The simulation of water quality in Chanba Ecological District

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Abstract. In order to investigate the characteristic of migration and transformation of various pollutants in rivers, the river in Chanba Ecological District was selected as the research object. The MIKE21 FM model coupled with Ecolab module was employed to establish the two-dimensional water quality model to simulate the distribution characteristic of different water quality parameters, which were Total Nitrogen (TN), Total Phosphorus (TP), Ammonium Nitrogen (NH₃-N), Chemical Oxygen Demand (COD), Chlorophyll a (Chla), and Dissolved Oxygen (DO) separately. The results demonstrated that the concentration values of TP, NH₃-N, and COD in Chanhe River were greater than them in Bahe River before the water flowed into the junction zone. The TN concentration value in the calculation zone except the region which had poor hydraulic conditions exceeded the standard of Grade V (GB3838-2002). Because the water in Bahe River was disturbed by water in Chanhe River and point sources in Bahe River, COD and NH₃-N concentration values increased clearly after the water passed from the NO.4 Dam in Bahe River.

1. Introduction

River, which plays a significant role in regional sustainable development, could supply an extensive ecological function, for example, irrigation, water supply, transportation, and entertainment, etc. Due to rapid urbanization and lagging rainwater management mode in China, numerous rivers get polluted, river water environment has been deteriorating, and ecological environment as well as human health has been endangered. Therefore, water environment management is an important task of current ecological construction. Water environment management is the data-based process, in other words, only a lot of water quality and hydrology data could facilitate the task of water environment management. However, water quality and hydrology data monitoring in the water environment management requires a lot of time and efforts. In order to promote the environmental management work efficiently, conveniently and economically, the hydrodynamic models, water quality models and eutrophication models are widely applied [1,2]. There have been various water quality models being widely used in different research and engineering fields [3]. MIKE21 FM model, one of the important water quality models, which could be used in the simulation of water quality in lake, estuary, wetland and river, is widely in the water environment management. Zhu et al developed the two-dimensional water quality by MIKE21 FM model to simulate the current situation of Erhai Lake to investigate the distribution characteristic of water quality [4]. Paliwal et al assess temporal and spatial variation in water quality of an estuary under the impact of effluent from an industrial estate based on the MIKE21 model [5]. Bahe and Chanhe Rivers, which are in Chanba Ecological District Xi’an Shaanxi China,
have been polluted seriously. In order to analyze the characteristic of pollution in spatial-temporal scale in Chanba Ecological District, the MIKE21 FM hydrodynamic model coupled with Ecolab module was utilized to develop a water quality model to investigate the process of migration and transformation for different pollutants.

2. Materials and methods

2.1. Study area
The Chanba Ecological District is located in the eastern region of Xi’an City (figure 1), and in the downstream area of ChangJiaWan and MaDuWang hydrology stations. The average annual temperature is 13.3 degrees Celsius. The prevailing wind direction in the region is northeast wind and southwest wind, and the annual mean wind-speed is 2.0 m/s. There are two rivers in Chanba Ecological District, which are Bahe River and Chanhe River respectively. Influenced by the industrial wastewater, domestic sewage, and gradual reduction in surface runoff compensation, the water in Chanhe River and Bahe River encounters severe pollution. The water in Chanhe River was disturbed by agricultural non-point sources before it flowed into Chanba Ecological District, and main pollutants were nutrients [6]. Moreover, the water in Bahe River was influenced by non-point sources and domestic sewage from LanTian County, and principal pollutants were organic matters [7]. The study area is situated in the northern region of the Chanba Ecological District (figure 1). The water in Chanhe River and Bahe River intersect in the junction zone, passes by the No. 4 Dam in Bahe River, and flow out from the calculation zone in the No. 1 Dam in Bahe River finally.

