SPECIAL TOPIC
Simulation and Regulation of Water Cycle in Haihe River Basin

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Integrated simulation and assessment of water quantity and quality for a river under changing environmental conditions

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The water cycle and water resources within river basins under changing environmental conditions undergo profound changes, which have significant effects on the water environment of the river. Owing to the water resources demanded for economic and social development, water quantity and quality are becoming the core constraints of water resources development and utilization. In this paper, the dual attributes of water resources, progress into research regarding water quantity and quality joint assessment and simulation and the shortcomings associated with these techniques are summarized and described with respect to water quantity and quality. The results indicated that under the current environmental conditions, the method used for traditional water quality assessment of single water bodies cannot meet the requirements for water resources management. Moreover, a coupled hydrodynamic and water quality numerical model for river networks and lakes that applies to the river water environment system was developed for the river network flow and pollutant migration and transformation process and validated. This validation revealed that the error between the simulated values calculated by the model and the monitored values was small, meeting the application requirements and realizing the integrated and dynamic simulation of water quantity and quality of the river water environmental system. On this basis, the integrated simulation model was applied to the Luanhe River Basin.

changing environment, water quantity and quality, integrated simulation and assessment, Luanhe River Basin

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The demand for water is continually increasing in many regions of the world owing to the growing population, which is leading to increased pressure on global water resources as a result of consumption, land use changes, urbanization and climatic changes [1]. These factors all exert individual and synergistic effects on global water resources and are gradually changing the global environment. All of the aforementioned pressures contribute to the quality and quantity of water resources, and the results of many studies have predicted that climatic changes can influence the supply of water and the corresponding quantity and quality [2–4]. In addition, pressure brought by anthropogenic activities such as land use, urbanization, population growth, energy utilization and economic growth can have a greater impact on the global water cycle than that of recent or the expected climatic changes [5]. Because of the interdependent nature of water resources under global climatic changes and the uncertainty of global pressures, the main target of river water resource management is meeting the demands of water quantity, water quality and protection of the ecological environment [6]. In this study, a coupled model of hydrodynamics and water quality for river networks and lakes that applies to the river water environment system was developed based on the evolving nature of the water cycle of river basins under climatic changes [7–9] and the migration and conversion process of river networks flow and pollutants. The developed model was then applied in the Luanhe River Basin.

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1 The background of integrated simulation of water quantity and quality

In nature, water quantity and quality are basic attributes of aquatic systems that are mutually dependent on each other for existence; therefore, neither can be omitted. In response to the demands for water resources management, many domestic and foreign scholars have conducted a great deal research to enable assessment and simulation of water quantity and quality. Tetsuya et al. [10] constructed and implemented a comprehensive model of water quantity and quality for the Weihe River Basin. Xia et al. [11–13] summarized the comprehensive management method for water quantity and quality and corresponding obstacles and developed an integrated assessment method to investigate surface water inflow and consumption. Gabriel et al. [14,15] combined the water resource allocation and impact analysis of water quality to construct decision support tools for integrated water quantity and quality management. Chen et al. [16,17] investigated the effects of water use in agriculture on the quality of water in the Yellow River and provided a comprehensive assessment of the water quantity and quality in the Yellow River Basin. Aertgeerts [18] introduced the management situation of water resources quantity and quality in Europe and Central Asia based on health criterion. Tao et al. [19] developed an optimal operation model for water quantity and quality directed at drainage basins. Through randomly dimming the artificial neural network. Chaves et al. [20] generated a reservoir operation strategy that concerns both the water quantity and quality. Chaparro et al. [21] investigated the regular patterns of spatial variability of the water quantity and quality of the Orontes River. Jochen et al. [22] investigated the dynamic effects of operation of the THC-Tuyamuyun reservoir on water quantity and quality. Using the element free method, Gu et al. [23] investigated seasonal variations in total nitrogen and total phosphorus in the Miyun Reservoir. Zeng et al. [24–26] investigated the use of numerical simulations of river water quality including model coupling and improvement. Furthermore, many scholars [27–32] have employed integrated assessment theory to determine surface water quantity and quality.

