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Simulating Water Quality of Wei River with QUAL2K Model, a Case Study of Hai River Basin in China

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Abstract. QUAL2K model is used to simulate the water quality of Wei River and the verification results are analyzed in this paper. For the actual situation of pollution in Wei River Basin, COD, ammonia nitrogen and total phosphorus are chosen as indexes of water quality prediction. The degradation coefficient of them, being one important water quality parameter, is calculated as 0.2428, 0.1019 and 0.2554, respectively. Conduct parameter setting and compared with the measured values combining comprehensive one-dimensional water quality model formula, with the measured data, then make adjustments to get new degradation coefficient with the values are 0.3631, 0.2046 and 0.2545, respectively. The simulation results are verified and showed that the predicted values fit with the measured ones well, the relative errors of COD, ammonia nitrogen and total phosphorus concentration are within 10%, and the simulation effect is good.

1 Introduction

Water quality simulation is important to master the variation law of pollutants in water body, reduce the risk of water pollution and its loss, and ensure the water safety and water environment quality. Research on water quality model is mainly in Europe and other developed countries where theoretical foundation and applied research of the model has been very mature [1]. While it starts relatively late, and is still in the exploratory stage of theoretical research and applications in China. QUAL2K model that evolved in QUAL2E is one of QUAL series models developed by the United States Environmental Protection Agency and applies to small and medium-sized dendritic rivers which mix well [2-4]. In order to solve some water quality problems, Seok Soon Park et al. [5] applied the above-mentioned two models to the Nakdong River, Korea and found simulated results of QUAL2K model was relatively more consistent with the measured values. Guo et al. [6] discussed water quality trends of the middle and lower reaches of Hanjiang River by QUAL2E and QUAL2K model with BOD as the predictor, and the results indicated that QUAL2K reflected the field data better than QUAL2E. Kalburgia et al. [3] conducts a study using the water quality model QUAL2K to develop the BOD-DO model and evaluation of the results for a 50 km stretch of river, and the results show that the values predicted by the model are in close agreement with measured values.

Wei River is the tributary of Hai River in China. It is the key of water pollution remediation area that required by *the 12th Five Year Plan* in China. According to the local *Environmental Quality Bulletin*, the water quality of Wei River was severe pollution from 2009 to 2014. Therefore, to provide a scientific basis for reducing water pollution risk and its losses, this study chooses a typical reach of Wei River and uses QUAL2K model for its water quality simulation.

2 Introduction of QUAL2K Model

QUAL2K model belongs to comprehensive one-dimensional water quality model and mainly simulates the main stream of rivers [2]. It is suitable for modeling the migration and transformation of BOD, N, P and other pollutants in well mixed dendritic river. The simulation with the elements as the basic unit, is a steady flow balance for each model element, namely:

$$Q_i = Q_{i-1} + Q_{in,i} - Q_{out,i} \tag{1}$$

where Q_i (m^3/d) is outflow from element i to i+1; Q_{i-1} (m^3/d) is inflow from element i-1; $Q_{in,i}$ (m^3/d) is inflow from point and non-point sources; $Q_{out,i}$ (m^3/d) is outflow from point and non-point sources of element i; there exists for any water quality components.

$$\frac{\partial C}{\partial t} = \frac{\partial\left(A_x E_x \frac{\partial C}{\partial x}\right)}{A_x \partial x} - \frac{\partial(A_x \overline{u} C)}{A_x \partial x} + \frac{dC}{dt} + \frac{S}{V} \tag{2}$$

where C(mg/L) is the concentration of a constituent; x(m) is the distance; t(s) is the time in days; A_x (m^2) is the river cross-sectional area from x; E_x (m^2/s) is the dispersion coefficient; $\overline{u}$ (m/s) is the average flow velocity; S(mg/L) is the external sources or sinks of the constituent; V(m^3) is the volume of each calculation unit. The four on the right side of the equation are respectively diffusion, advection, component reaction and the external sources or sinks of the constituent.

The model mainly simulates the water quality of the river main stream. The import tributary is regarded as a point source, and non-point source and its outlet are seen as a line source and line outlet. Firstly the river is divided into a series of steady nonuniform reaches according to the water quality, and then the reaches are divided into a number of calculation units. It conceptualizes the simulation river as a series of well mixed, end-to-end units formed through transport and diffusion by dividing reach units. Each unit is an ideal mixing reactor and the smallest calculation unit, and single unit calculate the corresponding equation based on the law of substance balance during the simulation. Among them, the substance balance includes water convection and dispersion. Not only will the substance of each unit increase or decrease along with the external water into or output, but also the concentration will rise or lower because of internal biological effect. Simulation generally includes the following basic steps: 1. material collection and field investigation; 2. divide reach and unit; 3. determine the model parameters; 4.validation and application of the model [2].