![Figure 1. Location of study area.](image)

2.2. Model setup
In this thesis, the Chanhe River and Bahe River were selected as study area (figure 1). There are eight rubber dams and 6 point sources in this calculation area (figure 1). The point sources in this calculation area were characterized by the water quality indexes, which were Chemical Oxygen Demand and Ammonia Nitrogen. The two-dimensional hydrodynamic model and Ecolab module were employed to develop the water quality model to investigate the characteristic of migration and transformation of various water quality parameters, whose process of migration and transformation is shown on figure 2. The calculation mesh was generated by the method of unstructured triangular grid, the grid independent analysis showed that 9245 grid cells would ensure the accuracy of calculation results, and the governing equations of the water quality model was spatially discretized by the finite
volume method. The simulation period is from July 10, 2012 to October 15, 2012, and the time step is set as 10 seconds. The flow volume of the inlet was given by one-dimensional data (dfs0), and the outlet was set as constant water level, 368.7 meters (1985 National Elevation Benchmarks). Additionally, the calibrated eddy viscosity was set as 0.28. The bed resistance, which was Manning’s coefficient in this paper, was given by data file (dfsu) [8]. The initial conditions for all parameters were set as measured values on July 10, 2012. Finally, other parameters are shown on table 1.

![Diagram of water quality parameters](image)

**Figure 2.** The frame graph of migration and transformation of water quality parameters.

**Table 1. Description of parameters.**

| No. | Parameters | Description                           | No. | Parameters | Description                           |
|-----|------------|---------------------------------------|-----|------------|---------------------------------------|
| 1   | $K_2$     | The rate for the reaeration           | 14  | $K_{11}$   | Carbon to oxygen ratio at primary production |
| 2   | Cs        | Saturated dissolved oxygen concentration | 15  | $K_8$      | Death rate of chlorophyll-a           |
| 3   | $P_{max}$ | Maximum production at noon            | 16  | $K_4$      | Nitrification rate at 20°C             |
| 4   | $\varphi$ | Time correction for at noon           | 17  | $\theta_4$ | Temperature coefficient for nitrification |
| 5   | Cresp     | Respiration rate                      | 18  | $Y_1$      | Yield factor for oxygen               |
| 6   | $\theta_2$| Temperature coefficient for respiration | 19  | $HS_{nitrif}$ | Half saturation concentration for nitrification |
| 7   | Resp_DO   | Half-saturation concentration for respiration | 20  | $Y_{2d}$ | Ammonia nitrogen content in dissolved COD |
| 8   | $K_{d3}$  | Degradation rate for COD at 20°C      | 21  | $K_N$      | Degradation rate for total nitrogen    |
| 9   | $\theta_3$| Arrhenius temperature coefficient     | 22  | $Y_{3d}$ | Total phosphorus content in dissolved COD |
| 10  | HS_COD    | Half saturation oxygen concentration for COD | 23  | $K_P$      | Degradation rate for total phosphorus  |
| 11  | KSN       | Half saturation concentration for nitrogen | 24  | $H$        | Water depth                           |
| 12  | KSP       | Half saturation concentration for phosphorus | 25  | $SD$       | Secchi disk depths                    |
| 13  | $K_{10}$  | Chlorophyll-a to carbon ratio         | 26  | $T$        | Temperature                           |

The processes of migration and transformation for various pollutants are generalized as bellows...
formulas.

- **DO**

\[
\frac{d(\text{DO})}{dt} = K_d * (C_s - \text{DO}) + \left( P_{\text{max}} * e^{-\frac{H_n}{SD}} \right) \frac{\text{SUNINF}}{H} - \frac{\text{DO}}{\text{DO} + \text{resp}_\text{DO}} \frac{C_{\text{resp}} \cdot \theta_2^{T-20}}{H} - K_{d3} \cdot \theta_3^{T-20} \cdot \text{COD} \cdot \frac{\text{DO}}{\text{DO} + \text{HS}_\text{COD}} - Y_3 \cdot K_4 \cdot \theta_4^{T-20} \cdot \text{NH}_3 - N \cdot \frac{\text{DO}}{\text{DO} + \text{HS}_\text{nitrif}}
\]

(1)

- **COD**

\[
\frac{d(\text{COD})}{dt} = -K_{d3} \cdot \theta_3^{T-20} \cdot \text{COD} \cdot \frac{\text{DO}}{\text{DO} + \text{HS}_\text{COD}}
\]

(2)