However, owing to gradual amplification of the cumulative effects of the environment on water quality, many aquatic systems cannot meet the demands for water resource development and utilization. From a general point of view, the water quantity and quality simulation and assessment method has several shortcomings, which are as follows: (1) Separate assessment. The water quantity and quality interaction mechanism is undefined and the assessment is separate. (2) Static assessment. The integrated assessment of water quantity and quality can only evaluate the static water without considering changes in the temporal and spatial properties. (3) Limit of spatial and temporal scale. The simulation and evaluation scale of the integrated assessment of water quantity and quality do not match. (4) Single evaluation object. Currently, many assessments of water quantity and quality only consider a single water body of rivers and lakes, while studies providing comprehensive assessments of multiple properties of water bodies within a river system are not common.

To address these problems, it is necessary to combine the comprehensive assessment method with the currently available water resources [33] and consider pollutants generated from the processes involved in the water cycle such as runoff generation, runoff pooling, development and utilization, and drainage to reveal the interaction mechanism of water quantity and quality of different water bodies. In addition, dynamic methods should be implemented to further establish a new scientific system for integrated simulation and assessment of river water quantity and quality to provide powerful support for the management and protection of water resources.

2 Integrated assessment model for river water quantity and quality

River water environments are primarily composed of water bodies of river networks and reservoirs. The water flows constantly in the space of existing forms and features of water resources, and the pollutants migrate, proliferate, degrade, absorb, and subside with the flow of the natural water bodies, which is directly influenced by hydrology and hydraulic factors. Therefore, the distribution of water quality within a river can be comprehensively understood through construction of a hydrodynamic and water quality model for the river water environment system to simulate dynamic changes in water quantity and quality.

2.1 Mathematical model equations of hydrodynamics and water quality for river networks

(1) One-dimensional unsteady flow equation. Apply Saint-Venant equations [34] to describe the flow form of the river water body, and the basic equation is:

Continuity equation:

$$B\frac{\partial z}{\partial t}+\frac{\partial Q}{\partial s}=q\,, \tag{1}$$

Momentum equation:

$$g\frac{\partial z}{\partial s}+\frac{\partial}{\partial t}\left(\frac{Q}{A}\right)+\frac{Q}{A}\frac{\partial}{\partial s}\left(\frac{Q}{A}\right)+g\frac{|Q|Q}{AC^2R}=0\,, \tag{2}$$

where Q is the flow rate (m^3/s), z is the water level (m), t is time (s), s is the channel length (m), q is the lateral inflow rate (m^3/s), B is the width of the water surface (m), A is the sectional area (m^2), C is the Chezy coefficient ($m^{1/2}/s$), R is the hydraulic radius (m), and g is the acceleration of gravity (m/s^2).

(2) One-dimensional model of water quality. Based on the hydrodynamic model of river networks and lakes, the longitudinal and one-dimensional water quality control equation [35] is:

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}=\frac{\partial}{\partial x}\left(E\frac{\partial C}{\partial x}\right)+\sum S_i\ , \qquad (3)$$

where, C is the concentration of pollutants in rivers and canals as x=x (mg/L), x is the distance from the drain outlet (x=0) to the water flow (m), t is time (h), u is the mean flow rate of river and canal water at the cross section (m/s), E is the river dispersion coefficient (m^2/s), and S_i is the source sink term of pollutants (mg/(L h)). The source sink term includes the sidewise influx of pollutants, as well as the degradation and synthesis of pollutants.

Because the time-varying item, migration item, and proliferation item are basically the same in comprehensive water quality models, the models primarily differ in how many water quality variants are considered. Therefore, when considering the water quality variants (e.g. NH_3-N, COD_{Mn}, TN, TP and DO), the influence of the relationships of physics, chemistry and biology among all variants are reflected in the source and sink terms.

(3) Junction equation. In the hydrodynamic model equations for river networks, the junction equation is established based on two assumptions: (i) The water levels of all sections at the junction are equal, which refers to $z_i=z_j=\cdots=\overline{z}$. As a result, i and j represent the code of each section obtained through junction points, and $\overline{z}$ represents the mean water level at junction points. (ii) The water retention capacity at the junction is zero, and flows into the junction are equal to the flow out of the junction, which refers to $\sum Q_i=0$.

