MIKE 11 model-based water quality model as a tool for the evaluation of water quality management plans

J. Liang, Q. Yang, T. Sun, J. D. Martin, H. Sun and Lei Li

ABSTRACT

Water quality models are important tools to test the effectiveness of alternative management plans on the water quality of water bodies. The main aim of this study was to develop and demonstrate use of a water quality model as a tool for evaluation of alternative water management scenarios for the river basin of Beijing, China. Considering Lao Hewan river landscape water circulation patterns and water quality protection programme, hydrodynamic module, structure operation module, advection/dispersion module and ECOlab module in the MIKE 11 model system, the circulating water drainage system and water quality model have been developed for water protection measures. Modelled results indicate the simulated biochemical oxygen demand, chemical oxygen demand, ammonia and total phosphorus concentration evolve in a general increasing trend for the first scenario since there are no water purification measures taken in this scenario; for the second scenario, the simulated water quality showed a slight decreasing trend in both sites, and better than that of scenario I due to considering the water circulation with a volume of 40,000 m^3/d in both sites and the purification function of the wetlands of the Centre Lake. Simulated concentrations of pollutants in scenario III are lower than in scenarios I and II, due to the strengthened purification measures (horizontal subsurface flow wetland and surface flow wetland) implemented.

Key words | Beijing, MIKE 11, modelling, water quality model

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INTRODUCTION

Water quality models are important tools to identify water quality modelling approaches that could be used to test the efficacy of alternative water management actions on water quality constituents. Various complex water quality models (one-dimensional (1-D), two-dimensional (2-D), or even three-dimensional (3-D)) have been developed and extensively applied to evaluate the response of a river water quality to several management scenarios. Many of these water quality models are basically extensions of the simple biochemical oxygen demand (BOD)-dissolved oxygen (DO) model (e.g., QUAL2K) whereas there are other more detailed analytical ecological models. During the last decades, the trend was to develop more detailed water quality models (Department of Energy and Resources Management 1968, 1970; Thomann 1998; Andersen *et al.* 2001; Shanahan *et al.* 2001; Butts *et al.* 2004; Parker *et al.* 2009; Ahmed 2010).

However, the models' increased complexity was not always associated with high precision of models' results, as discussed by Young *et al.* (1996). Therefore, the greatest challenge is to find a balance between models' complexity and reliability of the results (Noutsopoulos & Kyprianou 2014).

MIKE 11, which was developed by the Danish Hydraulic Institute (DHI), is a software package for modelling conditions in rivers, lakes, reservoirs, irrigation canals and other inland water systems (Danish Hydraulic Institute 2007a, b, c). It is an implicit finite difference model for 1-D unsteady flow computation and can be applied to looped networks and quasi-2-D flow simulation. MIKE 11 consists of a set of modules that allow users to specify the type of

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hydrologic process to simulate. In contrast to simpler models, MIKE 11 includes detailed heat balance calculations, and hence reliable calculation of water temperature, and a comprehensive set of interactions between water quality determinants. The model includes modules to handle various data types. One of these modules is the water quality module, ECOlab, which is a dimensionless ecological process toolbox (can be applied to MIKE 11, MIKE 21, MIKE 3 and MIKE SHE) and forms the basis of the water quality simulation that generally requires hydrodynamic (HD) and advection/dispersion (AD) inputs. ECOlab is an extension of the transport-dispersion module and is utilized to simulate the reaction processes of multi-compound systems and models a variety of biochemical interaction processes, including BOD and DO computations and simulations of nutrients, macrophytes and plankton. It has been extensively applied in water quality simulation (Snead 2000; Liu *et al.* 2009; Wang *et al.* 2009; Eisakhani *et al.* 2012).

Beijing, as the capital of China, initiates a programme of 'The Future Science and Technology Centre' (FSTC). The development of the FSTC orientates the development of applied science and technology in China, as a base for relevant industries in China to conduct applied research with the highest levels of talented innovation and entrepreneurship. The Science and Technology Waterside Forest Park is located in the northwest of the FSTC and is the core of the ecological zones of the FSTC. Therefore, the overall protection and long-term stability of the water quality of the FSTC Waterside Park is significantly important.

To better reflect environmental characteristics of the water of the Future Science and Technology Waterside Forest Park and to predict the temporal and spatial variations in water quality, in accordance with the water system features, a HD-water quality model is built to conduct simulations with different options. While selecting the model, comprehensive and integrative factors are considered, including data availability and advanced nature. Eventually, the HD module, structure operation (SO) module, AD module and ECOlab module of the MIKE were selected. The simulated pollutants include BOD, COD, ammonia and total phosphorus (TP) loads, with different water protection measures proposed incorporating water utilization schemes. The simulated results will provide useful insights for water quality improvement in the study area.

MATERIALS AND METHODS

Description of MIKE 11 model

MIKE 11 is a model for simulating flows, water quality and sediment transport in channels, rivers, irrigation systems and estuaries. The original channel simulation in MIKE SHE was relatively simple and had limited capabilities. MIKE SHE and MIKE 11 can be used independently or together (Danish Hydraulic Institute 1998a, b, 2001, 2003).

