Simulation of sudden benzene leakage water pollution events

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Abstract. Sudden water pollution incidents in rivers occur frequently, which has a serious impact on the ecological environment and residents' lives. After the sudden water pollution incident, determining the scale of the damage caused by the river water pollution event plays an important role in properly handling the accident. In this paper, the 3EWATER "hydrodynamic-water quality" numerical simulation system is used to simulate the concentration change of a certain pollutant in the river section during a certain period of time and realizes the visual expression of the simulation process. By simulating the sudden benzene leakage event in the Qin River, it was found that when the concentration of the leaked pollutant was \( 7 \times 10^{-3} \text{kg/m}^3 \), the concentration of benzene into the section of Yellow River reached a peak of 1.236mg/L after about 14 hours of leakage, and then began to decrease; after 20 hours of leakage, the concentration of pollutants dropped to the safe concentration of water; the pollutants moved from upstream to downstream in the form of "pollutant band" in the corresponding study area; The highest concentration of pollutants is near the center of the "pollutant band". The results of this case have strong practical value and provide decision-making basis for water environment planning management, water pollution prevention and emergency response to sudden water pollution incidents.

1. Introduction
Sudden water pollution incidents in the river not only make the water quality of water resources deteriorate rapidly in a short period of time, but also pose a great threat to human health and life safety. Such as: January 2000 Xiangjiang cadmium pollution; August 2006 Shaanxi Hancheng caustic soda pollution; 2013 Changzhi benzene leakage in Shanxi; 2013 Qingdao oil pipeline explosion eventually flow into Jiaozhou Bay and other events. When a sudden water pollution incident occurs, the environmental protection department should quickly enter the emergency state, start the water pollution event simulation system, quickly determine the type, concentration, pollution range and possible hazards of the pollutants, so as to properly handle the pollution accident. [1]

At present, research on sudden water pollution incidents in rivers has made some progress. Feng Wenzhao gave a software development method for early warning, emergency monitoring and treatment of sudden environmental pollution accidents, which satisfies the requirements of environmental protection departments for emergency monitoring and early warning services [2]. Chen Yuqing applied GIS technology to the emergency response system of sudden water pollution accidents, and provided a digital auxiliary system for the sudden warning of water pollution accidents and emergency decision-making through the calculation and analysis of the water pollution diffusion model [3-4]. Ding Tao used Matlab engineering software to establish a water quality analysis model for river sudden water pollution...
accidents, which can quickly calculate the water quality change process, the affected river section range and the over-standard time of each section downstream of the accident, and has the advantage of graphical display function [5]. The OTIS model system [6] is a one-dimensional water quality model for simulating the transport of dissolved matter in small rivers. It can simulate the regulation and storage of rivers and can also be used to simulate tracer tests. It can be seen that the above-mentioned studies are relatively weak for accurate numerical simulation and visualization techniques combined with GIS [7-8], and when the concentration gradient of pollutants in the lateral and vertical directions is not negligible, a one-dimensional model used for the simulation is not accurate enough.

This article uses the advanced Dutch 3EWATER hydrodynamic-water quality model system, which is the perfect combination of hydrodynamic-water quality equation, GIS accurate numerical simulation and visualization technology. 3EWATER software can use the 2D or 3D water quality model to decompose the target river section into several tiny grids and integrate them to calculate the water flow movement and pollutant concentration changes in the water environment system, and present the pollution diffusion visualization process.

This paper simulates a case where a truck turns over and causes benzene to leak into the Qin River to investigate the effects of water pollution caused by the diffusion of benzene pollutants at the point of leakage. By adjusting the leakage concentration, leakage time and water flow conditions, the pollutant concentration curve of the observation section set in the simulation time is derived and the flow process of the "pollutant band" is observed. Therefore, it provides scientific and effective technical support for environmental risk prevention, emergency treatment and disposal, damage identification and assessment, pollution repair and treatment of environmental pollution incidents.

2. Hydrodynamic-water quality model equation

2.1. Hydrodynamic equation

The hydrodynamic equation uses the Navier-Stokes equations, including the continuous flow equation and the momentum conservation equation.