In the water quality model equation for river networks, the pollutants in the water that flows into junctions are fully mixed, the water quality reaches a uniform status and the concentrations of pollutants at all junctions are equal. In the junction equation, the water retention capacity at the junction is not considered, and the water flows gently at the junction; therefore, no water level mutations exist.

2.2 Mathematical model equations of hydrodynamics and water quality for River-type Reservoirs

River-type reservoirs have attributes of both rivers and reservoirs [36], which necessitates the use of vertical and two-dimensional equations of mathematical physics to describe the progression of changes in water quantity and quality. For vertical and two-dimensional models, it is assumed that the water temperature, pollutants and concentrations remain constant at the cross section, while they change with water depth and in the horizontal direction, and the water body of the reservoir is divided into several control volumes along the horizontal and vertical directions, and through calculating the income and expenditure of water temperature, pollutants and nutrients in each control volume to achieve the goal of simulating internal water flow and substance transfer.

Continuity equation

$$\frac{\partial u}{\partial x}+\frac{\partial w}{\partial z}=0\,, \qquad (4)$$

Momentum equation in x direction

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+w\frac{\partial u}{\partial z}=-\frac{1}{\rho}\frac{\partial P}{\partial x}+\frac{\partial}{\partial x}\left(A_x\frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial z}\left(A_z\frac{\partial u}{\partial z}\right), \qquad (5)$$

Momentum equation in z direction

$$\frac{\partial P}{\partial z}=-\rho g\ , \qquad (6)$$

Matter balance equation

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+w\frac{\partial C}{\partial z}=\frac{\partial}{\partial x}\left(D_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial z}\left(D_z\frac{\partial C}{\partial z}\right)+\sum S_i\ , \qquad (7)$$

where, u and w represents the water flow rates along the horizontal and vertical direction (m/s), respectively, C is the substance concentration (mg/L), A_x and A_z represent the turbulent diffusion coefficient in the horizontal and vertical directions (m^2/s), respectively, D_x and D_z represent the dispersion coefficient in the horizontal and vertical directions (m^2/s), respectively, ρ is the water density (g/L), and the other symbols have the same meanings as described above.

2.3 Integrated simulation of river water environment

Currently, one and two-dimensional model coupling generally realizes the allocation solution according to the simulated water level and equal water flow at the joint sections. Figure 1 shows the transition unit used at the joint section to realize the coupling, which is a linkage unit of the one-dimensional model unit and the two-dimensional model unit. Linking conditions are set for the hydrodynamics and water quality according to river water depth and reservoir water lift height. As a result, the linkage for hydrodynamics requires identification of water depth, water flow rate and the inlet and outlet water amount, while the linkage for water quality requires identification of the concentration of water quality variables and pollutant amounts.

3 Validation of integrated simulation model for river water quality and quantity

The integrated simulation model can simulate the hydraulic parameters of different water bodies and water quality variables. According to the characteristics of the simulated and

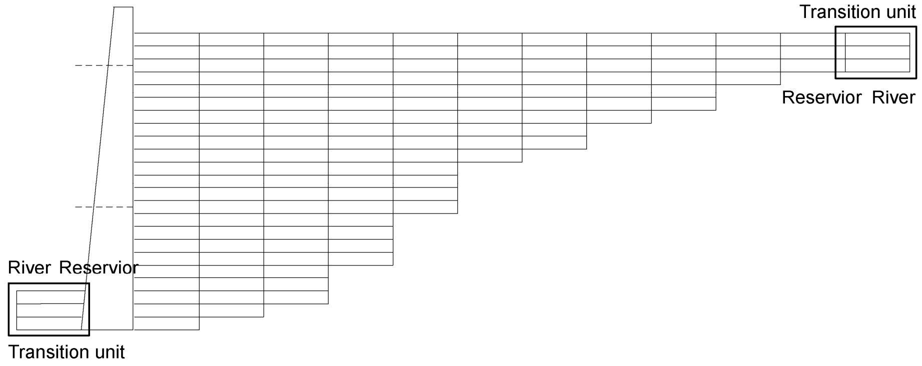

Figure 1 Schematic diagram of one and two-dimensional linkages.

assessed target water bodies and the available monitoring data, validations are conducted to distinguish different water bodies. However, under the current conditions, the hydraulic parameters of the reservoir water can only be analyzed regularly, and the focused water quality variables of river water and reservoir water are different.