3 Modeling process for WEI River

3.1 Study area introduction

Wei River originates in the Taihang Mountain of Shanxi Province, with a total length of over 900km and length of 399km in Hebi range. The catchment area is totally 15830km^2. Its northwest is mountain with an area of about 6280km^2 and southeast is plain with an area of approximately 9010 km^2. There are many kinds of water pollutants and with wider range of pollution. We selected Chaiwan - Wuling which is the typical provinces controlled sections of the Wei river， with total length of 38.17km. There are two general monitoring sections， Xunxian bridge and Tunzi bridge with total length of 38.17km. Chai Wan to Xunxian bridge is 13.9km, Xunxian bridge to Tunzi bridge is 8.44 km, and Tunzi bridge to Wuling is 15.83 km. The entire river slopes slightly from south to north without significant pollution source, and pollutants are easily well-mixed in the lateral and vertical.

3.2 Basic data and river course generalization

When using the model, data needed to input mainly include river boundary conditions, reach data, meteorological data, model parameters, point and non-point sources pollutants, etc., so required data generally include watershed hydrology and spatial information, weather data, initial conditions, boundary conditions, node data of each reach monitoring sections and monitoring data that the model parameters calibration and verification require. The output includes calculation of the input data, temperature data, hydraulic and water quality data, modeling water quality components and variation curve in water [2,4]. According to the actual situation of Wei River, March, April and May in 2013 were determined as the model parameters calibration period and May 2012 as the verification period. We select COD, NH_3-N and TP as simulation pollutants, and the length of the calculation unit is 2km, the whole with a total of 19 (Table 1).

Table 1. The division of Wei River reach and calculation units.

Reach number	The starting point	Length (km)	Distance from the upstream boundary(km)	Calculation unit
1	Chaiwan-Xunxian bridge	13.9	13.9	7
2	Xunxian bridge -Tunzi bridge	8.44	22.34	4
3	Tunzi bridge -Wuling	15.83	38.17	8

3.3 Parameters calibration of the model

3.3.1 The boundary conditions

Take the parameters of Weihui estuary monitoring sections in the upstream water bifurcation as the boundary conditions of water quality simulation, which include design flow, design temperature, the initial concentration of COD, NH_3-N and TP and the relevant hydraulics parameters. According to the annual monitoring data, use the average annual flow as a design flow, take the mean of pollution indicators average measured concentration nearly 10 years in Wehui monitoring sections as the initial concentration of water quality modeling, and use the average temperature of the monitoring period as design temperature, in Table 2.

Table 2. Water quality and quantity parameters of source.

Temperature (℃)	Flow (m³/s)	COD (mg/L)	NH_3-N(mg/L)	TP (mg/L)
17.53	7.07	29.33	8.71	1.79

3.3.2 Water quality parameters

The degradation coefficient' determination at home and abroad are mainly data projections, experience estimation method, inverse model estimation method, water mass tracing valuation method and laboratory simulation method, etc. According the one-dimensional river water quality model[7], the degradation coefficient can be calculated with formula 3 (Table 3).

$$K = 86.4(\ln C_0 - \ln C \frac{\overline{u}}{L}) \quad (3)$$

where C(mg/L) is pollutants concentration monitoring values of next section; C_0 (mg/L) is pollutants concentration of previous section; $\overline{u}$ (m/s) is the average flow velocity; L(km) is the distance from next section to previous section; $K(d^{-1})$ is degradation coefficient.

Table 3. The initial value of degradation coefficient.

Degradation coefficient (d^{-1})	Chaiwan-Xunxian bridge	Xunxian bridge - Tunzi bridge	Tunzi bridge-Wuling	Mean
K_{COD}	0.3362	0.2704	0.2218	0.2428
$K_{NH3\text{-}N}$	0.1188	0.0816	0.1053	0.1019
K_{TP}	0.2586	0.2341	0.2735	0.2554

3.3.3 Hydraulic parameters

In view of the property of the existing materials, the flow curve formula and Manning formula demand for data, flow curve formula was used to describe hydraulics characteristics [8-11]. Thus, the hydraulic parameters are mainly related to the flow curve parameter and the diffusion coefficient K.

1) The flow curve

QUAL2K model assumes steady stream hydraulic characteristics, namely $\partial Q / \partial t = 0$, and hydraulic characteristics of each river meet the following form:

$$\overline{u} = aQ^b \quad H = cQ^d \quad (4)$$

where Q (m^3/s) is flow; $\overline{u}$ (m/s) is the average flow velocity; a, b, c and d are the experience coefficient gotten by the velocity curve of drainage and water drainage curve, where b and d must meet the Table 4, and the sum of the two is not greater than 1.

Table 4. The parameter values of the flow curve.

Formula	Letter	Calibration value	Range of values
$\overline{u} = aQ^b$	b	0.43	0.4-0.6
$H = cQ^d$	d	0.45	0.3-0.5

Sectional area and width of the river can be gotten by formula 5.

$$A_x = Q / \overline{u} \qquad B = A_x / H \quad (5)$$

Then, the surface areas and volumes of reach units can be calculate by formula 6.

$$A_x = B\Delta x \qquad V = BH\Delta x \quad (6)$$

In this study, using the measured data of multi-sectional flow, flow velocity and depth, the values of a, b, c, d by the least squares method are 0.3, 0.28, 0.15, 0.45, respectively.

