for Q improvement, $RMSE_C$ increased by 1.75% from 2.359 to 2.390 mg/L, while $RMSE_Q$ decreased by 68.08% from 276.83 to 166.87 m³/s. The ECQ values ranged from -2.56 to -0.18 with the mean of -0.90 . Thus, the runoff simulation was obviously improved from the unsatisfactory rating to the good rating, although $\text{NH}_4\text{-N}$ simulation became a little weaker. For runoff simulation, the values of $Nbias$, r and NS changed from -0.103 (good) to 0.077 (very good), from 0.837 (good) to 0.895 (very good), from 0.432 (unsatisfactory) to 0.797 (very good), respectively. For $\text{NH}_4\text{-N}$ simulation, these three evaluation criteria changed slightly from 0.080 (very good) to 0.025 (very good), from 0.818 (good) to 0.791 (satisfactory) and from 0.624 (good) to 0.614 (good), respectively.

Fig. 7 presented the comparisons between the observations and simulations of runoff and $\text{NH}_4\text{-N}$ concentration with extreme objective function values in the Pareto front. When $RMSE_Q$ had the minimum (159.460 m³/s) and $RMSE_C$ had the maximum value (2.713 mg/L) (named as: $Q_{\min}\text{-}C_{\max}$), the simulated runoff matched well with the observations. All of these three indices were in the very good performance rating, i.e., 0.070 for $Nbias$, 0.901 for r and 0.812 for NS . However, the $\text{NH}_4\text{-N}$ concentration was typically underestimated, particularly before the flood season (January to

May). The performance was good for $Nbias$ (0.249), satisfactory for both r (0.786) and NS (0.503), respectively. When $RMSE_C$ got the minimum (2.359 mg/L) and $RMSE_Q$ was the maximum value (276.833 m³/s) (named as: $Q_{\max}\text{-}C_{\min}$), the simulated $\text{NH}_4\text{-N}$ concentration was obviously improved, especially the $Nbias$ in the very good rating (0.080). In addition, the other two indices were in the good rating, viz., 0.818 (r) and 0.624 (NS), respectively. However, the concentrations were still underestimated in March and April. For the runoff simulation, it was underestimated in the non-flood season (October to June), but obviously overestimated in the flood season (July to September). The performance was good for $Nbias$ (-0.103) and r (0.837), but unsatisfactory for NS (0.432) due to the mismatch of peak flow. The overall performance for runoff simulation was in the unsatisfactory rating. Thus, runoff and $\text{NH}_4\text{-N}$ calibrations were highly mutually affected and the trade-off was clear. The simulation of $\text{NH}_4\text{-N}$ concentration was quite sensitive to low flow variation.

4.3. Model validation

Along the Pareto front, the $RMSE_Q$ values ranged from 113.605 to 177.244 m³/s, while the $RMSE_C$ values ranged from 1.913 to 2.162 mg/L in the validation period. The variations of both $RMSE_Q$ and $RMSE_C$ were generally similar with those in the calibration period except the $RMSE_C$ in the dominated section for Q improvement (Fig. 8). All of these errors were also probably caused by the uncertainty of model structure. The simulation performances of runoff varied from the satisfactory to good ratings and those of $\text{NH}_4\text{-N}$ were from the unsatisfactory to satisfactory ratings. The $\text{NH}_4\text{-N}$ simulations were also not as good as the runoff simulations.

In the dominated section for $\text{NH}_4\text{-N}$ improvement, the performances of runoff simulation were in the satisfactory rating, although the r and NS values were in the very good rating. The performances of $\text{NH}_4\text{-N}$ simulation were in the unsatisfactory rating, although the $Nbias$ values were in the very good rating. The values of r and NS increased continuously from 0.691 to 0.723 and from 0.434 to 0.465 , respectively. In the trade-off section between $\text{NH}_4\text{-N}$ and Q , all the r and NS values of the runoff simulation were also in the very good rating and the $Nbias$ values were still in the satisfactory rating, varying from 0.175 to 0.239 . However, all the criteria of $\text{NH}_4\text{-N}$ simulation improved significantly and the performances shifted from the unsatisfactory to satisfactory ratings. The overall optimal between Q and $\text{NH}_4\text{-N}$ also appeared in this section. In the dominated section for Q improvement, the performances of

Fig. 6. The variation of all the evaluation criteria ($RMSE$, $Nbias$, r and NS) along the Pareto front during the calibration period.