- **Chla**

\[
\frac{d(\text{Chla})}{dt} = \left[ \left( P_{\text{max}} * e^{-\frac{H_n}{SD}} \right) \frac{\text{SUNINF}}{H} - \frac{\text{DO}}{\text{DO} + \text{resp}_\text{DO}} \frac{C_{\text{resp}} \cdot \theta_2^{T-20}}{H} \right] K_{11} \cdot K_{10} \cdot F(N, P) - K_{\text{Chla}}
\]

(3)

- **NH3-N**

\[
\frac{d(\text{NH}_3 - N)}{dt} = Y_{d} \cdot K_{d3} \cdot \theta_3^{T-20} \cdot \text{COD} \cdot \frac{\text{COD}}{\text{COD} + \text{HS}_\text{COD}} - K_{d3} \cdot \theta_3^{T-20} \cdot \text{NH}_3 - N \cdot \frac{\text{DO}}{\text{DO} + \text{HS}_\text{nitrif}}
\]

(4)

- **TN**

\[
\frac{d(\text{TN})}{dt} = -K_{\text{TN}} \cdot \text{TN}
\]

(5)

- **TP**

\[
\frac{d(\text{TP})}{dt} = Y_{d} \cdot K_{d3} \cdot \theta_3^{T-20} \cdot \text{COD} \cdot \frac{\text{DO}}{\text{DO} + \text{HS}_\text{COD}} - K_{\text{TP}} \cdot \text{TP}
\]

(6)

3. Results and discussions

3.1. Model verification and assessment

In this thesis, the four measure of goodness of fit, which are the absolute mean error (AME), the coefficient of determination (R²), the root mean square error (RMSE), and the mean absolute value of relative error (I) separately, were utilized to evaluate the model performance. The AME, R², RMSE, and I are calculated as follows:

- The absolute mean error (AME)

\[
AME = \frac{1}{n} \sum_{i=1}^{n} \left| P_{mi} - P_{ni} \right|
\]

(7)

- The coefficient of determination (R2)
\[ R^2 = 1 - \frac{\sum_{i=1}^{n}(P_{mi} - P_{si})^2}{\sum_{i=1}^{n}(P_{mi})^2} \]  

(8)

- The root mean square error (RMSE)

\[ RMSE = \sqrt{\frac{\sum_{i=1}^{n}(P_{mi} - P_{si})^2}{n}} \]  

(9)

- The mean absolute value of relative error (I)

\[ I = \frac{1}{n} \sum_{i=1}^{n} \left| \frac{P_{mi} - P_{si}}{P_{mi}} \right| \]  

(10)

The values of \( R^2 \), AME, RMSE, and I for state variables [9], which are from S1 point to S4 point, is shown on table 2. The results showed that the values of \( R^2 \) and RMSE were extremely closed, which suggested that the error between time series measured and simulated values held same order of magnitude. The smaller the I value is, the higher the precision of water quality model is, and the I value was within about 30% in this thesis. Referring the RMSE value calculated by Elshemy M [10], the conclusion would be drawn that the water quality model calibrated by the measured values could guarantee the accuracy and precision.

### Table 2. Performance measures for comparison of observed and simulated parameters.

| State Variables       | Point Position | AME | \( R^2 \) | RMSE | I/% |
|-----------------------|----------------|-----|-----------|------|-----|
| Total Nitrogen (TN)   | S1             | 0.11| 1.00      | 0.12 | 5   |
|                       | S2             | 0.53| 0.96      | 0.55 | 20  |
|                       | S3             | 0.41| 0.97      | 0.47 | 15  |
|                       | S4             | 0.45| 0.97      | 0.49 | 17  |
| Total Phosphorus (TP) | S1             | 0.01| 0.97      | 0.01 | 13  |
|                       | S2             | 0.01| 0.97      | 0.01 | 24  |
|                       | S3             | 0.03| 0.93      | 0.03 | 24  |
|                       | S4             | 0.03| 0.91      | 0.04 | 21  |
| Ammonium Nitrogen (NH\(_3\)-N) | S1     | 0.13| 0.91      | 0.16 | 28  |
|                       | S2             | 0.18| 0.94      | 0.20 | 24  |
|                       | S3             | 0.28| 0.94      | 0.31 | 22  |
|                       | S4             | 0.30| 0.97      | 0.35 | 13  |
| Chemical Oxygen Demand (COD) | S1     | 1.22| 0.99      | 1.46 | 7   |
|                       | S2             | 1.12| 0.99      | 1.36 | 6   |
|                       | S3             | 1.06| 1.00      | 1.11 | 6   |
|                       | S4             | 1.47| 1.00      | 1.62 | 19  |
| Chlorophyll a (Chla)  | S1             | 0.00| 0.99      | 0.00 | 20  |
|                       | S2             | 0.00| 0.91      | 0.01 | 27  |
|                       | S3             | 0.01| 0.76      | 0.01 | 22  |
|                       | S4             | 0.00| 0.96      | 0.00 | 30  |
| Dissolved Oxygen (DO) | S1             | 0.25| 1.00      | 0.28 | 11  |
|                       | S2             | 0.55| 0.99      | 0.64 | 12  |
|                       | S3             | 0.28| 1.00      | 0.34 | 12  |
|                       | S4             | 0.19| 1.00      | 0.20 | 9   |
3.2. The analysis of pollutants’ concentration field