The continuous flow equation is as follows:

\[
\frac{\partial \xi}{\partial t} + \frac{1}{G_{\xi\xi} \sqrt{G_{\eta\eta}}} \frac{\partial}{\partial \xi} [(d + \zeta)U \sqrt{G_{\eta\eta}}] + \frac{1}{G_{\xi\xi} \sqrt{G_{\eta\eta}}} \frac{\partial}{\partial \eta} [(d + \zeta)V \sqrt{G_{\eta\eta}}] = Q
\]  

(1)

The momentum equation is as follows:

\[
\frac{\partial u}{\partial t} + \frac{u}{G_{\xi\xi}} \frac{\partial u}{\partial \xi} + \frac{v}{G_{\eta\eta}} \frac{\partial u}{\partial \eta} + \frac{\omega}{G_{\xi\xi}} \frac{\partial u}{\partial \zeta} - \frac{v^2}{G_{\xi\xi} \sqrt{G_{\eta\eta}}} \frac{\partial}{\partial \xi} \sqrt{G_{\eta\eta}} + \frac{uv}{G_{\xi\xi}} \frac{\partial}{\partial \eta} \sqrt{G_{\eta\eta}} = P_{\eta} + F_{\eta} + \frac{1}{(d + \zeta)^2} \frac{\partial}{\partial \zeta} (vV \frac{\partial u}{\partial \sigma}) + M_{\eta}
\]

\[\quad - fV = - \frac{1}{\rho_0 \sqrt{G_{\xi\xi}}} \frac{\partial}{\partial \xi} \left( \frac{1}{(d + \zeta) \omega} \frac{\partial}{\partial \sigma} \frac{\partial u}{\partial \sigma} \right) + M_{\xi}
\]

\[
\frac{\partial v}{\partial t} + \frac{u}{G_{\xi\xi}} \frac{\partial v}{\partial \xi} + \frac{v}{G_{\eta\eta}} \frac{\partial v}{\partial \eta} + \frac{\omega}{G_{\xi\xi}} \frac{\partial v}{\partial \zeta} + \frac{uv}{G_{\xi\xi} \sqrt{G_{\eta\eta}}} \frac{\partial}{\partial \xi} \sqrt{G_{\eta\eta}} - \frac{u^2}{G_{\xi\xi} \sqrt{G_{\eta\eta}}} \frac{\partial}{\partial \eta} \sqrt{G_{\eta\eta}} = P_{\eta} + F_{\eta} + \frac{1}{(d + \zeta)^2} \frac{\partial}{\partial \zeta} (vV \frac{\partial u}{\partial \sigma}) + M_{\eta}
\]

\[\quad + fu = - \frac{1}{\rho_0 G_{\eta\eta}} \frac{\partial}{\partial \eta} \left( \frac{1}{(d + \zeta) \omega} \frac{\partial}{\partial \sigma} \frac{\partial u}{\partial \sigma} \right) + M_{\eta}
\]

(3)
2.2. Water quality equation

The water quality equation uses a convection-diffusion equation with the following equation:

$$\frac{\partial (d + \zeta)c}{\partial t} + \frac{1}{\sqrt{G_{\xi \zeta} G_{\eta \eta}}} \left[ \frac{\partial [\sqrt{G_{\eta \eta}} (d + \zeta)uc]}{\partial \xi} + \frac{\partial [\sqrt{G_{\xi \xi}} (d + \zeta)uc]}{\partial \eta} \right] + \frac{\partial \omega c}{\partial \sigma} = \frac{d + \zeta}{\sqrt{G_{\xi \xi} G_{\eta \eta}}}
$$

$$\left[ \frac{\partial}{\partial \xi} (D_{\eta \eta} \frac{\partial c}{\partial \xi}) + \frac{\partial}{\partial \eta} (D_{\xi \xi} \frac{\partial c}{\partial \eta}) \right] + \frac{1}{d + \zeta} \frac{\partial}{\partial \sigma} (D_{\eta \eta} \frac{\partial c}{\partial \sigma}) - \lambda_d (d + \zeta)c + S$$

(4)

2.3. Variable Description

Table 1 gives the meaning of the symbols used in the hydrodynamic and water quality equations.