Fig. 7. The simulated runoff and $\text{NH}_4\text{-N}$ concentration with extreme objective function values ($Q_{\min}\text{-}C_{\max}$, $Q_{50\%}\text{-}C_{50\%}$ and $Q_{\max}\text{-}C_{\min}$) and the step-by-step calibration (single) during the calibration period.

Fig. 8. The variation of all the evaluation criteria ($RMSE$, $Nbias$, r and NS) along the Pareto front during the validation period.

$\text{NH}_4\text{-N}$ simulation were in the satisfactory rating while the runoff simulation varied from the satisfactory to very good ratings. Here the NS values changed most remarkably, i.e., from 0.558 (satisfactory) to 0.818 (very good).

Fig. 9 illustrated the comparison between the observations and simulations of runoff and $\text{NH}_4\text{-N}$ concentrations with extreme objective function values in the Pareto front. For the parameter set of $Q_{\min}\text{-}C_{\max}$, the runoff simulation was in the satisfactory rating, i.e., 0.157 for $Nbias$ (satisfactory), 0.898 for r (very good) and 0.784 for NS (very good), respectively. But the $RMSE_C$ ($2.15 \text{ m}^3/\text{s}$) was very close to the maximum value ($2.162 \text{ m}^3/\text{s}$) and the concentrations were also underestimated before the flood season (January to April), but overestimated in and after the flood season. The simulation performance of the $\text{NH}_4\text{-N}$ concentrations was in the unsatisfactory rating. For the parameter set of $Q_{\max}\text{-}C_{\min}$, the

performance of runoff simulation was also the worst, particularly for the NS (0.558). However, the simulation of $\text{NH}_4\text{-N}$ concentrations was obviously improved and the performance was in the satisfactory rating, i.e., -0.197 for $Nbias$ (good), 0.777 for r (satisfactory) and 0.516 for NS (satisfactory), respectively. Only the simulated values obviously increased in the non-flood season of year 2007, but they still mismatched with observations remarkably. The trade-off between runoff and $\text{NH}_4\text{-N}$ simulations was also clear in the validation period.

4.4. Parameter sets of Pareto front

Fig. 10 gave the variations of normalized hydrological and water quality parameter values along the Pareto front. Over 70% of the normalized parameters showed no significant variations with

Fig. 9. The simulated runoff and $\text{NH}_4\text{-N}$ concentration with extreme objective function values ($Q_{\min}\text{-}C_{\max}$, $Q_{50\%}\text{-}C_{50\%}$ and $Q_{\max}\text{-}C_{\min}$) and the step-by-step calibration (single) during the validation period.

Fig. 10. Normalized hydrological and environmental parameter sets along Pareto front.

ranges of less than 0.25. However, there were still three parameters (g_1 , K_g and $K_{scu}(\text{NH}_4)$) having variation ranges of over 0.50 due to their trade-offs between the runoff and $\text{NH}_4\text{-N}$ objectives, i.e., these parameters had positive correlations with the runoff simulation performance, but negative correlations with the $\text{NH}_4\text{-N}$ simulation performance.

The correlations between each pair within the full suite of 31 parameters (435 pairs) were tested by Pearson's correlation coefficient and t -tests. Although nearly half of total pairs had significant correlations at a 95% confidence level, the correlations were quite low and only 3.21% of pairs had strong correlations (i.e. $r \geq 0.75$)

(Table 3). Thus, most parameters of HEQM were well defined and could be calibrated using the multi-objective optimization algorithm. The hydrological parameters (g_1 , g_2 , T_g and K_{sat}) were negatively correlated with $RMSE_Q$, but obviously positively correlated with $RMSE_C$ except T_g and K_{sat} . The correlations of K_{ET} with $RMSE_Q$ and $RMSE_C$ were just the opposite. Moreover, water quality parameters ($R_{set}(\text{COD})$, $K_d(\text{COD})$, $K_d(\text{NH}_4)$ and $K_{scu}(\text{NH}_4)$) had positive correlations with $RMSE_C$, but only the correlation coefficients of $K_d(\text{COD})$ and $K_{scu}(\text{COD})$ were greater than 0.75. Thus, in order to improve the simulation performances of runoff and $\text{NH}_4\text{-N}$ concentrations, the variations of hydrological (g_1 , g_2 and

Table 3

The highly correlated parameter pairs and their correlation coefficients.