The time-average concentration field for TN, TP, NH$_3$-N, COD, DO, and Chla is shown on figure 3. TN concentration exceeded the standard of Grade V (GB3838-2002). The cloud picture for TP concentration filed showed that the TP concentration in Bahe River varied from 0.02 mg/L to 0.1 mg/L, and it in the region of outlet increased to range between 0.1 and 0.2 mg/L.

The TP concentration in Chanhe River ranged from 0.1 to 0.2 mg/L. The NH$_3$-N concentration in Bahe River along with the direction of water flow could be divided into five regions, whose concentration values were 0.15-0.5 mg/L, 0.5-1.0 mg/L, 1.0-1.5 mg/L, and above 2.0 mg/L respectively. The dominant concentrations were 0.5-1.5 mg/L and 1.5-2.0 mg/L, which were corresponding to the standard of Grade III and Grade V (GB3838-2002). The dominant NH$_3$-N concentration values were 0.5-1.0 mg/L and 1.5-2.0 mg/L.

The COD dominant concentration values were 15-20 mg/L and 30-40 mg/L. The phenomenon that COD concentration field could be divided into three regions, whose concentration values were 15-20 mg/L, 20-30 mg/L, and 30-40 mg/L, was induced by sewage drainage from point sources. For the disturbance of the water in Chanhe River and sewage discharge of point source in the downstream of No. 4 Dam, the COD concentration fields in the junction zone and downstream of No. 4 Dam forms two transition zones, whose area was relatively small, and concentration values were 20-30 mg/L and above 40 mg/L.

The cloud picture of DO concentration field suggested that DO concentration values in Chanhe River and Bahe River before entering the junction zone were better than the standard of Grade I (GB3838-2002). For the disturbance from the water in Chanhe River entering into the junction zone and the sewage discharge from point sources in the downstream of No. 4 Dam, DO concentration value in Bahe River decreased from above 7.5 mg/L to 6-7.5 mg/L. However, DO concentration value in all study area was better than the standard of Grade II (GB3838-2002).

The TN concentration in the upstream of Chanhe River exceeded 7.5 mg/L.
Figure 3. The time-average pollutants concentration field.
For the disturbance of sewage discharge from point sources, the DO concentration value in Chanhe River decreased to 6.0-7.5 mg/L after the water passed from No.3 Dam in Bahe River.

DO concentration value in the region, which held poor hydraulic conditions, ranged from 3.0-5.0 mg/L, and it was obviously lower than DO dominant concentration value. This was because the water in this region basically maintained still, so the atmospheric oxygen enrichment rate was less than it in other regions. Moreover, from the cloud picture of Chla concentration value, we could get the information that Chla concentration value in the region, which held poor hydraulic conditions, was obviously lower than it in other regions. At the same time, the transformation process of COD and NH$_3$-N needed oxygen consumption.

The time-average concentration values for TP, NH$_3$-N, COD, and DO in the junction zone are shown on figure 4. The figure 4(b) showed that TP concentration value in Chanhe River, which was greater than it in Bahe River, varied from 0.1 to 0.2 mg/L, before the water flowed into Bahe River. For the difference in TP concentration between Chanhe River and Bahe River, there would be a region in the left bank of the junction zone holding the greater TP concentration value, which ranged from 0.1 to 0.2 mg/L after the water in Chanhe River entering into the junction zone.

