Study on simulation and prediction of environmental risk material leakage in an Equipment Manufacturing Industrial Park

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Abstract. From the perspective of environmental risks, the groundwater pollution, surface water pollution, and fire and explosion scenarios were simulated and predicted with the analytical method in an equipment manufacturing industrial park in Shenyang. The results showed that: after the accident, the maximum migration distance of COD pollution factor leakage in groundwater in the next ten years could reach 1500m, and its peak concentration was 786.35mg/L; the leakage of WSCLC wastewater treatment system would affect Xihe river, and its hazard range mainly concentrated within 17m downstream of the discharge port; the vapor cloud explosion of the HCBM enterprise oil tank caused slight damage to the equipment, and the maximum radius of minor injuries was 15.3m.

1. Introduction

In recent years, various industrial parks in my country have risen rapidly. While bringing huge economic benefits, they also make huge environmental risks. Especially after the 8ꞏ12 Tianjin Port explosion and the 3ꞏ21 Xiangshui explosion accident, the environmental risk prevention and emergency response work were put in an important position. In order to prevent the occurrence of various environmental emergencies from the source, the scholars are committed to the establishment of an environmental risk prevention system on the one hand, and on the other hand strengthen the research on the theory of environmental risk prediction \cite{1}. The environmental risk prediction models have begun to study at abroad since the 1970s and 1980s \cite{2}. The related research in China started relatively late. In 1989, the former National Environmental Protection Agency established the Office of Toxic Chemicals Management, which marked the formal promotion of risk assessment and management on the agenda in China \cite{3}. After decades of development, the environmental risk research in China has begun to take shape, but due to the complexity and timeliness of emergent environmental events, the research work still has a long way to go \cite{4,6}. A national equipment manufacturing industrial park in Shenyang City was taken as an example. By analytical methods, the possible environmental emergencies were simulated, which contained three major environmental emergencies impact on the surrounding environment. The results would provide scientific basis of environmental risk prevention and emergency work for the environmental management department.

2. Study Area

The equipment manufacturing industrial park is located in the west of Shenyang City, belonging to the mid-latitude northern temperate monsoon-type semi-humid continental climate zone.
The statistical results of the accumulated annual meteorological value in Shenyang since 2018, the annual average temperature in the area was 8.1℃, the lowest average temperature in January was -11.6℃, and the highest average temperature in July was 24.6℃. The annual precipitation was 714mm, mostly in July and August. The main surface water in the study area was Hunhe River and Xihe River. The thickness of the silty clay layer below the ground in the study area was about 2.0~5.5m, and its permeability coefficient was 10^{-7}~10^{-4}cm/s. It has medium water permeability and medium water and pollution resistance. The permeability coefficient and poor runoff conditions of the aquifer were large. Once polluted, the diffusion process would proceed slowly. The lithology of the aquifer is mainly medium sand, and the lower part has gravel sand, medium sand and gravel sand, which were the main water-rich parts.

According to the principle of high probability of occurrence and large scope of influence, three types of key environmental risk companies in the area were screened out: HCBM, WSCLC, and RYC. Among them, according to the identification of major hazards [7], HCBM companies have major risk sources, and the hazardous chemicals they use and store were mainly gasoline, diesel, and acetylene.

3. Research Method
The analytical method was adopted for simulation and prediction, which was the most common method used in environmental risk prediction simulations and recommended by the Technical Guidelines for Environmental Risk Assessment of Construction Projects (HJT 169-2018). According to the analysis results of the largest credible accidents. The groundwater pollution accidents caused by sewage leakage, Xihe pollution accidents caused by sewage leakage, and fire and explosion accidents that may occur in the park would be analyzed and predicted in the article.

3.1. One-dimensional infinitely long porous medium cylinder, instantaneous tracer injection model
The one-dimensional steady flow and one-dimensional hydrodynamic model—no smell and no on-site porous medium body, instantaneous tracer injection model was often used for the groundwater pollution accident caused by sewage leakage. The specific formula was as follows:

\[ C(x, t) = \frac{m/W}{2n_{e} \sqrt{\pi D_{L} t}} e^{-\frac{(x-u t)^{2}}{4D_{L} t}} \]  

Where \( C(x, t) \) is tracer concentration at point \( x \) at time \( t \), g/L; \( m \) is the injected pollutants quality, kg; \( W \) is the cross-sectional area, m²; \( u \) is the flow velocity, m/d; \( n_{e} \) is the effective porosity; \( D_{L} \) is the longitudinal dispersion coefficient, m²/d.