This study adopts the MIKE 11 model system's HD module, which is currently the most widely used HD simulation software, offering features of computational stability, high precision and reliability etc., making simulation of gates, water pumps and various types of hydraulic structures convenient and flexible, where it can be used in the situation of several buildings and for complexity control. This model is based on 1-D non-constant flow equations established by Saint-Venant Abbott using the six-point non-central implicit scheme adopted in pursuit of a solution.

ECOlab is a recently developed water quality and ecological modelling tool (Figure 1) developed by the DHI on the basis of the conventional water quality model. It was developed using advanced concepts and techniques, and it not only allows the modification of the module in accordance with the actual situation, but is also able to create other water quality response models. This not only meets the requirements of the various water reaction processes, but also makes the water quality modelling more flexible and convenient. ECOlab is accompanied by the water quality template, which is divided into six levels, from the simplest BOD-COD relationship model to providing complex water quality response models in processes such as nitrification, denitrification, sediment precipitation and resuspension, and sediment oxygenation, etc. At the same time, the model system consists of eutrophication models and heavy metals within the model. In eutrophication models, the nitrogen cycle, oxygen balance, and the growth and distribution of aquatic organisms,

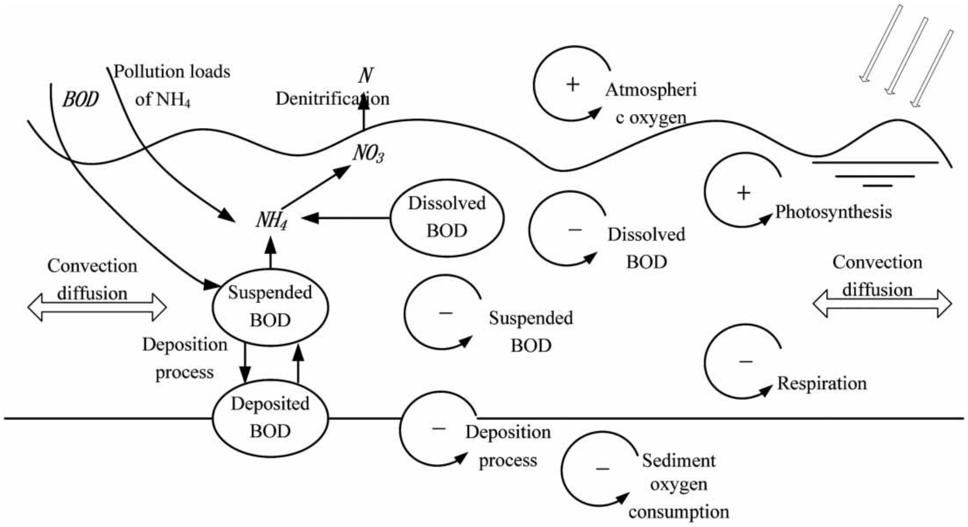

Figure 1 | ECOlab model of water quality reaction process.

phytoplankton and underwater plants are simulated in the water body. The heavy metal model is used to stimulate the contamination diffusion of metals and their chemical substances resulting from various causes, and can stimulate the metal concentrations in various forms such as dissolution, suspension and adsorption or deposition, and can be conducted as inverse analysis.

The choice of water quality indicators should be able to reflect upon the current situation as well as the possible water quality that may appear in the future. If the consideration of indicators is excessively complicated, it often not only fails to improve the model simulation accuracy, but on the contrary, introduces too many uncertainties that will reduce the simulation accuracy. On the basis of currently available data, the key water quality indicators of the selected model are the following five items: DO, BOD_5, total nitrogen (TN) ($NH_3 + NO_3$-N), TP (OP + PP) and COD. Their biochemical reactions are described according to first-order kinetics equation.

DO balance equation

In the river water, the two processes, namely oxygen production and oxygen consumption, occur simultaneously. The process of oxygen production primarily comes from atmospheric reaeration and photosynthesis of algae and aquatic plants. The process of oxygen consumption in the river mainly includes the oxidation of carbon and nitrogen compounds and other reducing substances, the respiration of aquatic animals, plants and microbes, and sediment oxygen consumption.

Combining these factors, the water oxygen balanced equation can be written as

$$\begin{aligned}\frac{\mathrm{dDO}}{\mathrm{d}t} &= +K_2(C_S - \mathrm{DO}) - K_3\mathrm{BOD}\theta_3^{(T-20)}\frac{\mathrm{DO}^2}{K_S + \mathrm{DO}^2} \\ &\quad - Y_1K_4\mathrm{NH}_4\theta_4^{(T-20)}\frac{\mathrm{DO}^2}{K_S + \mathrm{DO}^2}R\theta_2^{(T-20)} + P_1 - B_1\end{aligned} \tag{1}$$

where K_2, K_3 and K_4, at 20 °C are the atmospheric reaeration coefficient (1/d), BOD degradation coefficient (1/d) and nitrification coefficient (1/d), respectively; DO, NH_4 and BOD represent concentrations of dissolved oxygen, ammonia and biochemical oxygen demand (mg/L), respectively; C_s is the concentration of saturated dissolved oxygen (mg/L); K_s as half-saturation constant of dissolved oxygen (mg/L); Y_1 is the conversion rate of BOD generating ammonia (mg ($NH_4 - N$)mg (BOD)); R represents the respiration rate at 20 °C ($g(O_2)/m^2/d$); θ_3, θ_4 and θ_2 are the Arrhenius temperature coefficients of the respiration during BOD degradation process and nitrification process; B_1 is the constant for sediment oxygen demand ($g(O_2)/m^2/d$); P_1 is the photosynthetic oxygen production rate ($g(O_2)/m^2/d$).