3.1 Validation of the hydrodynamics and water quality model for river networks

The model of river hydrodynamics was validated based on the water level and flow duration at the monitoring section of the trunk of the Luanhe River. The model validation was conducted through a final comparison with data collected at Guojiatun Station and Sandaohezi Station of the Luanhe River in 2006, and simulation to calculate the water level and flow process at these sections of the river channels. Comparisons of the simulated and monitored results are shown in Figures 2 and 3. The results revealed 85% and 82% flow errors at Guojiatun Station and Sandaohezi Station controlled under 10%, as well as 90% water level errors controlled under 10%, which fully satisfies the accuracy requirements for application of the model.

Take the simulated water flow process by hydrodynamics model as the input of water quality model validation, and according to the pollution sources amount investigated in 2006 at the trunk of the Luanhe River, conduct simulation validations for pollutant indicators in each month of 2006 at the sections of Guojiatun Station and Sandaohezi Station, like NH_3-N and COD_{Mn}. The validation results are shown in Figure 4. Comparison of the monitored values of the two stations revealed that there are 83% and 80% concentration errors at Guojiatun Station and Sandaohezi Station are both controlled under 18%, and the trend of simulated value is identical with monitored value generally, satisfying the application requirements.

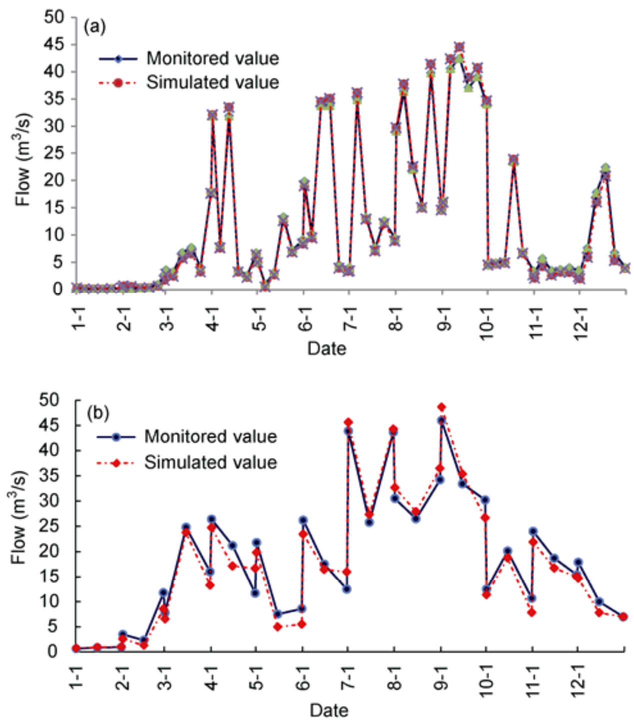

Figure 2 (Color online) Comparative analysis of the simulated value and monitored value of flow at the monitored section of the trunk of the Luanhe River. (a) Guojiatun Station; (b) Sandaohezi Station.

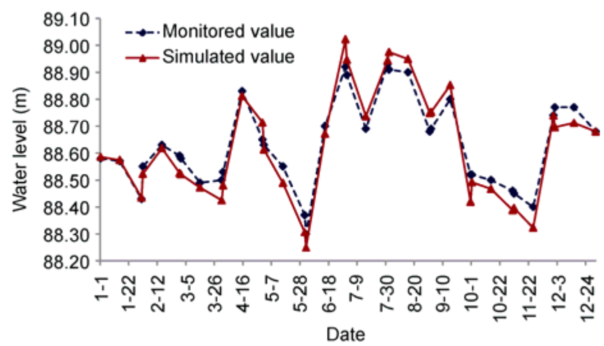

Figure 3 (Color online) Comparative analysis of the simulated and monitored water levels at the Sandaohezi section on the trunk of the Luanhe River. For the influence of Fengning power station, except blood, all has lost representativeness, the average daily water level validation at Guojiatun Station is not considered.

