Simulation of Water Pollution Accidents Based on FORTRAN and Its Application on Heshangshan Drinking Water Source Area

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Abstract. Developing a water quality model which is based on FORTRAN to simulate the distribution of pollutant concentration after water pollution accidents and to apply it to the drinking water source area of Heshangshan is the intention of this research. Taking ammonia nitrogen as the main water environment index, the spatial and temporal distribution and flow rate of pollutants at the inlet of Heshangshan drinking water source were analysed, and compared with those before and after the dispatching. The upstream discharge of water source area is selected from dry period, fall period, flood season and storage period respectively. The results show that the influent pollutant concentration decreases gradually with the increase of upstream flow in the source area. Moreover, the higher the upstream flow rate, the faster the decrease of influent concentration and the easier to reach level III.

1. Introduction
Water is the source of life and indispensable for people's long-term survival and development. However, water pollutions still happens frequently in many countries. For example, after the tailings slag rainstorm of Xichuan Lanjiang Electrolytic Manganese Plant in Sichuan Province, it flows into the Minjiang River with the mudslide water body, causing the water body index of more than 200 kilometers to exceed the standard on July 21 this year. The extremely large water pollution accident of Tuojiang River in 2004 has been listed as the largest water pollution accident nationwide in recent years by the state environmental protection administration. As a result of the large amount of high-concentration industrial wastewater flowing into Tuojiang River, the direct economic loss has reached 219 million Yuan. Chongqing municipality is the central municipality directly under the central government of our country, the centre of political, economic, cultural and others of the upper reaches of the Yangtze River. Once a major environmental emergency occurs, it will bring about a wide range of social impact. Located in Jiulongpo district, Heshangshan drinking water source is the water supply source for residents in Daping, Yanzhiping, Shiqiaopu and Zhongliangshan areas as well as Yuzhong district and Shapingba district of Chongqing. The protection of Heshangshan drinking water source is directly related to the stable development of social economy and people's daily life. The pollutants in the three gorges reservoir area mainly come from non-point sources, and the proportion of ammonia and nitrogen input load non-point sources is 65.45\% [1]. The excessive application of chemical fertilizer and the discharge of untreated sewage from chemical plants are the reasons for exceeding the...
standard of ammonia nitrogen in Heshangshan drinking water source. So the prediction results can provide scientific basis for making decision and reference for water resources management.

At present, the research on water quality model has been mature, and the water quality models commonly used abroad included: The effects of estuaries on lake water quality are simulated and quantified which is used by data driven water quality model by Mohamed Shaban [2]. Lale Balas applied model HYDROTAM-3D to simulate the wind driven circulations, hydrodynamics and basic water quality parameters in coastal waters [3]. Doan Quang Tri developed a 1D–2D coupled model to evaluate the water quality in Ca Mau Peninsula, Vietnam [4]. Moreover, the water quality of coastal estuaries in 2016 was evaluated by a 2D model. However, these methods still have some limitations. The first one is that the aforementioned studies emphasize water quality simulation without a comparative analysis of spatial and temporal distribution and pollutant concentration before and after dispatching. In addition, few studies predict the source of drinking water.

A dynamic water quality model of the 2D was developed by FORTRAN platform. Apply the water quality model to the Heshangshan drinking water source area (HSSWSA) and then simulate the temporal-spatial change of water velocity and the concentration of ammonia nitrogen after the hypothetical water pollution accident, and build a complete system of theoretical systems.

2. Materials and methodology

2.1. Study area

Located in the southwestern part of Chongqing, Chongqing Jiulongpo District is surrounded by the Yangtze River and the Jialing River and forms the main part of the Yuzhong Peninsula. The scope is from 106°31'40" to 106°32'25"E, 29°30'43" to 29°31'22"N, covering an area of 432km², is adjacent to Yuzhong District, Shapingba District, Daishan County and Jiangjin District, and is located on both sides of the Yangtze River in the Nan'an District and Banan District[5]. The area is 36.12km in the north-south direction and 30.4 km in the east-west direction .Heshangshan Water Source Protection Area is an important water source of Jiulongpo District (Figure 1). Jiulongpo District constitutes the topography of “two mountains and one water”: the north-south direction consists of the Zhongliang Mountain Range, the west side has the Jinyun Mountain Range, and the Yangtze River flows from the west to the east [6]. The land area is larger than the water area. The highest and lowest points of altitude are 698.5m and 170m respectively. The hills account for about half of the area of Jiulongpo, mainly medium and low hills, between 200 to 350m. The Jiulongpo District Yangtze River and Heshangshan Water Source Protection Area is level III, with the length of the upper and lower reaches of the water intake 1km and 0.1km respectively, and the width is the same side waters with the Zhongyu line as the boundary.