Balance equation of BOD

The main processes that affect the BOD content in river water include organics degradation, deposition and resuspension. The balance equation for BOD is as follows:

$$\frac{\mathrm{dBOD}}{\mathrm{d}t} = -K_3\mathrm{BOD}\theta_3^{(T-20)}\frac{\mathrm{DO}^2}{K_S+\mathrm{DO}^2} + S_1/h_1 - K_5\mathrm{BOD}/h_1 \tag{2}$$

where S_1 represents the BOD resuspension rate $(\mathrm{g(O_2)/m^2/d})$, when BOD is less than a certain critical flow velocity, resuspension does not occur; K_5 is the sedimentation rate for the BOD suspension; h_1 is the depth (m), when BOD is greater than a certain critical flow velocity, sedimentation does not occur.

Balance equation of ammonia

The main processes that affect the ammonia content in river water include production of ammonia during organics degradation, absorption of ammonia by micro-organisms and plants, consumption of ammonia by nitrification reactions, etc. The balance equation for ammonia is

$$\frac{\mathrm{dNH_4}}{\mathrm{d}t} + Y_1K_3\mathrm{BOD}\theta_3^{(T-20)}\frac{\mathrm{DO}^2}{K_s+\mathrm{DO}^2} - K_4\mathrm{NH_4}\theta_4^{(T-20)} \frac{\mathrm{DO}^2}{K_s+\mathrm{DO}^2} - 0.66(P-R) - 0.109K_3\mathrm{BOD}\theta_3^{(T-20)}\frac{\mathrm{DO}^2}{K_s+\mathrm{DO}^2} \tag{3}$$

Balance equation of nitrate

The main processes that affect the nitrate content in river water include nitrification and denitrification. The balance equation for nitrate is

$$\frac{\mathrm{dNO_3}}{\mathrm{d}x} = +K_4\mathrm{NH_4}\theta_4^{(T-20)}\frac{\mathrm{DO}^2}{K_s+\mathrm{DO}^2} - K_6\mathrm{NO_3}\theta_6^{(T-20)} \tag{4}$$

Balance equation for COD

Since the COD variable includes not only organics, but also some inorganic substances, in response to water ecology, there is some overlap with other variables and it is difficult to divide, therefore the ECOlab model will not consider COD as a measure acting on water quality reactions, and at present, there is no template. When taking into account the water quality of the environment in China, the evaluation of COD is usually an important indicator of pollution. Thus study refers to the BOD reaction equation, using ECOlab to establish the COD reaction template.

$$\frac{\mathrm{dCOD}}{\mathrm{d}t} = -K_{\mathrm{COD}}\mathrm{COD}\theta_{\mathrm{COD}}^{(T-20)}\frac{\mathrm{DO}^2}{K_s+\mathrm{DO}^2} + S_{\mathrm{COD}}/h_1 - K_{\mathrm{RE-COD}}/h_1 \tag{5}$$

where K_{COD} is the degradation coefficient of COD at 20 °C (1/d); θ_{COD} is the Arrhenius temperature coefficient of COD degradation; S_{COD} is the resuspension rate of COD $(\mathrm{g/m^2/d})$; $K_{\mathrm{RE-COD}}$ is the sedimentation rate for COD suspension.

RESULTS AND DISCUSSION

Model overview

The simulated domain is located at the Western District (indicated with a box in Figure 2). To conduct the HD simulation of the river, first, the drainage network is generalized reasonably within the simulation scope, ensuring that on the basic principles of the generalizations of river networks, it reflects the basic hydraulic characteristics of the natural river, that is, the river network after the generalizations regarding carrying capacity and regulation and storage capacity is close to those of the actual river, and is as simple as possible under the preconditions of meeting the research. The four rivers are considered in the model, and the detailed lengths are listed in Table 1. According to the landscape design plan, the Future Science and Technology Waterside Forest Park including the Lao Hewan, the Centre Lake, the Cascade Bloom, the Wetland Landscape and other water bodies have been generalized. Among the generalizations regarding the Lao Hewan, the Centre Lake and the Wetland Landscape, the generalizations of the river length are carried out based on the length and width of the actual design, mainly to ensure the water balance.