2) The diffusion coefficient

There are many methods to determine diffusion coefficient, and the study adopted the formula of QUAL2K model [2, 4].

$$E_x = 3.82 K n \overline{u} H^{5/6} \quad (7)$$

where E_x is the Longitudinal dispersion coefficient; K is the Longitudinal diffusion constant, and the empirical average is 5.93; n is Manning roughness coefficient; $\overline{u}$ is the average flow velocity; H is the average depth.

Wei River bend is with narrow and deep river channel, so Manning coefficient of it is relatively large. Contrasting with the common channel Manning coefficient, its value is ultimately determined 0.05.

4 Solution and verification of the model

4.1 Solution of the model and parameter adjustment

We model the water quality using the partial differential equations and solve it by the improved Euler Finite difference Scheme [2-4]. The solution process is omitted here, and the measured values are compared in Table 5.

Table 5. Simulation and measured values of parameter initial values.

Section	COD(mg/L)			NH3-N(mg/L)			TP(mg/L)		
	CV	MV	RE (%)	CV	MV	RE (%)	CV	MV	RE (%)
Xunxian bridge	28.85	25.01	15.35	10.45	9.27	12.73	0.93	0.84	10.71
Tunzi bridge	30.31	23.87	26.98	11.89	9.43	26.09	1.02	0.86	18.60
Wuling	26.89	24.12	11.48	10.12	9.06	11.70	0.95	0.71	33.80

Note: CV is Calculated Value; MV is Measured Value; RE is Relative Error; AE is Absolute Error.

It shows that the relative errors and the measured values are larger, especially Xunxian bridge-Tunzi bridge. It is advised to decrease the river longitudinal diffusion coefficient and to increase pollutant degradation coefficient. After repeated modification, the parameter values are as follows (Table 6).

Table 6. The determination results of model parameters.

Model parameter	Chaiwan-Xunxian bridge	Xunxian bridge - Tunzi bridge	Tunzi bridge - Wuling	Mean
$K_{COD}(d^{-1})$	0.4507	0.4839	0.1547	0.3631
$K_{NH3\text{-}N}(d^{-1})$	0.1277	0.2079	0.2782	0.2046
$K_{TP}(d^{-1})$	0.2588	0.2346	0.2701	0.2545

4.2 Analysis of the modelling results

Use routine monitoring data in May 2012 for model validation and the results are shown in Table 7. It shows that, except that the COD concentration simulation value at Tunzi bridge is slightly larger than the measured value, and the measured values of the other sections are less than the calculated values. The calculated and measured values of COD are with the same trends over reach distance, with a high correlation. There is little change in water quality from Chai Wan to Xunxian bridge, and it is deteriorating from Tunzi bridge to Wuling.

The measured values of NH_3-N concentration are slightly less than the calculated ones. Different from COD, the maximum error between NH_3-N model calculated and measured values is Tunzi bridge. The smallest error is in Wuling section with the relative error of 1.36% and the absolute error of 0.15.

The concentration calculated and measured values of TP have the same trend with NH_3-N, that pollutant concentrations increases from Xunxian bridge to Tunzi bridge and begins to decline after reaching a peak in Tunzi bridge.

In a whole, the relative errors of the concentrations of COD, NH_3-N and TP are within 10%. The calculation value of each water quality indicator significantly correlated to the measured ones. It indicates that the parameter values are relatively reasonable, and the model has high authenticity and reliability.

Table 7. Concentrations' comparison of calculated value and measured one for different river sections.

Section	COD(mg/L)				NH_3-N(mg/L)				TP(mg/L)			
	CV	MV	RE(%)	AE(mg/L)	CV	MV	RE(%)	AE (mg/L)	CV	MV	RE(%)	AE(mg/L)
Xunxian bridge	27.81	27.27	1.98	0.54	11.55	11.39	1.40	0.16	0.81	0.8	1.25	0.01
Tunzi bridge	27.55	28.36	-2.86	-0.81	11.65	11.45	1.75	0.2	0.85	0.82	3.66	0.03
Wuling	32.33	30	7.77	2.33	11.18	11.03	1.36	0.15	0.68	0.73	-6.85	-0.05

Note: AE is Absolute Error.

5 Conclusion

In this paper, QUAL2K model is used to simulate and verify the water quality of Wei River, which COD, ammonia nitrogen and total phosphorus are chosen as indexes of water quality prediction. Through the parameter optimization, mainly degradation coefficient, the modeling results show that the predicted values fit with the measured ones well. The relative errors of COD, ammonia nitrogen and total phosphorus concentration are all within 10%, and the effect is good. QUAL2K model relying Microsoft Office Excel interface, equipped with relatively simple VB programming, is easy to handle and learn. Meanwhile, to determine the water quality parameters is particularly important in the course of solving the model. To promote the results' rationality, we make appropriate adjustments of the parameters, mainly degradation coefficient. In the future, we should conduct more studies on the methods to optimize the parameter of the model for different river, especially for those without enough data.

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