3.2 Vertical and two-dimensional model validation of Panjiakou reservoir

Under normal water level conditions, the area of the Panjiakou Reservoir can extend to the Chehekou section, which

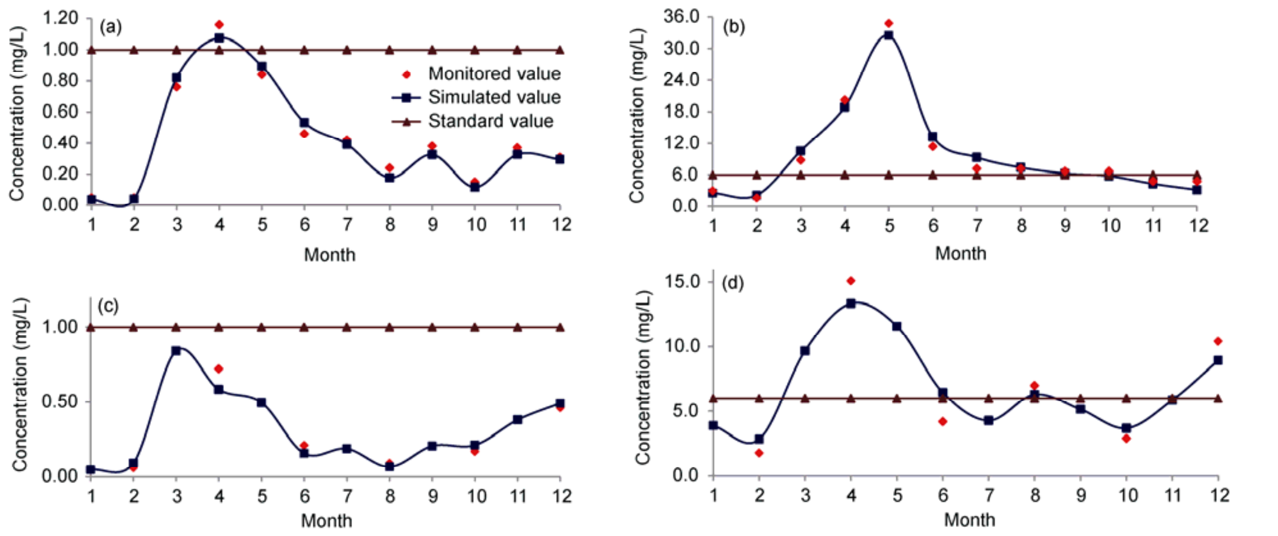

Figure 4 (Color online) Comparison of the simulated concentration value and monitored concentration value for both Guojiatun and Sandaohezi Stations. The monitored and simulated monthly concentration of ammonia nitrogen (a) and CODMn (b) at Guojiatun Station; the monitored and simulated monthly concentration of ammonia nitrogen (c) and CODMn (d) at Sandaohezi Station.

is 64 km from the dam. The greatest water depth is 69 m and the elevation of the reservoir bottom gradually rises from the frontier area of the dam to the upper stream. Taking 1 km in the horizontal direction and 1 m in the vertical direction as the computing unit for the vertical and two-dimensional model of reservoir water gives a maximum of 64 grid cells in the horizontal direction and 69 grid cells in the vertical direction. According to the actual landform, there are 2246 final calculated grid cells. The actual measured data obtained at time divisions from October, 29 to 31 2010 and the corresponding calculated results for the models indicate that the calculation results of this model can properly reflect the water flow characteristics and movement rules of the reservoir. In addition, the water characteristics of reservoir were validated based on the measured TN and TP. The validation results are shown in Figure 5.

Comparative analysis of the monitored and simulated values of TP and TN revealed that the average error of each section is 12% and 9%, respectively. Although some sections had relatively large errors, the model can satisfy the application requirements overall.