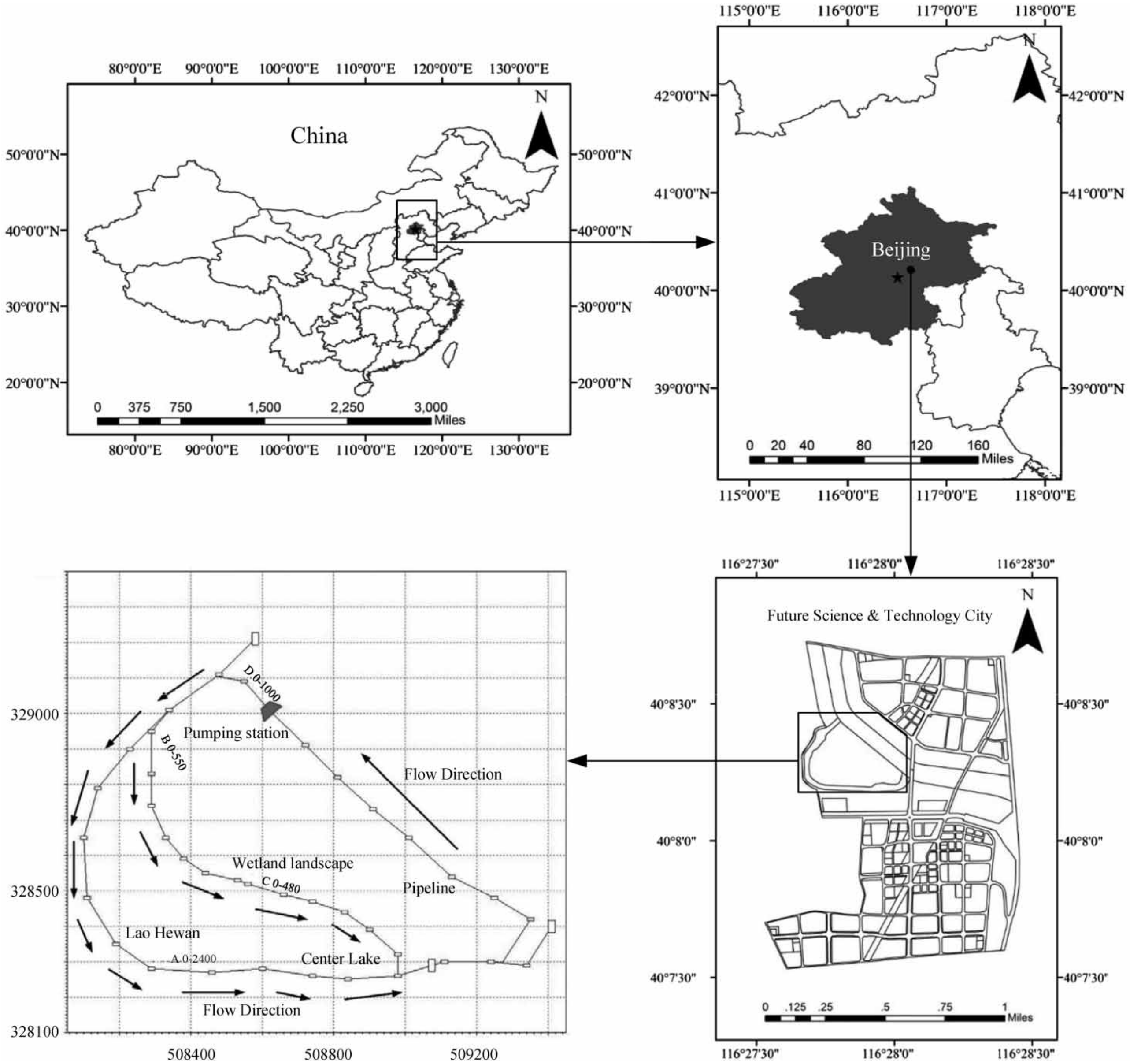

Figure 2 | Location map of study area and conceptualized 1-D HD model.

Table 1 | The rivers included in 1-D river network model

	Mileage (m)			
River name	**Upstream**	**Downstream**	**River width (m)**	**Length (m)**
Lao Hewan	0	2,400	72.92	2,400
Wetland landscape	0	550	109.1	550
Centre water	0	480	187	480
Connection canal	0	1,000	26	1,000

The generalization is illustrated in Figure 2, in which the pumping station accomplishes the head to tail connection of Lao Hewan, and thus, achieves the water cycle. The model takes into account the water balance as shown in the following equation:

$$\begin{aligned}\text{Water demand} &= \text{Evaporation} + \text{Infiltration amount}\\ &\quad + \text{Irrigation capacity} - \text{Rainfall}\end{aligned}$$

Parameter selection for HD model

The roughness rate of the riverbed has a direct impact on the calculation of HD force and is the most critical factor in the HD simulation. The riverbed roughness rate can initially be set according to the actual situation, obtained again by model calibration. Since the water system is in the design stage, there are no monitoring values. Therefore, in this study, the roughness rate is set at 0.025 according to the basic situation of river course in Beijing city.

Basic conditions setting of the model

In this simulation, because the project has not yet been carried out, the water quality monitoring data of the river during the engineering running was not obtained; therefore, it is not possible to conduct the model validation and parameter calibration.