| Number | Symbol | Units | Meaning |
|--------|--------|-------|---------|
| 1      | \(v\)  | m/s   | Fluid velocity in the y- or \(\eta\)-direction |
| 2      | \(u\)  | m/s   | X- or \(\xi\)-direction fluid velocity |
| 3      | \(\omega\) | m/s | Velocity in the \(\sigma\) direction in the \(\sigma\)-coordinate system |
| 4      | \(\sigma\) | J/m/s\(^4\) | Stefan-Boltzmann's constant |
| 5      | \(d\)  | m     | Depth below a certain horizontal reference plane (reference plane) |
| 6      | \(G_{\xi \xi}\) | m | The coefficient used to transform the curve into Cartesian coordinates |
| 7      | \(G_{\eta \eta}\) | m | The coefficient used to transform the curve into Cartesian coordinates |
| 8      | \(\xi\), \(\eta\) | m | Horizontal and curvilinear coordinates |
| 9      | \(\zeta\) | m | The water level is above a horizontal reference plane (reference plane) |
| 10     | \(c\)  | kg/m\(^3\) | Concentration |
| 11     | \(\lambda_d\) | 1/s | First order attenuation coefficient |
| 12     | \(S\)  | ppt   | Salinity |
| 13     | \(D_s\) | Dimensionless particle size |
| 14     | \(V\)  | m/s   | Depth average speed in the y or \(\eta\)-direction |
| 15     | \(Q\)  | m/s   | Source or sink per unit area |
| 16     | \(t\)  | s     | Time |
| 17     | \(\rho_0\) | kg/m\(^3\) | Reference water density |
| 18     | \(P_\eta\) | kg/m\(^3\)s\(^2\) | Gradient hydrostatic pressure in the \(\eta\)-direction |
| 19     | \(f\)  | 1/s   | Coriolis parameter (inertial frequency) |
| 20     | \(F_s\) | m/s\(^2\) | Directional flow flux |
| 21     | \(M_s\) | m/s\(^2\) | Momentum source or sink in the direction |

3. Simulation of benzene leakage pollution incident in Qin River

3.1. Overview of benzene pollution events

This paper simulates that at 8 o'clock on June 20, 2018, a truck fell over and fell into the river next to the G222 provincial road in B Town, Qinyuan County, Shanxi Province, causing one death and one injury. The car is equipped with 400 barrels of pure benzene solution, gearbox, wooden floor, electric mosquito coil and mosquito coil. Some of the pure benzene solution barrels are damaged. After being properly disposed, benzene leaking for about two hours into the Qin River is caused. After the accident, the B Town government and the Municipal Environmental Protection Bureau immediately added reinforcement personnel to set up an on-site emergency headquarters and carried out emergency disposal
work, while tracking and monitoring the water quality of the Qin River. After nearly 20 hours, as of 4:00 am on June 21, 2018, the water quality standard was reached near the accident point and into the section of Yellow River.

3.2. Water flow conditions, pollutant release conditions table
According to the historical data of the Qin River, it is determined that the river flow during the simulation is 4.41 m$^3$/s and the average speed of the river is 0.68 m/s. The simulated pollutant is benzene, the attenuation coefficient of benzene in the Qin River is 0.2766 1/Day, and the safe concentration of pollutants is 0.0006 kg/m$^3$. After setting the above parameters, the simulation is carried out by adjusting the concentration of released pollutants. The detailed parameters are shown in Table 2.

| Number | Name                                      | Content            |
|--------|-------------------------------------------|--------------------|
| 1      | Simulation time (h)                       | 24                 |
| 2      | Simulation time step (min)                | 1                  |
| 3      | Contaminant                                | benzene            |
| 4      | Result output time frequency (min)        | 30                 |
| 5      | Initial conditions of pollutant           | 0                  |
| 6      | Inflow boundary water flow conditions (m$^3$/s) | 4.41               |
| 7      | Outflow boundary water flow condition (m$^3$/s) | 0                  |
| 8      | Inflow/outflow boundary transmission conditions (m$^3$/s) | 0                  |
| 9      | Transmission material decay rate (1/Day)  | 0.0006             |
| 10     | Safety concentration (mg/L)              | 0.2766             |
| 11     | Dangerous concentration (mg/L)            | 0.000689           |

3.3. Drawing a grid
RGFGRID is a dedicated mesh drawing tool that generates a smooth and orthogonal curved mesh by loading the water boundary of GISMODEL. First, load the river profile file, then draw Splines along the river profile, which should include two sets of curves in different directions, and finally mesh the operation to form the grid, as shown in Figure 1.

![Figure 1. Qin River Basin research section grid map.](image)

3.4. Description of simulation section and pollutant leakage point
The simulation research section started in Youyi Village, Qinyuan County, Shanxi Province, and finally reached Wushe County, Jiaozuo City, Henan Province, with a total length of about 200 kilometers. Most of the research sections are very curved.

The dumping position of the truck is located at the G222 Provincial Road in Qinyuan County, Shanxi Province and the leaking point is located at the Youyi Bridge in Qinyuan County, Shanxi Province. As
shown in the following figure, it is located in the upper part of the research section, about 20 kilometers away from the starting point of the research section. The map of the Qin River research section and the leakage point is shown in Figure 2.