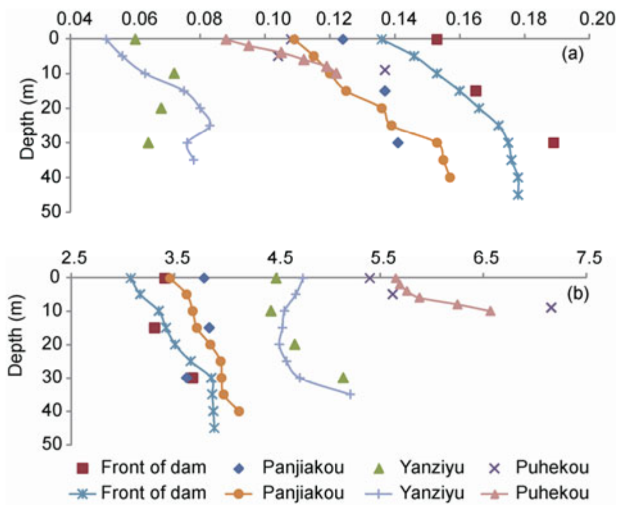

Figure 5 (Color online) Validation results of TP (a) (mg/L) and TN (b) (mg/L) for the water quality model of the Panjiakou Reservoir. The scattered points with data markers are the actual measured values; the values marked by the smooth curve and data are the simulated values.

4 The integrated assessment of water quantity and quality at the trunk of the Luanhe River

4.1 Brief introduction to the Luanhe River Basin

The Luanhe River Basin is located in the north east of north China, at 39°10′ to 42°35′N and 115°40′ to 119°20′E. The basin originates from Dagudao ditch on the southern slope of Xiaoliang Mountain in the City of Fengning in Hebei Province, after which it flows through 27 cities in Inner Mongolia, Liaoning and Hebei Province and then drains into the Bohai Sea at the City of Leting in Hebei Province. The total length of the basin is 888km and the drainage area is 44900 km^2 (Figure 6(a)). The Panjiakou Reservoir is located in the Village of Yangchazi in Qianxi, which is at the midstream portion of the Luanhe River. The controlled drainage area above the reservoir is 33700 km^2, which accounts for more than 75% of the total drainage area. The submerged area and sections of the Panjiakou Reservoir are shown in Figure 6(b).

Economic and population growth, as well as changes in the natural environment are influencing the water quantity, water movement and changes in water quality during each step of the water cycle. As a result, the water environment in the Luanhe River Basin has changed greatly in recently 44 years, and these changes have primarily been manifested as a gradual decrease in runoff depth in the river basin [37],