In this simulation model, all the required parameters of water quality largely draw reference from the results of model parameter calibration from recent simulation studies of Beijing lakes and reservoirs.

The diffusion in the river is mainly dispersion; the diffusion coefficient as a calibration parameter is an important fundamental parameter of conducting the water quality model, and usually can make use of a conservative substance to carry out the calibration. The diffusion coefficient is the hybrid diffusion coefficient including molecular diffusion, turbulent diffusion, shear diffusion and other factors. Empirical values are: Brook 1–5 m^2/s; River 5–20 m^2/s. According to these characteristics of river, the diffusion coefficient is taken as 5 m^2/s and the related water quality modelling parameters are summarized in Table 2.

Analysis and design of model source concourses

Using the inflow water quality conditions of Class IV of 'Surface Water Environmental Quality Standards' (GB3838-2002 2002), the maximum concentration of inflow water quality indicators is shown in Table 3. The temperature data using the average daily value from 1956 to 2000, are shown in Figure 3.

Multi-year average value of precipitation is listed in Table 4. The water quality indicator of precipitation used in the model is the average of multiple monitoring data from 1956 to 2000, which is listed in Table 5.

Table 2 | Water quality parameters used in the model

Definition and unit	Parameter range	Parameter value
Reaction rate of first-order nitrification at 20 °C, day^{-1}	0.01–0.3	0.105
Temperature coefficient of first-order nitrification, °C		1.088
Reaction rate of first-order denitrification at 20 °C, day^{-1}	0.05–0.3	0.1
Temperature coefficient of first-order denitrification, °C		1.16
Rate of first-order degradation of COD at 20 °C, day^{-1}	0.1–0.2	0.13
First-order reaction rate of BOD at 20 °C, day^{-1}	0.1–0.2	0.13
Temperature coefficient of first-order reaction rate of BOD, °C	1.02–1.09	1.07
Oxygen demand for nitrification, $g/O_2/gNH_3$-N		4.57
Amount of ammonia absorbed by plants, g/NH3-N/g/O_2		0.066
Typical output rate of phosphorus release in BOD degradation, gP/gO_2	0.01–0.09	0.08
Amount of phosphorus absorbed by plants, gP/gO_2		0.091
Degradation rate of particulate phosphorus (PP), day^{-1}	0.1–0.2	0.1
Oxygen production rate of photosynthesis	According to the formula, related to temperature and flow rate	
Oxygen demand for nitrification 4.57 $g/O_2/gNH_3$-N		4.57

Table 3 | Inflow concentration index

Input indicator	Ammonia	TN	TP	COD	DO	BOD_5
Concentration (mg/L)	1.5	10	0.3	30	3	6

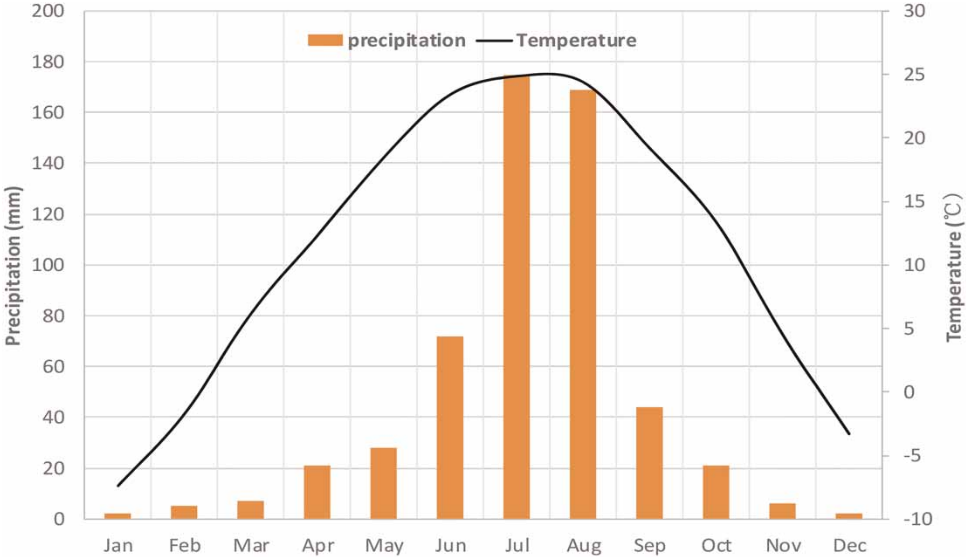

Figure 3 | The average monthly temperature and precipitation in Beijing plains from 1956 to 2000.

Table 4 | The monthly average precipitation in Beijing

Month	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Rainfall (mm)	2	5	7	21	28	72	175	169	44	21	6	2

Table 5 | The water quality concentration of precipitation

Input indicator	Ammonia	TP	COD	DO	BOD_5
Concentration (mg/L)	4	0.1	10	7.5	1

Scenario analysis

Three scenarios considering the present and future water development schemes, are proposed, which are summarized in Table 6.