Parameters	g_2	K_{ET}	T_g	$R_{set}(\text{COD})$	$K_d(\text{COD})$	$K_d(\text{NH}_4)$	$K_{scu}(\text{COD})$	$RSEM_Q$	$RSEM_C$
g_1	0.82	−0.88	0.89		0.92		0.85	NR	0.88
g_2		−0.92	0.94				0.82	NR	0.76
K_{ET}			−0.94				−0.79	PR	−0.83
T_g					0.76		0.84	NR	
K_{sat}				0.76				NR	
$R_{set}(\text{COD})$						0.92			PR
$K_d(\text{COD})$									0.76
$K_d(\text{NH}_4)$									PR
$K_{scu}(\text{COD})$									0.75

Note: “NR” means negative correlation whose coefficient is between −0.75 and 0.00; “PR” means positive correlation whose coefficient is between 0.0 and 0.75.

T_g) and water quality parameters ($R_{set}(\text{COD})$, $K_d(\text{COD})$, $K_d(\text{NH}_4)$ and $K_{scu}(\text{COD})$) were consistent, which were just opposite with the variation of K_{ET} .

4.5. Comparison with traditional step-by-step procedure

The objective function values of Pareto optimal solutions were also compared with the results of the traditional step-by-step procedure. In the calibration period, the function values of the step-by-step procedure were located in the middle of the dominated section for $\text{NH}_4\text{-N}$ improvement, and tended to the objective function value of ($Q_{\min}\text{--}C_{\max}$) solution (Figs. 5a and 6). Although the runoff calibration reached the optima ($N_{bias} = 0.007$, $r = 0.901$ and $NS = 0.812$), there was still a potential to improve $\text{NH}_4\text{-N}$ simulation (Table A1). The $RMSE_C$ was 2.574 mg/L, which was 9.1% greater than the optimal value (2.359 mg/L). Particularly in the dominated section for $\text{NH}_4\text{-N}$ improvement, the ECQ was 7.22 and $RMSE_C$ decreased by 2.60% from 2.574 to 2.507 mg/L by a slight increase of $RMSE_Q$ (0.36% from 159.460 to 160.041 m^3/s). The values of N_{bias} , r and NS of $\text{NH}_4\text{-N}$ simulation would also be improved. Although the r values changed very slightly, the N_{bias} decreased most obviously, from 0.216 (good) to 0.150 (very good) while the NS values increased from 0.553 (satisfactory) to 0.576 (satisfactory). However, the model performance of runoff was still at the very good rating.

In the validation period, the function values of the step-by-step procedure were also located in the dominated section for $\text{NH}_4\text{-N}$ improvement (Fig. 8). The runoff simulation criteria of the step-by-step procedure were the same as those of the ($Q_{\min}\text{--}C_{\max}$) solution ($RMSE_Q = 123.722 \text{ m}^3/\text{s}$, $N_{bias} = 0.157$, $r = 0.898$ and $NS = 0.784$, i.e., the satisfactory rating), but the $\text{NH}_4\text{-N}$ performance was even worse. The $RMSE_C$ and r values increased from 2.150 to 2.176 mg/L and 0.691 to 0.694, but the N_{bias} , r and NS values decreased from 0.005 to −0.050 and from 0.440 to 0.426, respectively. Thus, the traditional step-by-step procedure did not reach the reasonable optima of all the objectives of HEQM in the validation period either.