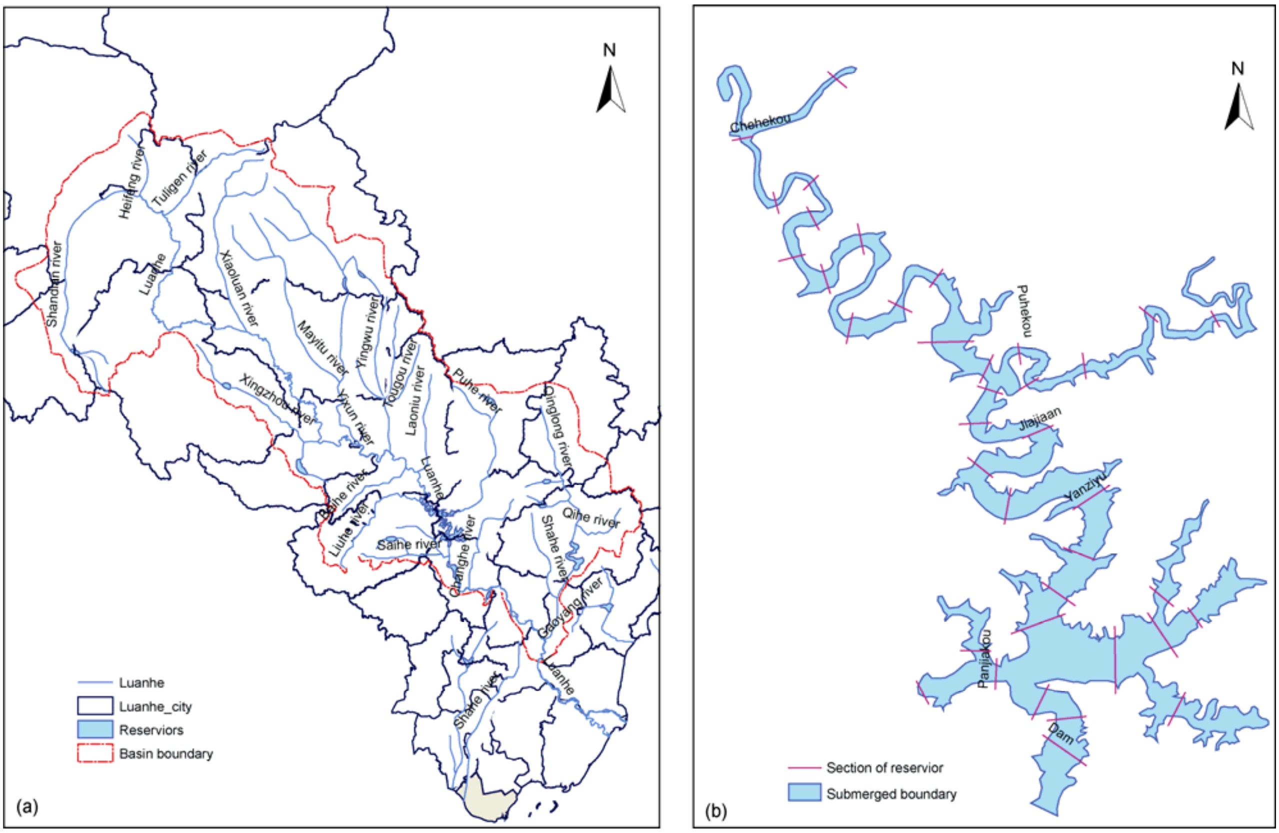

Figure 6 (Color online) Schematic diagram of the water system of the Luanhe River Basin and the Panjiakou Reservoir area. (a) Rivernet system and regionalism of Luanhe River Basin; (b) submerged area and sections of Panjiakou Reservior.

gradual deterioration of the water environment, and new types and diversification of pollutants, such as heavy metals and estrogen pollution etc. [38].

4.2 Integrated simulation and assessment of water quantity and quality for Luanhe River

In this study, the water environment system in the Luanhe River Basin primarily consists of the water quantity and quality assessment of the trunk stream water body and the Panjiakou Reservoir water body. Evaluation of the characteristics of target water bodies revealed differences between the simulation model control equation and numerical solution. For example, in the river network system simulation, the calculated time step of water flow is 15 min and the calculated time step of water quality is 1 h, while in the reservoir water body simulation the calculated time step is 9 s. Therefore, the integrated simulation and assessment of the river water environment system employs a 1 h interval and a space step of 1 km, meeting the requirements for joint calculation of transition units.

The simulation and assessment were conducted in 2006. During this year, the actual amount of precipitation in the Luanhe River Basin was 428 mm, making it a dry year. The simulation covered the area from Wulongji Station on the trunk of the Luanhe River to the dam of the Panjiakou Reservoir. The dissolved oxygen, ammonia nitrogen, hypermanganate index, total phosphorus, and total nitrogen were calculated using the integrated simulation and assessment model for water quantity and quality of the river environment system, realizing joint simulation of water quantity and water quality of the river water environment. However, classification of the quality of the water body at the trunk of the stream was conducted based on the ammonia nitrogen and the hypermanganate index, while the water quality classification of the reservoir was conducted based on the total phosphorus and total nitrogen. Therefore, statistical analyses were conducted according to the calculated time interval. The quantities of trunk streams with different water qualities during each month are shown in Table 1. The water quantities of type I to type V water bodies in the Luanhe River were 11.9%, 16.9%, 32.3%, 14.2%, 19.4% and 5.3%, respectively. Analysis by month revealed that 89.3% of the water in January is superior to type III water quality, and the maximum water quantity for water quality superior to type III is 60402000 m^3 in July.

According to the requirements for TN and TP concentration in reservoirs in the Environmental Quality Standards for Surface Water (GB3838-2002), the main water body of the Panjiakou Reservoir is inferior to type IV. The distributions of TN and TP are shown in Figures 7 and 8. With the climatic changes and influences brought by anthropogenic

Table 1 The quantities of water in systems with different water qualities at the trunk of the Luanhe River in 2006 (units: 10^4 m^3)