Scenario I

The landscape drainage system will require 7,000 m^3/d of recycled water, and the required amount of 6,449 m^3/d water of the Western District (evaporation leakage, irrigation and external discharge) will be diverted to Lao Hewan. The amount of water required as the source term and the external displacement will be taken as the source of the input model; in the case that no measures are taken, the simulation of water quality changes in the Western District drainage system is carried out as shown in Figure 4.

It can be seen from Figure 4 that the Class IV water is introduced into the landscape water body; in the case that no measures are taken, gradual deterioration of water quality occurs with time, and the indicators within 1 year after the replenishment exceed standards of Class V. An exception occurs with ammonia, where it can be observed that the maximum concentration of ammonia appears about September, which corresponds to later summer/early fall in Beijing.

Table 6 | The regulation scenarios

Scenario designation	Scenario description
Scenario I: advanced treatment of recycled water to supplement the lake	The use of advanced treatment of recycled water to supplement the lake (Surface Water Quality Standard Class IV), do not take any circulation and purification measures
Scenario II: replenishment of recycled water + circulation + wetland landscape	The use of advanced treatment of recycled water to supplement the lake (Surface Water Quality Water Standard Class IV), consider the water circulation of 40,000 m^3/d and wetland landscape
Scenario III: replenishment of recycled water + circulation + wetland landscape + enhanced treatment measures	The use of advanced treatment of recycled water to supplement the lake (Surface Water Quality Water Standard Class IV), consider the water circulation of 40,000 m^3/d and wetland landscape, and increase enhanced purification measures (water cycle and aeration)

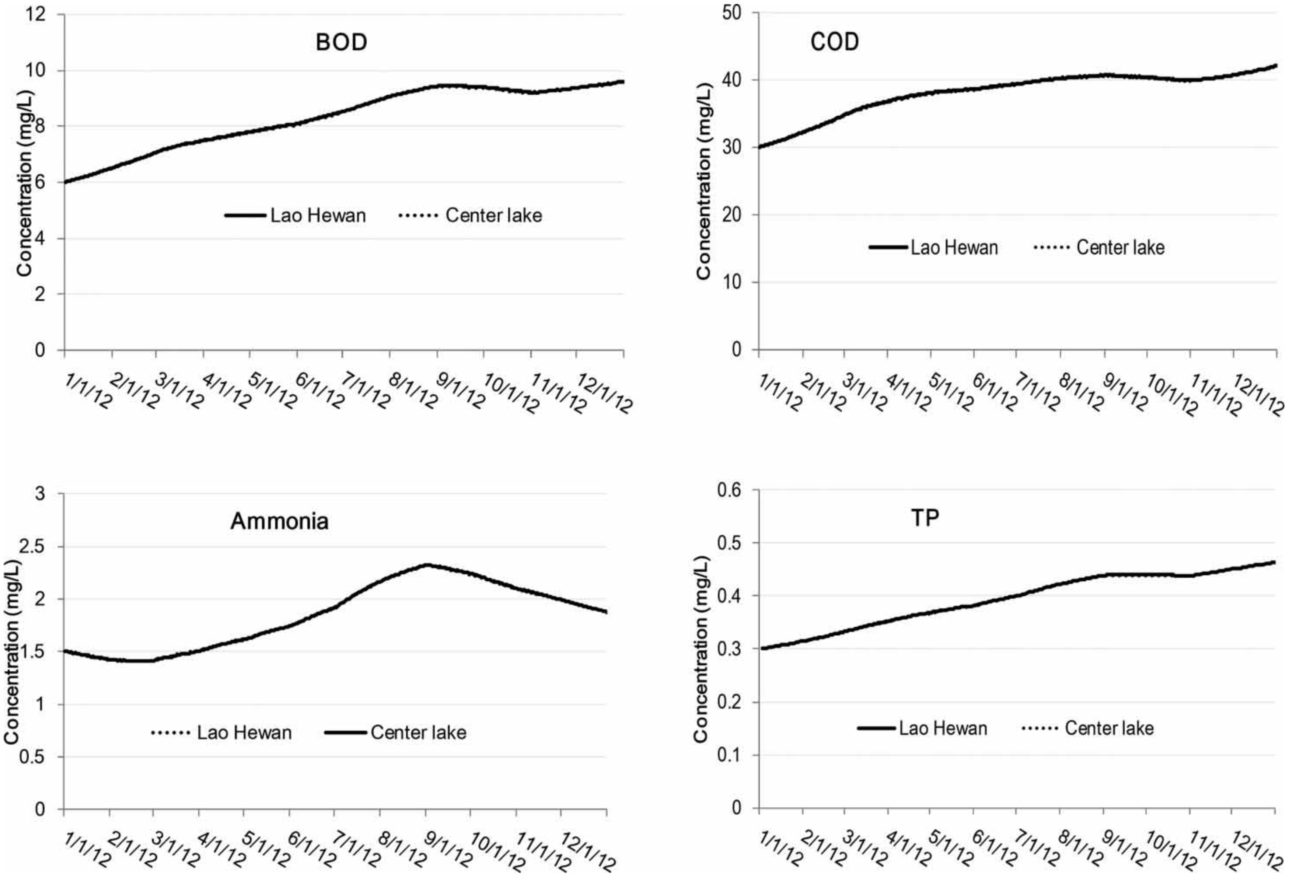

Figure 4 | Changing trends of water quality in scenario I.