3.2. One-dimensional Convection and Diffusion Model of Instantaneous Emission Source River
The pollution accident of Xihe River caused by sewage leakage adopts the instantaneous discharge model—the concentration distribution formula of the instantaneous discharge source river one-dimensional convection diffusion equation was as follows:

\[ C(x, t) = \frac{M}{A \sqrt{4 \pi E_{t}}} \exp(-kt) \exp\left[\frac{(x-ut)^{2}}{4E_{t}}\right] \]  

At time \( t \), the peak pollutant concentration at \( x=ut \) downstream from the pollution source is as follows:

\[ C_{\text{max}}(x) = \frac{M}{A \sqrt{4 \pi E_{t}}} \exp(-kt / u) \]  

Where \( C(x, t) \) means the pollutant concentration at time \( t \) at the distance from the discharge port \( x \), mg/l; \( x \) means distance from the discharge port, m; \( u \) means the flow velocity, m/d; \( E_{t} \) means the longitudinal diffusion coefficient of pollutants, m²/s; \( K \) means the comprehensive attenuation coefficient of pollutants, s⁻¹.
3.3. Mathematical Model of Steam Cloud Explosion

The TNT equivalent method is used to describe the energy release degree of an explosion accident in the fire and explosion accidents. The damage caused by an explosion accident is equivalent to the damage caused by an $X$ kg TNT explosion, which means that the mass of the explosive fuel is converted into TNT equivalent. The specific formula is as follows:

$$W_{\text{TNT}} = \frac{\alpha W_f Q_f}{Q_{\text{TNT}}}$$  \hspace{1cm} (4)

Where $W_{\text{TNT}}$ is the TNT equivalent of the steam cloud, kg; $W_f$ is the mass of fuel leaked into the air, kg; $\alpha$ is the explosion factor of the steam cloud, usually 4%; $Q_f$ is the fuel combustion heat involved in the steam cloud explosion accident, MJ/kg; $Q_{\text{TNT}}$ is the heat of explosion of TNT, generally 4.52 MJ/kg.

The TNT equivalent method is used to calculate the fuel mass in the combustion range which could describe the fire accident. And then the Equation 4 is used to calculate the equivalent TNT mass of the vapor cloud explosion accident:

$$W_{\text{TNT}} = \frac{W_f Q_f}{Q_{\text{TNT}}}$$  \hspace{1cm} (5)

In the formula, $W_f'$ is the mass of fuel in the combustion range (kg) in the mixture.

The distance range of the buried oil tank's damage caused by the explosion is calculated by the empirical formula of the relationship between the overpressure of the Lekhoff explosion shock wave and the distance, which is:

$$R = \left( \frac{0.8W_{\text{TNT}}}{P} \right)^{\frac{1}{3}}$$  \hspace{1cm} (6)

Where $R$ is the blast damage distance, m; $P$ is the explosion shock wave overpressure (MPa).

The damage caused by the blast shock wave is mainly based on the shock wave overpressure "injury-destruction criterion", which is in Table 1.

| No. | $\Delta P$/MPa | Harm                        |
|-----|---------------|-----------------------------|
| 1   | 0.02~0.03     | Minor damage                |
| 2   | 0.03~0.05     | Hearing damage or fracture  |
| 3   | 0.05~0.10     | Serious internal organ damage or casualties |
| 4   | >0.10         | Most people died            |

Destructive effects of shock wave overpressure on buildings

| No. | $\Delta P$/MPa | Harm                                               |
|-----|---------------|----------------------------------------------------|
| 1   | 0.005~0.006   | Partially broken doors and windows                 |
| 2   | 0.006~0.015   | Most of the door and window glass on the pressure surface broken |
| 3   | 0.015~0.02    | Damaged window frame                               |
| 4   | 0.02~0.03     | Wall crack                                         |
| 5   | 0.03~0.05     | Strong cracks, roof tiles fall                     |
| 6   | 0.05~0.07     | The column of the wooden building workshop broken and the frame loose |
| 7   | 0.07~0.10     | Brick wall collapsed                               |
| 8   | 0.10~0.20     | Earthquake-proof reinforced concrete damage, small house collapse |
| 9   | 0.20~0.30     | Large steel frame structure failure                |
4. Results and Discussion

4.1. Groundwater pollution scenario

4.1.1. Scene setting and source strength
This scenario setting considers the impact of non-continuous and constant discharge of wastewater from enterprises in the park on the surrounding groundwater environment under abnormal conditions. According to the characteristics of wastewater quality, the predictive factor in the scenario was COD.

Assuming that the domestic sewage drainage system and the workshop process water cleaning system have serious failures during operation, according to the principle of maximum risk, the pollutants have not undergone any pre-treatment, and the pollutants leak directly from the source of the pollutants. The highest concentration of pollutants discharged was chose as the source strength, in which the COD=1000mg/L (100 times the lower limit of the five types of water quality standards).

