Numerical Simulation for Impact of Groundwater Environment in a Chemical Industry Park in the Southwest of Shandong Province Based on GMS

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Abstract. The establishment of chemical industry park can bring great pressure on local groundwater environment, and even cause serious groundwater pollution problems. This study armed at a chemical industry park in southeast of Shandong province and developed a three-dimensional groundwater solute transport model through GMS software, selected dichloromethane as the typical contaminant, simulated and predicted the transport characteristic of groundwater contaminant in different conditions. The results showed that after 20 years, the dichloromethane can separately transport 820m and 1,000m under different hypothetical conditions, the greatest affected area can separately reach $32 \times 10^4$ m$^2$ and $21 \times 10^4$ m$^2$; it indicated that the studied area would be polluted under these simulated conditions, so measures must be done to improve the ability of seepage-proofing of this chemical industry park and to enhance the management and the monitoring of groundwater in this studied area.

1. Introduction
The construction and operation of chemical industry often cause pressure on regional groundwater environment that result in groundwater pollution increasingly threatening the safety of drinking water to a certain extent [1-3]. Prevention and remediation strategies for groundwater pollution can be successfully carried out only after well known for the scope and characteristics of pollutants [4-5]. Numerical simulation model of groundwater solute transport can effectively simulate the transportation and distribution of pollutants in groundwater, which can provide useful information for groundwater pollution control and effective remediation [6-10].

In this paper, we established solute transportation numerical model by GMS based on a chemical industry park in southwest Shandong province to simulate and predict spatial and temporal distribution of leaked dichloromethane under different working conditions, and assessed the potential groundwater environment risk in this chemical industry park.

2. General situation of study area
The study area locates in the plain between the Luxi Plains and the Luzhong Mountains. The terrain is low in the west and south, and high in the north and east. The east and north which are hilly terrain locates in the edge zone of the southern and middle Lu Mountain, takes up 46% of the total area and the elevation is generally between 80-480m. The western part is the deposition area and composed of river sediments. The southern hills have a low elevation compared with north which is between 100-140m, as shown in Figure 1.

3. **Groundwater numerical model**

3.1. **The conception of the study area**

Study area can be divided into two groundwater layers by analyzing the geology, hydrogeology and borehole data of the study area. The first layer is the porous rock unconfined layer, the total thickness of the aquifer is 5-50m; the second layer is limestone shale karst confined layer, thickness is about 80-260m.

Groundwater flow to the aquifer through the bedrock mountainous area, which can be treated as the flow boundary. The northern area has a close hydraulic connection with rivers, which can be treated as the general head boundary. The north-west area and the south-east boundary are determined as the general head boundary according to the flow field, of which the northwest side is mainly the discharge boundary, and the southeast side is the recharge boundary. The southwest side and the south side of the confined aquifer also accept the lateral recharge of the bedrock mountainous area, which is treated as the flow boundary. The northwest and south-eastern sides which perpendicular to the direction of groundwater flow can be treated as the flow boundary and was divided into discharge boundary and the recharge boundary. The depth of the aquifer in the northeast and north border is large, and the boundary is the same as the groundwater flow, so it can be generalized as zero flux boundary.

3.2. **hydraulic feature**

Taking account to lots of water exchange between unconfined and confined aquifers, we can generalize the movement of groundwater in the aquifer into a spatial three-dimensional flow. The annual supply and exploitation of the study area change little and can be generalized as stable flow. The
hydrogeological parameters change with the spatial change, but there is no obvious change in the horizontal direction, so it can be summarized as isotropic.

In summary, the hydrogeological conceptual model can be generalized into heterogeneous and three-dimensional stable flow.

3.3. Hydrogeological parameter
The relevant hydrogeological parameters in the study area are mainly determined by parameter calibration, previous work results, hydrogeological data and field hydrogeological tests, as shown in Figure 2 and Table 1-2.