Scenario II

Scenario II is based on scenario I, in addition to the volume of water circulation increased to 40,000 m^3/d, it considers wetland landscape of the Centre Lake. The simulated concentrations of pollutants are illustrated in Figure 5.

After increasing the water circulation of Lao Hewan and the Centre Lake, as well as considering the purification function of the wetlands in Centre Lake, the water quality

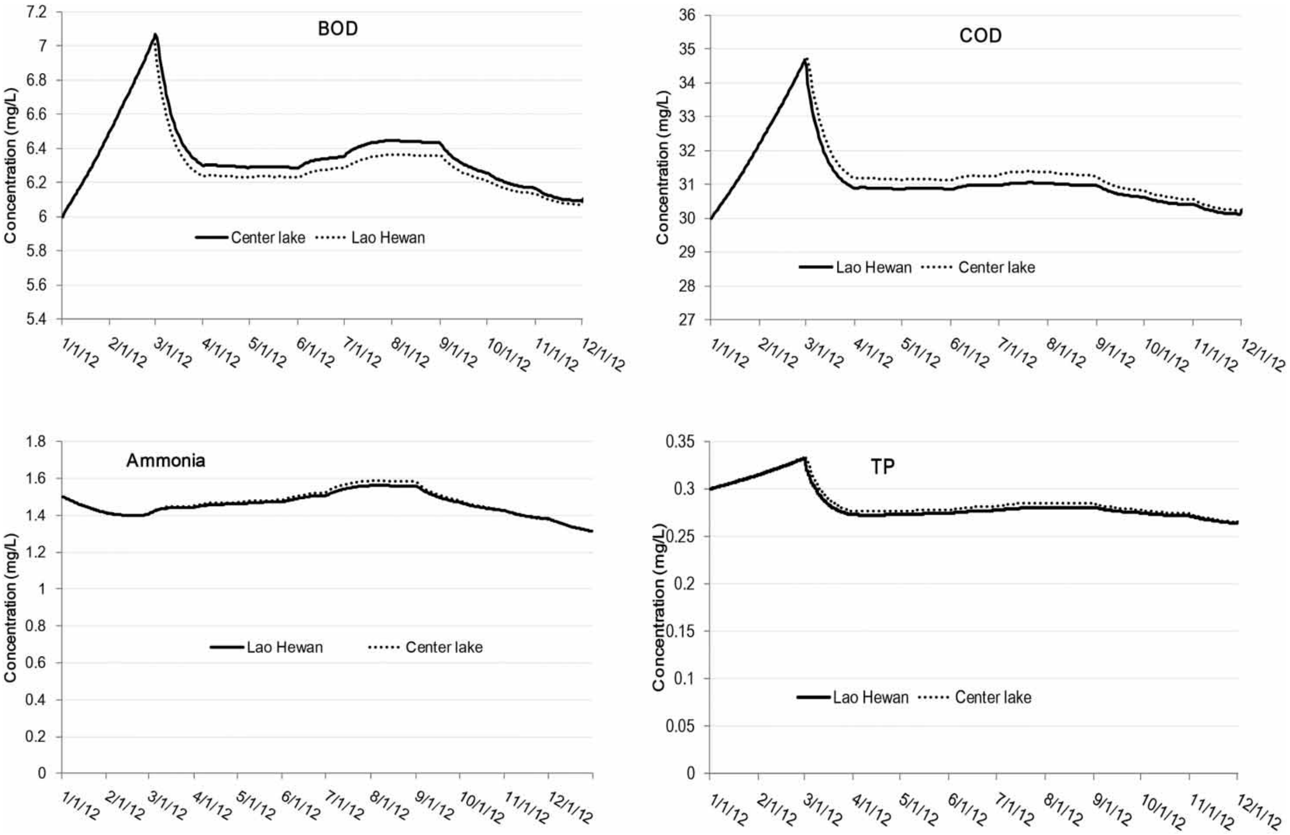

Figure 5 | Changing trends of water quality in scenario II.

conditions in scenario II are better in comparison to those of scenario I; however, it still does not satisfy the objectives and requirements of water quality, thus strengthening measures should be enhanced for pure water.

Scenario III

Scenario III is based on scenario II, the strengthening purification measures are enhanced, and the strengthening measures include horizontal subsurface flow wetland and surface flow wetland. The simulation results are shown in Figure 6.

As can be seen from Figure 6, after considering water circulation on the basis of the surface stream wetland and the horizontal subsurface flow wetland, the water quality conditions improved significantly, and satisfy the requirements of Class IV most of the time. In actual operation, increasing water volume circulation, extending aeration time and other measures can be taken into account to ensure water quality to meet the requirements.