Furthermore, it was proved that the traditional step-by-step procedure just achieved the local optima of the first objective. It was more difficult to get the optima if the calibration was at the higher stage. On the one hand, the errors of pre-calibrated processes were gradually accumulated to the post-calibrated processes; On the other hand, the observation sources were only used to calibrate their dominated processes, and the underlying information of other related processes was always ignored. Thus, it was impossible to get the holistic optima of all the processes for the water system model using the step-by-step calibration procedure. Generally, the existing models usually had a dominated process to connect all of these subsystems, such as hydrological process of SWAT and HEQM, biochemical process of DNDC (Li et al., 1992; Deng et al., 2011). Nevertheless, along with the absorption of multiple data sources from different processes, it

was no longer suitable to calibrate the dominated processes and other processes sequentially. Moreover, the concerned objectives might be significantly improved at the slight expense of the dominated process or other processes simulation. Simultaneous multi-process calibration by Pareto- optimization was an effective and scientific approach to achieve the holistic optima of the water system model, and to take full advantage of all the useful observation sources instead of the traditional step-by-step procedure.

5. Conclusions

The global optimization of an integrated water system model is difficult due to the complicate interactions among the water-related processes and the integration of multi-source observations. The traditional step-by-step calibration approach was usually unable to achieve reasonable solutions for all objectives, especially for the high-order objectives (last few objectives) in the multi-stage calibration. In this study, a combined auto-calibration of water quantity and quality for the integrated water system model (HEQM) was presented using a multi-objective evolutionary algorithm (NSGA-II). Moreover, the rationality and feasibility of this approach was tested by parameter analysis and comparison with the results of traditional step-by-step calibration. The results of our study demonstrated that:

- (1) Hydrological and water quality processes were symbiotic and closely interactive. Although the hydrological cycle was one of the driving factors for the migration and degradation of water quality variables, several water quality processes also acted on the hydrological cycle. For example, the loss of nutrient substance along with water routing, would restrict plant growth due to nitrogen stress and indirectly affect the plant transpiration process. Moreover, water quality observations could help constrain the hydrological processes. Water quality concentration observations could act as a reference to calibrate low flow regimes.
- (2) Pareto optimal solutions were formed between $RMSE$ of simulated runoff and $\text{NH}_4\text{-N}$ concentration by NSGA-II at our study station. The integrated water system model could capture runoff and $\text{NH}_4\text{-N}$ concentration reasonably in both calibration and validation periods. Along the Pareto optimal solutions, the runoff simulation varied from the very good rating to unsatisfactory rating, while the $\text{NH}_4\text{-N}$ simulation varied from the unsatisfactory rating to good rating in the calibration period. In the validation period, the runoff simulation also varied from the good rating to satisfactory rating, while the $\text{NH}_4\text{-N}$ simulation varied from the unsatisfactory rating to satisfactory rating. Thus, the simulation performances of runoff and water quality were highly mutually affected and the trade-off was clear in both the calibration and validation periods. The slight reduction in runoff simulation accuracy significantly improved the simulation

Table A1
The list of all criteria results along Pareto front in the calibration and validation periods.