![Figure 2](image-url) Figure 2 Hydrogeological parameters of unconfined and confined aquifers
Table 1 Hydrogeological parameters of unconfined aquifer

| Partition | Horizontal conductivity (m/d) | Vertical conductivity (m/d) | Effective porosity |
|-----------|-------------------------------|-----------------------------|-------------------|
| 1         | 18.00                         | 0.05                        | 0.30              |
| 2         | 6.00                          | 0.40                        | 0.30              |
| 3         | 8.00                          | 0.20                        | 0.30              |
| 4         | 4.00                          | 0.30                        | 0.30              |

Table 2 Classification of hydrogeological parameters of confined aquifers

| Partition | Horizontal conductivity (m/d) | Vertical conductivity (m/d) | Effective porosity |
|-----------|-------------------------------|-----------------------------|-------------------|
| 1         | 5.00                          | 0.03                        | 0.25              |
| 2         | 6.00                          | 0.40                        | 0.25              |
| 3         | 7.00                          | 0.40                        | 0.25              |

4. Simulation of pollutant transport in chemical industry park

The chemical industry park in this study would cause a potential threat on the local ecological environment which mainly manufactured pesticides and chemical fertilizer including nitrobenzene, aniline, cyclohexylamine and benzene. The typical pollutants produced in the production process, dichloromethane (C₂H₄Cl₂), is chosen to simulate the risk posed to local groundwater environments when part of pollutants get into the aquifer during normal production process or an accident occurred respectively.

4.1. Under normal operating conditions

Under normal operating conditions, leakage would occur in the facilities such as sewage pipe network or sewage treatment pond in the factory area, resulting in the waste water which containing dichloromethane contaminants infiltrated into the aquifer for a long time. Dispersion effect is mainly considered in the process of pollutant transport simulation in which the longitudinal dispersion is 18 m²/d and vertical dispersion are 6 m²/d. According to the factory report, it is assumed that the amount of sewage leakage is 100m³/d (about 1/3 of the total amount of sewage), the concentration of dichloromethane in the waste water is 5 mg/L, and the simulated pollution threshold is 0.03 mg/L.

It can be seen from the simulation results (Figure 3) that the pollutants in the aquifer continue to move in the factory as time goes by, and then began to move to the northwest after 10 years. The main reason is that on the one hand, the chemical plant has exploited too much groundwater leading local flow field has changed. The pollutant was located in the groundwater hydraulic capture area, indicating that the human effect factors have an important impact on the transportation of groundwater pollutants. On the other hand, the transport of pollutants is affected by the flow of groundwater itself.

With the prolonging of the leaking time, the concentration of pollutants on the leaking point gradually increased. The concentration of dichloromethane was about 2.0 mg /L after 20 years which exceed concentration limits a lot in groundwater, and the farthest distance of dichloromethane is 820 m, the maximum impact area is 32×104 m².
4.2. Under extreme operating conditions
Chemical plant accidents could result in a large number of toxic and hazardous substances leaking. Then assumed that an accident happened in the chemical plant and in which a large number of high concentrations of dichloromethane (99%) leaked from the storage device while the leakage was 5t. What's worse, high-concentration dichloromethane directly entered and dissolved in the aquifer due to improper handling. Then simulate the transport of dichloromethane in the aquifer and predict the impact of the analysis on the aquifer. The simulated cut-off threshold was 0.03 mg/L. A fact can be seen from the simulation results that the aquifer suffered pollution with the passage of time. (Figure 4)

One year after the accident, the concentration of dichloromethane contaminants in the aquifer near the leak can reach 9 mg/L and the polluted area is $12 \times 10^4$ m². Pollutants spread with the water flow to the factory and the northwest as time goes by, the longest distance is about 1000m. Dichloromethane contaminant concentration in the leakage point gradually reduced and less than 0.03 mg/L ultimately. The maximum contaminated area appears in the fifth year which the polluted area is about $21 \times 10^4$ m². Twenty years later, the pollution plume gradually become slender mainly because of the large surrounding groundwater exploitation which changed the local groundwater hydraulic characteristics artificially, so pollution plume affected by human factors.

5. Conclusion
In this simulation, dichloromethane are selected as typical contaminant to simulate the transportation
of pollutants in the aquifers under different working conditions and the potential impact on the aquifers. It can be seen from the simulation results:

(i) As time goes by, the pollutants move roughly along the direction of the water flow and cause a certain degree of pollution to the aquifer.

(ii) The transportation range is an ellipse-like polluted area with the infiltration point as the centre of the circle and the main flow direction as the long axis. The concentration of the pollutant in the infiltration centre is the largest and decreasing outward.

(iii) Under different working conditions, the dichloromethane can be transported at 820m and 1000 m respectively after 20 years, and the maximum impact area can reach $32 \times 10^4 \text{ m}^2$ and $21 \times 10^4 \text{ m}^2$ respectively.

(iv) The transport of pollutants in aquifers is greatly influenced by human factors. Artificial exploitation of groundwater can change the hydraulic characteristics of groundwater, then change the transportation path and pollution range of pollutants.

(v) Prevention and remediation strategies need to be strengthened and the intensity of groundwater pollution monitoring should be increased.

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