![Figure 1. Location of HSSWSA](image-url)
2.2. Methodology

2.2.1. Establishment of Water Quality Model. Most of the urban water supply type is surface water, and some of which is groundwater [7]. This paper builds a model of sudden water pollution accident, which is based on the planar two-dimensional water quality control equations.

\[
\frac{\partial h}{\partial t} + \frac{\partial hu}{\partial x} + \frac{\partial hv}{\partial y} = q
\]  

(1)

\[
\frac{\partial hu}{\partial t} + u \frac{\partial hu}{\partial x} + v \frac{\partial hu}{\partial y} = -gh \frac{\partial h}{\partial x} - g\nu \left( \frac{u^2 + v^2}{h^3} \right) + \frac{\partial}{\partial x} \left( \epsilon_x \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \epsilon_y \frac{\partial u}{\partial y} \right)
\]  

(2)

\[
\frac{\partial hv}{\partial t} + u \frac{\partial hv}{\partial x} + v \frac{\partial hv}{\partial y} = gh \frac{\partial h}{\partial y} - g\nu \left( \frac{u^2 + v^2}{h^3} \right) + \frac{\partial}{\partial x} \left( \epsilon_x \frac{\partial y}{\partial x} \right) + \frac{\partial}{\partial y} \left( \epsilon_y \frac{\partial y}{\partial y} \right)
\]  

(3)

\[
\frac{\partial hc}{\partial t} + u \frac{\partial hc}{\partial x} + v \frac{\partial hc}{\partial y} = \frac{\partial}{\partial x} \left( E_x \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left( E_y \frac{\partial c}{\partial y} \right) + H \sum S_i
\]  

(4)

where \(x\) and \(y\) were the longitudinal and transverse flow distances of the river, \(m\); \(u\) and \(v\) were the water velocity in the \(x\) and \(y\) directions, respectively; \(\epsilon_x\) and \(\epsilon_y\) were the eddy viscosity coefficient in the \(x\) and \(y\) directions, respectively; \(E_x\) and \(E_y\) were the sum of molecular diffusion coefficient, turbulent diffusion coefficient and discrete coefficient of \(x\) and \(y\) directions, respectively; \(n\) was the river reach roughness, \(\sum S_i\) was the source term of water pollutants in the river.

2.2.2. Discrete method. For formula (1) to formula (4), the formula (5) [8] was discretized by the finite volume method:

\[
\alpha_p \phi_p = \alpha_x \phi_x + \alpha_w \phi_w + \alpha_n \phi_n + \alpha_s \phi_s + b
\]  

(5)

2.2.3. Solution of equations. In this paper, the ADI method is used to solve the problem. After the generalization, the shape of the water in the study area is relatively complex. It is necessary to identify the scanning lines in the horizontal and vertical directions of the study area separately to generate hundreds of scan lines. Finally, the two-dimensional water quality model is written based on FORTRAN language.

2.3. Data

Water quality model parameters are the major factors that determined the accuracy of water quality simulation. The HSSWSA was small and there was no ready-made topographic data of water sources area. Therefore, the study through data collection, obtaining the data on a section of HSSWSA. The method of GIS is used to process the data, and the DEM diagram of HSSWSA is generated. (Figure 2). In order to ensure the simulation of the model was stable, the Zhutuo station was selected as the upper boundary, and the daily flow process of Zhutuo station was used, the Cuntan station was selected as the downstream boundary, and the daily water level process was used (Figure 3).