The NH$_3$-N concentration value, which was greater than it in the junction zone, varied from 1.5 to 2.0 mg/L, before the water in Chanhe River flowed into the junction zone. For the difference in NH$_3$-N concentration value between Chanhe River and Bahe River, there would be a region, whose NH$_3$-N concentration value was 1.0-1.5 mg/L, which was greater than it in Bahe River, but lower than it in Chanhe River, in the junction zone.

COD concentration value in Chanhe River was obviously greater than it in Bahe River before the two water bodies flowed into the junction zone, which was because the water in Chanhe River was disturbed by the sewage discharge from point sources.

There would be the region, which held lower DO concentration value, in the left bank of the junction zone. DO concentration value was greater than the standard of Grade II (GB3838-2002) on the whole.
Figure 4. The time-average pollutants concentration field in junction zone.

4. Conclusions
The water quality model developed by the MIKE21 FM hydrodynamic model and Ecolab module could analyse the processes of migration and transformation of different water quality parameters clearly, and it would be used to study the distribution characteristic of water quality. The conclusions would be drawn as follows:

- The water quality induced by the MIKE21 FM hydrodynamic model and Ecolab module could be utilized to simulate the processes of migration and transformation for different water quality parameters and to study spatial variation of water quality accurately.
- The water quality in Bahe River was disturbed largely by water quality in Chanhe River.
- There was a large spatial heterogeneity for COD, NH$_3$-N and DO.
- DO concentration value in the region, which held poor hydraulic conditions, was limited by the atmospheric oxygen enrichment rate and Chla concentration value.
- TN concentration value in the calculation zone exceeded the standard of Grade V (GB3838-2002), which meant the water was be inferior to Grade V.
- The COD and NH$_2$-N concentration values would increase after the water passed from the No. 4 Dam in Bahe River.
- The TP, NH$_3$-N, and COD concentration values in Chahe River were greater than them in Bahe River before the water flowed into the junction zone.

Acknowledgments
The research was supported by the Major Basic Research Projects in Natural Science of Shaanxi Province (2017ZDJC-20), and the Key Technology Project from Power Construction Corporation of China (DJ-ZDXM-2018-38).
References

[1] Hull V, Parrella L and Falcucci M 2008 Modelling dissolved oxygen dynamics in coastal lagoons *Ecol. Model.* 211 468-80

[2] Najah A, El-Shafie A, Karim O A *et al* 2013 Application of artificial neural networks for water quality prediction *Neural Comput. Appl.* 22 187-201

[3] Qi H, Lu J, Chen X, Sauvage S and Sanchez-Pérez J-M 2016 Water age prediction and its potential impacts on water quality using a hydrodynamic model for Poyang Lake, China *Environ Sci Pollut R* 23 13327-41

[4] Zhu C J, Liang Q, Yan F and Hao W 2013 Reduction of waste water in Erhai Lake based on MIKE21 hydrodynamic and water quality model *Sci. World J.* 2013 1-9

[5] Paliwal R and Patra R R 2011 Applicability of MIKE 21 to assess temporal and spatial variation in water quality of an estuary under the impact of effluent from an industrial estate *Water Sci. Technol.* 63 1932

[6] Wang Z P 2009 Water quality actuality and control countermeasures for the surface water in Bahe River *Journal of Water Resources & Water Engineering* 20 145-7

[7] Li Z Z and Zhang X B 2011 Water pollution situation assessment in lower reach of Chan and Ba River in Xi’an city *Journal of Water Resources & Water Engineering* 22 151-6

[8] Xia Y F 2002 Research on application of 3D hydrodynamic, sediment transport model with non-staggered curvilinear grid for tidal rivers (Nanjing, China: Hohai University)

[9] Chen J 2018 Study on numerical simulation of water environment in Chan Ba Ecological District (Xi’an, China: Xi’an University of Technology)

[10] Elshemy M, Khadr M, Atta Y and Ahmed A 2016 Hydrodynamic and water quality modeling of Lake Manzala (Egypt) under data scarcity *Environ Earth Sci* 75 1329