![Figure 2. Study area and leak location map.](image)

3.5. Diffusion simulation process
According to the general experience to determine the leakage time, water flow conditions and the parameters in Table 1, due to the uncertainty of the sudden event, it is necessary to compare the leakage concentration. The concentration of pollutants into the section of Yellow River is taken as the observed value, and the simulated leakage concentration set when the observed value falls below the safe concentration is the actual leakage concentration.

This case has a total of 4 selections, numbered from Case 1 to Case 4. The pollutant concentrations are: $5 \times 10^{-3}$kg/m$^3$, $9 \times 10^{-3}$kg/m$^3$, $11 \times 10^{-3}$kg/m$^3$, $7 \times 10^{-3}$kg/m$^3$. The data of the comparison result can refer to Table 3.

| Case | Leaked benzene concentration | Benzene concentration at control point |
|------|------------------------------|----------------------------------------|
| 1    | $11 \times 10^{-3}$kg/m$^3$  | 0.6978mg/L                             |
| 2    | $9 \times 10^{-3}$kg/m$^3$   | 0.4872mg/L                             |
| 3    | $7 \times 10^{-3}$kg/m$^3$   | 0.2752mg/L                             |
| 4    | $5 \times 10^{-3}$kg/m$^3$   | 0.0653mg/L                             |

After the simulation, the curve of Case 4 is the best curve, and the concentration of pollutants into the section of Yellow River in the simulation time (24 hours) reaches the benzene safety concentration of the environmental quality standard. The best curve is shown in Figure 3.

![Figure 3. Case 4 of the pollutant concentration curve into the section of Yellow River.](image)
According to Figure 3, after 6 hours of leakage of contaminants, traces of benzene are detected in the section of Yellow River; after about 10 hours of leakage, the concentration of benzene in the section of Yellow River exceeds the safe concentration of benzene; from the sixth hour to the 10 hours after the leak is the slow rise of pollutant concentration; from the 10th to 14th hour after the leakage is the extremely high rise of pollutant concentration; the concentration of benzene in water pollutants continues to rise until the peak of 1.236mg/L in the 14th hour after the leakage and then begins to decrease; from the 14th hour to the 18th hour after the leak, the pollutant concentration drops rapidly; the 18th hour after the leak is the flat drop of the pollutant concentration; finally, the pollutant drops to the safe concentration of the water body until the 20th hour after the leak.

3.6. Simulation of pollutant diffusion based on optimal parameters
(1) The pollutants move from upstream to downstream in the form of "pollutant band" in the corresponding research basin. The darker the color in the figure, the higher the concentration of pollutants. The lighter the color, the lower the concentration of pollutants. The colors are red, orange, yellow, green, and blue in order from dark to light. That is to say, red represents the most polluted area, and the concentration of pollutants represented by orange, yellow and green decreases in turn, and the blue represents that the concentration of pollutants has fallen below the water quality standard.

Figure 4 shows the process of "pollutant band" migrating over time. It can be seen from these figures that the "pollutant band" gradually becomes lighter as the overall color of the movement changes, indicating that the concentration of pollutants gradually decreases with river migration. The reason for the decrease in concentration is the transport and degradation of pollutants by water bodies and the self-purification of rivers. Due to lateral diffusion and longitudinal diffusion, the contaminated area gradually increases from the upstream to the downstream of the target river section and is affected by its speed. The color of the "pollutant band" gradually deepens from the outside to the inside, indicating that the region with the highest concentration of pollutants is near the center of the "pollutant band".

![Diffusion status 6, 12, 18 and 24h after benzene leakage event](image)

4. Conclusion
(2) When the concentration of the leaked pollutant is 7*10^{-3}kg/m^3, trace benzene is detected in the section of Yellow River at the 6th hour after the leak; in the 10th hour after the leak, the benzene concentration in the section of Yellow River exceeds the safe concentration of benzene; at the 14th hour
after the leak, the benzene concentration reaches a peak of 1.236mg/L, and then begins to decrease; in the 20th hour after the leak, the pollutant concentration decreases below the safe concentration of the water.

(2) Contaminants move from upstream to downstream in the form of "pollutant band" in the corresponding research basin. During the process of pollutant migration, the concentration of pollutants in the river gradually decreases, and the area with the highest concentration of pollutants is near the center of the "pollutant band".

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