Months	I	II	III	IV	V	Inferior V
1	112.5	126.2	81.2	38.2	0.0	0.0
2	96.3	159.1	62.6	37.7	49.6	52.8
3	262.4	297.6	523.8	221.6	287.1	365.5
4	756.4	857.9	1510.2	638.9	1029.5	852.1
5	309.3	436.6	788.6	296.5	285.6	185.2
6	513.4	915.8	1614.0	643.2	878.4	0.0
7	817.5	1518.6	3704.2	1367.2	924.1	728.8
8	1165.4	1461.9	2925.6	1737.6	3122.1	523.1
9	555.1	783.6	1415.4	418.5	958.5	0.0
10	634.4	854.3	1162.5	536.8	788.8	0.0
11	583.0	864.1	1941.4	854.8	839.5	0.0
12	151.5	202.6	462.2	335.5	575.9	0.0

activities, the nutrient levels in Panjiakou Reservoir have gradually increased, resulting in higher concentrations of TP and TN. For example, in June of 2006 the lowest TP concentration in the water body was 0.068 mg/L, and the lowest TN concentration was 5.31 mg/L, both of which exceeded the type III standard indexes (0.05 and 1.0 mg/L) of surface water environmental quality.

5 Conclusions and discussion

Under the currently changing environmental conditions, the quantity and quality of river water has shown more distinctive characteristics of integration and dynamic changes; therefore, it is necessary to establish a new scientific system for integrated simulation and assessment of river water quantity and quality. In this study, an integrated simulation model for river system hydrodynamics and water quality was constructed and validated. The validation indicated that the error between the simulated and monitored value is comparatively small, satisfying the demands for application and having realized the integrated dynamic simulation of water quantity and quality.

Under the global climatic changes and the disturbance of highly-insensitive human activities, the water in the Luanhe River Basin has changed greatly. According to the results of the integrated and dynamic assessment model for water resource quantity and quality, the quantities of water in type I to type V water bodies of the upper stream of the Luanhe River Basin were 11.9%, 16.9%, 32.3%, 14.2%, 19.4% and 5.3%, respectively. In addition, the water quality of the main water body comprising the Panjiakou Reservoir is inferior to type IV.

The integrated simulation and assessment for water quantity and quality is required for effective water resources management. Although integrated simulation and assessment have been realized in river water environment systems, statistical analyses of the inflow pollutants during the water cycle and from point sources still need constant improvement. In addition, the current hydrology and water quality monitoring data series is relatively short, so the conclusions of integrated simulation and assessment can not reveal the effect by either anthropogenic activities or

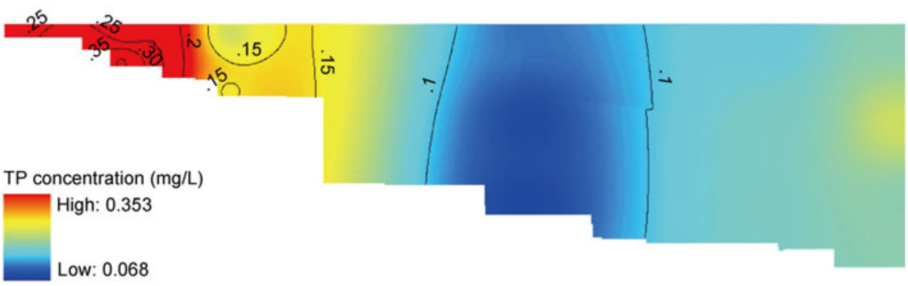

Figure 7 (Color online) TP distribution in Panjiakou Reservoir in June, 2006.

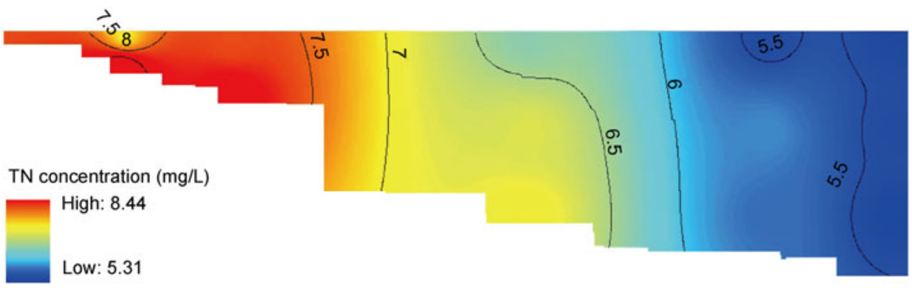

Figure 8 (Color online) TN concentration distribution in Panjiakou Reservoir in June, 2006.

climatic changes, and the research on the integrated simulation and assessment of water quantity and quality under changing environmental conditions still waits for strengthening.

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