Figure 2. Topographic map of HSSWSA. Figure 3. Hydrological information map of hydrological station in 2016.
The influence of the roughness of riverbed on the water velocity was reflected by the roughness coefficient \((n)\), which was the empirical coefficient of the water flow roughness in the resistance square zone under uniform flow conditions \([9]\). There are three general methods to determine the coefficient of roughness (Table 1).

| Method Name         | Method Basis                                                                 | Advantages and Disadvantages                                                                 |
|---------------------|------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------|
| Look-up table method| According to the surface characteristics of the riverbed beach, the roughness of river channel roughness is roughly estimated by querying the similar rivers with reference charts. | It is simple and quick, but the influence of human factors is great.                         |
| Trial-and-error method | The river roughness is calculated by the measured hydrological data. | The actual application is more, but when the number of the calculated river sections is large, the workload of the debugging is large. |
| Formula method      | By means of physical and mathematical analysis, the roughness of the river bed and the roughness of the side wall are determined. | The physical basis is good, but it is difficult to determine the corresponding parameters of the roughness formula. |

3. Case Study
A 2D model of water quality was used in this study. The generalized terrain is divided into 70,500 grids \((250 \times 282 (I \times J))\), and each grid is a 4m square. Hypothetical simulation method was used to simulate the pollution accident of HSSWSA. The main variable description and parameter values are shown in the following table (Table 2).

| No. | Index | implication                        | value |
|-----|-------|------------------------------------|-------|
| 1   | \(n\) | roughness factor                   | 0.03  |
| 2   | \(\varepsilon_x\) | Transverse eddy viscosity coefficient \((m^2/s)\) | 20    |
| 3   | \(\varepsilon_y\) | Longitudinal eddy viscosity coefficient \((m^2/s)\) | 20    |
| 4   | \(E_x\) | Transverse diffusion coefficient \((m^2/s)\) | 0.5   |
| 5   | \(E_y\) | Longitudinal diffusion coefficient \((m^2/s)\) | 0.5   |

4. Results and Discussion

4.1 Changes in ammonia nitrogen concentration in the water intake of HSSWSA in four water periods
According to the figure (Figure 4) below, we can know that the water source is polluted by the polluted water. The initial concentration of the water inlet is 2.0mg/L. Due to the small area of the water source, the water quality can reach the standard in a short time.

It can be concluded that the intake concentration gradually decreases with time and finally reaches the level III water quality standards. Moreover, the larger the flow rate, the faster the concentration is reduced.
Figure 4. The changes of inlet concentration in four different periods

4.2 Migration and diffusion of ammonia nitrogen in HSSWSA.

Figure 5 shows the change in ammonia nitrogen over 240 minutes. According to the first picture, most of the water in the water source area of HSSWSA are seriously polluted after a sudden water pollution incident. After an hour, as the water inlet continues to enter the water, it can be concluded that the ammonia nitrogen concentration in the water is gradually decreasing by the second picture. And some water bodies have reached water quality standards. There is a third picture showing that only a small part of the water is contaminated, and most of the water has been restored to the water quality standard. The fourth picture shows that the water has reached the level III water quality standards. It can be concluded that the concentration of ammonia nitrogen gradually decrease over time and eventually reach water quality standards.

Figure 5. Migration and diffusion of ammonia nitrogen concentration at 1h,2h,3h,4h after an accident

5. Conclusions

In this research, the water quality model could simulate the migration and diffusion process of pollutants based on FORTRAN. In the hypothetical water pollution accident, the water quality model is used to measure the change of concentration and simulate the temporal-spatial variation of ammonia nitrogen pollutants in HSSWSA. The simulation of the concentration in HSSWSA indicates that the upstream flow has a significant influence on the migration and diffusion rate under the scheduling situation, and the reduction rate of inlet concentration also increases with the increase of the upstream flow of the water source. The topography of HSSWSA also affects the temporal and spatial variation of ammonia nitrogen pollutants. In the same region, the deeper the water source area, the faster the ammonia nitrogen concentration diffuses. It takes 240 minutes for ammonia nitrogen to be transported and diffused to make the quality of water body meet the level III water quality standards.

In a word, the results of this paper can improve the ability of emergency response to sudden water pollution accidents and ensure the safety of water quality to the maximum extent. At the same time, it
can also supply the theoretical basis and help for the sustainable development of social economy and the happy life of human beings.

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