ID	Dominated area	ECQ	Calibration (2003–2005)								Validation (2006–2007)							
			Runoff				NH ₄ -N				Runoff				NH ₄ -N			
			RMSE_Q	Nbias	r	NS	RMSE_C	Nbias	r	NS	RMSE_Q	Nbias	r	NS	RMSE_C	Nbias	r	NS
Single-objective		–	159.460	0.007	0.901	0.812	2.574	0.216	0.804	0.553	123.722	0.157	0.898	0.784	2.176	–0.050	0.694	0.426
Multi-objective	Dominated section for NH ₄ -N improvement	–	159.460	0.007	0.901	0.812	2.713	0.249	0.786	0.503	123.722	0.157	0.898	0.784	2.150	0.005	0.691	0.440
		–352.91	159.464	0.012	0.901	0.812	2.686	0.240	0.787	0.513	124.457	0.163	0.897	0.782	2.162	–0.012	0.689	0.434
		–144.49	159.508	0.011	0.901	0.811	2.579	0.203	0.796	0.551	124.099	0.159	0.897	0.783	2.153	–0.057	0.699	0.438
		–8.88	159.550	0.013	0.901	0.811	2.573	0.197	0.794	0.553	123.959	0.161	0.898	0.784	2.149	–0.058	0.701	0.441
		–5.95	159.608	0.013	0.901	0.811	2.567	0.194	0.794	0.555	123.315	0.159	0.898	0.786	2.144	–0.060	0.702	0.443
		–22.58	159.622	0.017	0.901	0.811	2.562	0.194	0.796	0.557	123.564	0.163	0.898	0.785	2.138	–0.062	0.704	0.446
		–21.30	159.630	0.021	0.901	0.811	2.560	0.190	0.794	0.558	124.646	0.167	0.898	0.781	2.149	–0.065	0.701	0.441
		–15.13	159.665	0.014	0.901	0.811	2.551	0.184	0.794	0.561	122.682	0.159	0.899	0.788	2.132	–0.059	0.705	0.449
		–11.43	159.677	0.015	0.902	0.811	2.549	0.183	0.794	0.561	122.589	0.162	0.900	0.788	2.124	–0.066	0.708	0.453
		–10.19	159.699	0.024	0.901	0.811	2.545	0.176	0.792	0.563	123.395	0.173	0.899	0.786	2.122	–0.091	0.714	0.454
		–53.94	159.714	0.026	0.901	0.811	2.532	0.172	0.793	0.567	123.557	0.177	0.900	0.785	2.103	–0.086	0.718	0.464
		–0.50	159.811	0.031	0.901	0.811	2.532	0.170	0.793	0.567	124.079	0.180	0.900	0.783	2.112	–0.093	0.716	0.460
		–1.91	159.861	0.034	0.901	0.811	2.530	0.167	0.792	0.568	124.030	0.178	0.900	0.783	2.114	–0.088	0.715	0.459
		–0.39	159.921	0.033	0.901	0.810	2.530	0.168	0.793	0.568	123.305	0.170	0.900	0.786	2.112	–0.075	0.713	0.460
		–23.14	159.941	0.034	0.901	0.810	2.522	0.156	0.790	0.571	123.221	0.180	0.901	0.786	2.106	–0.096	0.718	0.463
		–51.53	159.947	0.034	0.901	0.810	2.517	0.159	0.793	0.572	122.989	0.181	0.901	0.787	2.106	–0.102	0.720	0.463
		–3.31	160.010	0.042	0.901	0.810	2.514	0.160	0.795	0.573	124.287	0.190	0.900	0.783	2.106	–0.114	0.723	0.463
		–13.72	160.041	0.040	0.901	0.810	2.507	0.150	0.795	0.576	123.599	0.187	0.901	0.785	2.101	–0.112	0.723	0.465
	Trade-off section between NH ₄ -N and Q	–0.69	160.249	0.032	0.901	0.810	2.505	0.151	0.794	0.576	122.287	0.175	0.902	0.789	2.095	–0.084	0.719	0.468
		–0.75	160.413	0.053	0.900	0.809	2.503	0.147	0.792	0.577	125.344	0.199	0.901	0.779	2.109	–0.125	0.724	0.461
		–1.08	160.426	0.044	0.900	0.809	2.503	0.151	0.795	0.577	123.292	0.190	0.903	0.786	2.095	–0.118	0.727	0.468
		–4.32	160.449	0.052	0.900	0.809	2.501	0.140	0.791	0.578	122.407	0.185	0.903	0.789	2.086	–0.108	0.727	0.473
		–2.12	160.510	0.041	0.900	0.809	2.499	0.142	0.792	0.578	123.368	0.193	0.902	0.786	2.104	–0.125	0.727	0.464