CONCLUSION

This paper presents a study on the development of a water quality model as a tool for the evaluation of alternative water management scenarios for the river basin of Beijing, China. According to the corresponding design plan, some of the critical techniques and key technologies in the modelling (such as river generalization, module coupling, contrast determination of boundary conditions, etc.) are employed to conduct the study. The HD module, SO module, AD module and ECOlab module in the MIKE 11 model system were employed to perform a simulation of water quality change considering the circulating water drainage system and water quality model have been

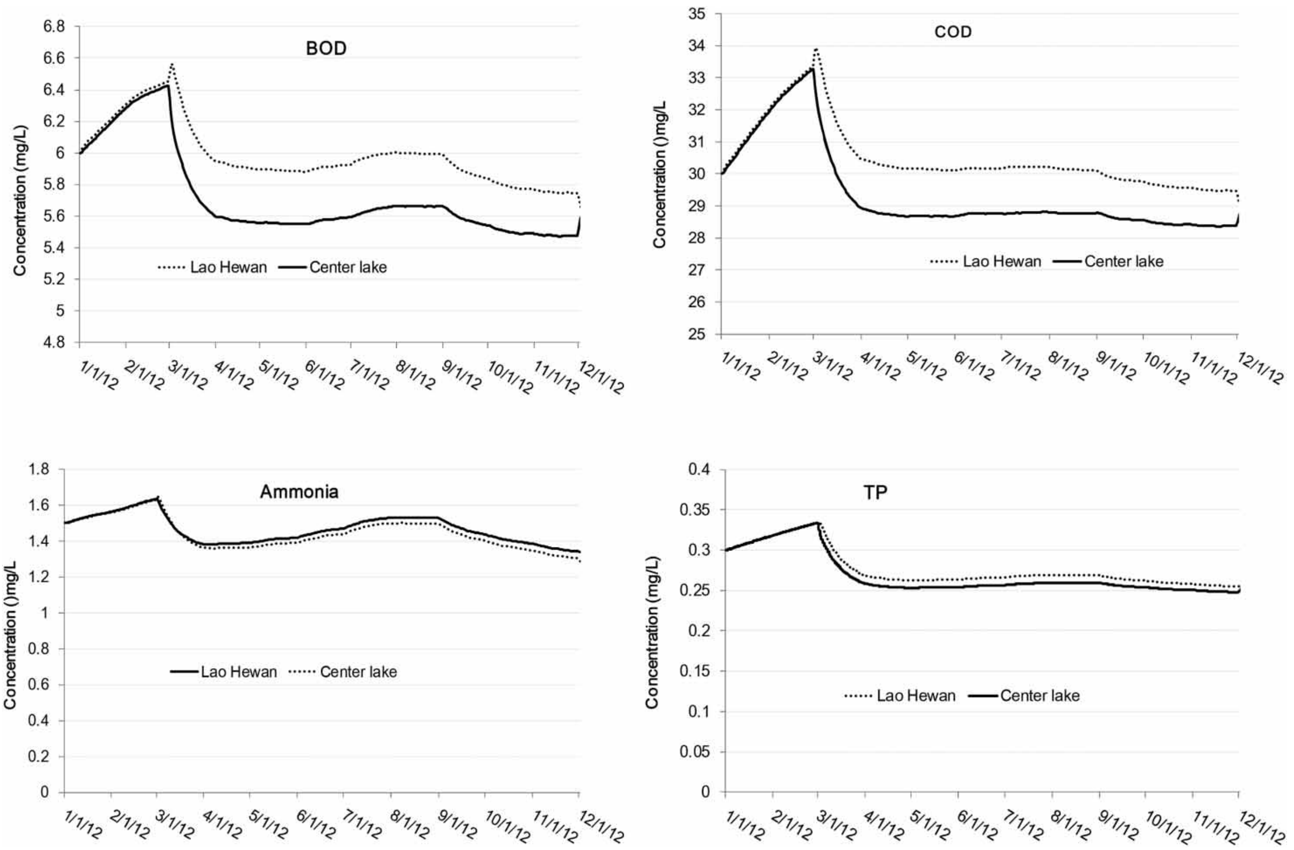

Figure 6 | Changing trends of water quality in scenario III.

applied for water protection measures and the simulation of the multi-programme evaluation. Results for simulated BOD, COD, ammonia and TP loads are presented in the form of time series for four different water development scenarios. The simulated pollutant loads for different scenarios indicate that if Class IV water is introduced into the landscape water body and no water protection measures are taken, water quality will gradually deteriorate, and exceed standards of Class V after 1 year. After increasing the water circulation, as well as considering the purification function of the wetlands, the water quality is improved to some degree; however, it still does not satisfy the objectives and requirements of water quality. Further, after considering water circulation on the basis of the surface stream wetland and the horizontal subsurface flow wetland, the water quality is improved significantly, and satisfies the requirements of Class IV most of the time. Increasing water volume circulation, extending aeration time and other measures can be taken into account to ensure water quality to meet the requirements.

The dynamic changes in water quality planning can be used to demonstrate the different planning scenarios in the study area, which greatly facilitates the comparison of different planning scenarios. The present method is conducive to the scientific selection and development of water quality maintenance programme and can be used to improve the efficiency of water management planning. Furthermore, an extension of the simple quality model in order to provide for uncertainty assessment should be conducted in the future.

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