4.1.2. Simulation result analysis
The hydrogeological conceptual model was generalized into a one-dimensional steady flow and one-dimensional hydrodynamic dispersion problem. The prediction model adopted the "one-dimensional infinite-length porous medium cylinder, and the tracer was injected instantaneously". According to formula (1), the simulation results are shown in Table 2 and Figure 1.

| Pollution Time (year) | Predicted concentration (mg/L) | Predicted distance (m) |
|-----------------------|--------------------------------|------------------------|
|                       | 100   | 200   | 300   | 400   | 500   | 1000  | 1500  | 2000  | 2500  |
| 1                     | 148.03 | 29.61 | 2.11  | 0     | 0     | 0     | 0     | 0     | 0     |
| 5                     | 777.17 | 304.97 | 41.19 | 4     | 0.33  | 0     | 0     | 0     | 0     |
| 10                    | 786.35 | 551.54 | 281.97 | 79.33 | 24.00 | 7.26  | 2.04  | 0     | 0     |

Figure 1. Changes in COD concentration at different distances at 1, 5, and 10 years.

The detection range of COD pollutants after one year was 300m, and the exceeding range was 200~300m. In the next ten years, the detection range and the exceeding range would increase significantly, the detection range would reach 1500m, and the exceeding range would reach 1000~1500m. The peak concentration was 786.35mg/L, which seriously affects the quality of groundwater. It could be seen that groundwater pollution was a long-term and hidden process. Once a leak occurred, it was extremely difficult to find, and it was easy to miss the most opportunity for disposal.
Therefore, take care of daily environmental risks. The investigation of hidden dangers was very important.

4.2. Surface water pollution scenario

4.2.1. Scene setting and source strength
The scenario was set as the failure of the sewage treatment system in the enterprise WSCLC or the equipment maintenance and debugging caused untreated sewage to be directly discharged into the Xihe River with the pipeline. Assuming that the sewage treatment plant was directly discharged into Xihe River without treatment due to some factors, the outlet flow of the sewage treatment plant into Xihe River was calculated at 1.5m³/s, and the leakage was discovered by employees after 5 minutes, and the corresponding plan was activated to stop the discharge to Xihe River, which meant that a total of 450m³ of untreated wastewater was discharged to Xihe River. The wastewater concentration was shown in Table 3.

| Pollutants | SS (mg/l) | BOD₅ (mg/l) | CODcr (mg/l) | NH₄-N (mg/l) | TP (mg/l) | TN (mg/l) |
|------------|-----------|-------------|-------------|-------------|----------|----------|
| Influent water quality | 67.0 | 46.5 | 186.0 | 18.4 | 3.16 | 18.4 |
| 2018.4 Inlet-water flow (t/d) | 135000 |
| Effluent water quality | 13.0 | 4.0 | 20.0 | 1.7 | 186 | 1.69 |
| 2018.4 Discharge flow (t/d) | 135000 |

4.2.2. Simulation result analysis
With the instantaneous source river one-dimensional convection diffusion model formula (3), the maximum concentration of COD at different distances downstream of the discharge outlet was calculated as shown in Table 4 and Figure 2. At 17m downstream of the sewage discharge outlet, the maximum concentration drops to 40mg/l, which meant that if the accident was found within 5 minutes and action was taken immediately after the accident had occurred, the impact range could be controlled within 17m downstream of the discharge port. Therefore, the impact of the instantaneous discharge of untreated sewage from a company mainly depends on the time it takes for the company to discover and take effective measures. The shorter the time, the smaller the scope of impact. If it was not found after treatment for a long time, it may affect the Hunhe River.

| x m | COD Cₘₐₓ(x) mg/l | Water quality standards V mg/l | x m | COD Cₘₐₓ(x) mg/l | Water quality standards V mg/l |
|-----|-----------------|------------------------------|-----|-----------------|------------------------------|
| 1   | 7394.136803     | 40                           | 15  | 52.47791635     | 40                           |
| 2   | 3150.433876     | 40                           | 16  | 41.92380982     | 40                           |
| 3   | 1789.74844      | 40                           | 17  | 33.62363685     | 40                           |
| 4   | 1143.842263     | 40                           | 18  | 27.0603859      | 40                           |
| 5   | 779.7744638     | 40                           | 19  | 21.84569031     | 40                           |
| 6   | 553.7333051     | 40                           | 20  | 17.68488584     | 40                           |
| 7   | 404.4517686     | 40                           | 20  | 17.68488584     | 40                           |
| 8   | 301.5696797     | 40                           | 40  | 0.360437462     | 40                           |
| 9   | 228.4273151     | 40                           | 50  | 0.058216855     | 40                           |
| 10  | 175.187626      | 40                           | 60  | 0.009794817     | 40                           |
| 11  | 135.7136795     | 40                           | 70  | 0.001695034     | 40                           |
| 12  | 106.0102716     | 40                           | 80  | 0.000299444     | 40                           |
| 13  | 83.38707187     | 40                           | 90  | 5.37392E-05     | 40                           |
| 14  | 65.98221999     | 40                           | 100 | 9.76479E-06     | 40                           |
4.3. Fire and explosion scenario