		–0.50	160.513	0.048	0.900	0.809	2.499	0.139	0.791	0.578	124.191	0.197	0.902	0.783	2.103	–0.126	0.726	0.464
		–1.64	160.591	0.054	0.900	0.809	2.497	0.139	0.792	0.579	124.398	0.200	0.902	0.782	2.104	–0.134	0.728	0.464
		–0.17	160.815	0.046	0.900	0.808	2.497	0.144	0.793	0.579	122.871	0.193	0.903	0.787	2.103	–0.136	0.729	0.464
		–1.72	160.871	0.048	0.900	0.808	2.495	0.129	0.789	0.580	122.842	0.190	0.904	0.788	2.081	–0.112	0.729	0.475
		–0.27	160.907	0.055	0.900	0.808	2.495	0.127	0.788	0.580	122.708	0.199	0.904	0.788	2.088	–0.138	0.735	0.472
		–23.79	160.912	0.058	0.900	0.808	2.493	0.123	0.787	0.581	123.647	0.205	0.903	0.785	2.109	–0.157	0.734	0.461
		–0.06	161.009	0.065	0.900	0.808	2.493	0.127	0.788	0.581	125.291	0.213	0.902	0.779	2.122	–0.163	0.732	0.454
		–1.39	161.051	0.053	0.900	0.808	2.492	0.132	0.791	0.581	123.292	0.190	0.903	0.786	2.084	–0.138	0.735	0.474
		–4.77	161.093	0.056	0.900	0.808	2.489	0.133	0.792	0.582	123.704	0.202	0.903	0.785	2.089	–0.150	0.737	0.471
		–1.22	161.359	0.070	0.899	0.807	2.484	0.120	0.789	0.584	125.373	0.216	0.903	0.779	2.101	–0.159	0.736	0.465
		–0.80	161.483	0.062	0.899	0.807	2.482	0.120	0.789	0.584	122.970	0.205	0.904	0.787	2.089	–0.150	0.737	0.471
		–1.19	161.604	0.057	0.900	0.806	2.480	0.113	0.788	0.585	122.217	0.206	0.904	0.790	2.103	–0.174	0.742	0.464
		–0.89	161.956	0.077	0.899	0.806	2.475	0.121	0.793	0.586	124.773	0.218	0.903	0.781	1.989	–0.122	0.754	0.521
		–0.03	162.258	0.059	0.898	0.805	2.475	0.135	0.797	0.587	122.352	0.198	0.904	0.789	2.018	–0.111	0.744	0.507
		–5.82	162.278	0.055	0.899	0.805	2.473	0.126	0.795	0.587	121.942	0.196	0.904	0.791	1.987	–0.108	0.751	0.522
		–1.48	162.368	0.065	0.899	0.805	2.471	0.104	0.787	0.588	122.345	0.210	0.904	0.789	2.054	–0.164	0.751	0.489
		–1.11	162.650	0.076	0.898	0.804	2.466	0.125	0.796	0.589	125.172	0.221	0.903	0.779	2.019	–0.143	0.752	0.506
		–1.26	162.879	0.076	0.898	0.803	2.462	0.116	0.794	0.591	124.157	0.217	0.904	0.783	1.984	–0.133	0.758	0.523
		–13.60	162.914	0.078	0.898	0.803	2.455	0.115	0.796	0.593	123.806	0.223	0.904	0.784	1.998	–0.153	0.760	0.517
		–0.55	163.318	0.080	0.898	0.802	2.451	0.110	0.796	0.594	123.285	0.222	0.904	0.786	1.981	–0.154	0.765	0.525
		–0.94	163.653	0.096	0.897	0.802	2.447	0.101	0.794	0.596	126.502	0.235	0.903	0.775	1.992	–0.163	0.764	0.519
		–3.49	163.689	0.097	0.897	0.801	2.445	0.107	0.797	0.597	125.522	0.239	0.904	0.778	1.991	–0.171	0.767	0.520
		–0.95	163.722	0.084	0.897	0.801	2.444	0.107	0.797	0.597	123.240	0.226	0.905	0.786	1.984	–0.160	0.766	0.523
		–0.02	163.982	0.094	0.897	0.801	2.444	0.125	0.804	0.597	123.408	0.226	0.905	0.786	1.965	–0.141	0.765	0.532
		–1.37	164.157	0.095	0.897	0.800	2.441	0.118	0.803	0.598	122.928	0.228	0.905	0.787	1.98	–0.160	0.766	0.525
		–5.16	164.353	0.095	0.897	0.800	2.426	0.069	0.791	0.603	120.458	0.222	0.906	0.796	1.924	–0.191	0.790	0.552
		–1.21	164.525	0.098	0.897	0.799	2.423	0.040	0.785	0.604	122.076	0.225	0.904	0.790	1.958	–0.221	0.792	0.535

(continued on next page)

Table A1 (continued)

ID	Dominated area	ECQ	Calibration (2003–2005)						Validation (2006–2007)					
			Runoff			NH ₄ -N			Runoff			NH ₄ -N		
			RMSE_Q	Nbias	r	NS	RMSE_C	Nbias	RMSE_Q	Nbias	r	NS	RMSE_C	Nbias
51		-27.47	164.532	0.090	0.897	0.799	2.420	0.074	120.618	0.219	0.905	0.795	1.924	-0.191
52		-2.09	164.566	0.089	0.897	0.799	2.419	0.055	120.108	0.216	0.906	0.797	1.936	-0.203
53		-6.11	164.659	0.105	0.896	0.799	2.410	0.047	121.844	0.232	0.906	0.791	1.942	-0.219
54		-12.73	164.708	0.097	0.896	0.799	2.401	0.036	121.213	0.222	0.905	0.793	1.942	-0.217
55		-0.27	165.166	0.086	0.896	0.798	2.399	0.053	119.617	0.213	0.905	0.799	1.924	-0.206
56		-0.43	165.621	0.086	0.896	0.797	2.396	0.035	119.413	0.213	0.906	0.799	1.951	-0.231
57		-4.13	165.644	0.078	0.896	0.797	2.395	0.056	118.952	0.205	0.905	0.801	1.913	-0.204
58	Dominated section for Q improvement	-0.25	166.874	0.077	0.895	0.794	2.390	0.025	119.505	0.205	0.903	0.799	1.963	-0.243
59		-0.11	169.864	0.060	0.893	0.786	2.386	0.028	118.716	0.189	0.902	0.802	1.958	-0.234
60		-0.01	171.116	0.056	0.892	0.783	2.385	0.037	119.121	0.184	0.901	0.800	1.949	-0.228
61		-0.10	172.240	0.049	0.892	0.780	2.384	0.030	117.160	0.174	0.904	0.807	1.978	-0.232
62		-0.03	178.182	0.028	0.889	0.765	2.382	0.034	117.418	0.159	0.903	0.806	1.916	-0.205
63		-0.02	179.299	0.032	0.888	0.762	2.381	0.033	119.219	0.162	0.900	0.800	1.988	-0.235
64		-0.02	193.277	-0.027	0.886	0.723	2.377	0.037	113.605	0.107	0.910	0.818	1.98	-0.217
65		0.00	207.119	-0.058	0.880	0.682	2.376	0.039	119.171	0.070	0.906	0.800	1.976	-0.189
66		-0.05	214.016	-0.061	0.878	0.661	2.372	0.036	121.776	0.078	0.904	0.791	1.952	-0.202
67		0.00	257.246	-0.076	0.844	0.510	2.371	0.068	166.637	0.063	0.844	0.609	1.987	-0.208
68		-0.13	262.046	-0.078	0.842	0.491	2.365	0.067	170.223	0.067	0.839	0.592	1.984	-0.213
69		-0.02	269.580	-0.089	0.838	0.461	2.364	0.084	175.975	0.048	0.835	0.564	1.995	-0.198
70		-0.07	276.833	-0.103	0.837	0.432	2.359	0.080	177.244	0.033	0.839	0.558	1.998	-0.197

performance of NH₄-N concentration. Managers and other stake-holders could choose a satisfying solution according to specific objectives.

- (3) The traditional step-by-step procedure just achieved the local optimum of runoff simulation, and there was a great potential to improve the NH₄-N simulation with the slight sacrifice of runoff simulation performance. This procedure was not able to deliver the reasonable solutions for all of the considered processes in the integrated water system model, due to the high level of interactions of the multi-process, the underutilization of the multi-source observations and error accumulations.

In our study, only the parameter uncertainty about the runoff and water quality simulations was investigated. Besides this uncertainty source, the simulation performances were also affected by the uncertainties of data input, model structure and calibration observations because of the complicated model structure and numerous indispensable input data sets (Yang et al., 2008; Li et al., 2010a; Zhang et al., 2016). More attentions should be paid to addressing the effects of all uncertainty sources. Advanced analysis technologies would benefit the future model improvement and parameter optimization, such as Bayesian method (Yang et al., 2007; Li et al., 2010c; Yen et al., 2014), autoregressive error models (Duan et al., 1988; Yang et al., 2008), data assimilation (Vrugt et al., 2005), and sequential data assimilation (Moradkhani et al., 2005).

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Appendix A.

See Table A1.

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