4.3.1. Scene setting and source strength

The environmental emergencies that may occur in the study area contain the leakage and proliferation or explosion of gasoline, diesel, natural gas, paint, etc., which could cause atmospheric environmental pollution around environmental risk sources. According to the rank about the ratio of the inventory of atmospheric environmental risk substances to the critical mass, the highest was the enterprise HCBM. Its main atmospheric environmental risk substances were gasoline, diesel, ethanol, glycol, etc., the following was the selection of plant oil depots and gas stations for leaks, fires and explosions. As this simulation scenario. The gasoline was taken as an example for simulation, whose maximum storage capacity was 97.6t. The most common fire and explosion scene modes were the empty tank explosion scene and the half tank fire explosion scene.

4.3.2. Simulation result analysis

According to the mathematical model of steam cloud explosion, the simulation results were as follows:

① The result of mathematical simulation calculation for the explosion scene of an empty oil tank: the oil and gas content in the oil tank was 2.36%, $W_f'=5.34$kg, $W_{TNT}=51.63$kg.

② The result of mathematical simulation calculation of the fire and explosion scene of the oil tank and half tank: The fuel involved in the second explosion in the fire and explosion scene of the oil tank and half tank should be related to the energy of the first explosion. It was assumed that 1/10 of the energy in the second explosion was used for gasoline vaporization, Calculated $W_f'=2.7$kg, and the energy used for vaporization $E=11799.0$kJ.

The mass of vaporized gasoline was about 35.2kg. The vaporized vapor of liquid droplets brought out by gasoline vapor and exploded was 6 times that of energy vaporization. The fuel mass in the vapor cloud was estimated to be $W_f = 211.3$kg. There were a lot of liquid droplets in the vapor. The fuel involved in the explosion of the vapor cloud accounts for a low percentage of the total fuel. T is taken as 1%, and the TNT equivalent was calculated as $W_{TNT} = 20.4$kg.

Use TNT equivalent to calculate the corresponding damage radius ($R_2$) and damage degree. The specific results were shown in Table 5.
Table 5. The degree of damage to the human body caused by the explosion wave of the oil tank.

| No. | Overpressure $\Delta P$/Mpa | Empty tank explosion damage distance $R_1$/m | Half tank explosion damage distance $R_2$/m | Damage to structures | Personal injury and destruction degree |
|-----|----------------------------|---------------------------------|---------------------------------|-------------------|--------------------------------------|
| 1   | 0.02~0.03                  | 11.1~12.7                       | 11.6~15.3                       | slight            | Minor injuries                       |
| 2   | 0.03~0.05                  | 9.4~11.1                        | 8.9~11.6                        | medium            | Serious injuries                     |
| 3   | 0.05~0.10                  | 7.4~9.4                         | 6.2~8.9                         | serious           | Serious internal organ or dead       |
| 4   | >0.1                       | <7.4                            | <6.2                            | Extremely serious  | Most people died                     |

Through the simulation calculation of the explosion process, it could be seen that the vapor cloud explosion of the oil tank caused slight damage to the equipment and the maximum radius of minor injuries to personnel was 15.3m. The main damage scope was around the oil and gas reservoir and inside the plant area, but the oil droplets splashed after the explosion. If the oil-water mixture produced during the fire extinguishing process was not contained in time, it may pollute the surrounding soil and groundwater.

5. Conclusions
The analytical methods were used to simulate and predict the environmental pollution accidents that may occur in an equipment manufacturing industrial park in Shenyang, and the conclusions were as follows:

1) In the groundwater pollution scenario, after the groundwater pollution occurs, the COD pollutants exceed the standard range of 200~300m within one year; after 10 years, the range of exceeding the standard would reach 1000~1500m, and the predicted peak concentration was 786.35mg/L.

2) In the surface water pollution scenario, the accidental discharge of the WSCLC wastewater treatment system would cause pollution to Xihe River and its downstream. If only 450m$^3$ of untreated wastewater was leaked, it would cause COD concentration within 17m downstream exceeding the Class V standard of "Surface Water Environmental Quality Standard".

3) In the fire explosion scenario, the HCBM enterprise oil tank empty tank explosion scene and the oil tank half-tank fire explosion scene caused the vapor cloud explosion of the oil tank to slightly damage the equipment, and the maximum radius of minor injuries to personnel was 15.3m, and the main damage area was around the oil and gas reservoir. If the oil droplets splashed after the explosion and the oil-water mixture produced during the fire extinguishing process were not contained in time, they may pollute the surrounding soil and groundwater.

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