Simulation and prediction of groundwater pollution based on GMS: a case study in Beijing, China

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Abstract. Groundwater is an important fresh water resource, which is very important for human survival. In this study, the hydrogeological information of the study area was obtained through field investigation and data reference, and the groundwater flow field in the study area was constructed using GMS (Groundwater Modeling Systems) software. The actual drilling water level data was used for verification. Based on the groundwater flow field, combined with pollution source sampling and testing data, a groundwater pollutant transport model was constructed, and the pollution situation was comprehensively evaluated. The results showed that once the landfill leachate and lead-acid battery plant waste liquid leaked in the study area, the groundwater in more than 40% of the study area will be greatly affected and it was not easy to recover. Therefore, predicting and simulating the transport of groundwater pollutants has a certain value, and can provide a scientific basis for preventing and controlling environmental degradation and protecting groundwater resources.

1. Introduction
Groundwater is one of the important freshwater resources. In China, groundwater has always been an important source of water supply. In 2018, 16.2% of China's water supply was groundwater, while in northern cities, this proportion could reach more than 50%[1]. Located in the North China Plain, Beijing has a small annual rainfall, a large population, and lack of fresh water resources. The status of groundwater is even more important. However, due to the rapid population growth and the vigorous development of industry and agriculture, the groundwater environment has been damaged to varying degrees. Therefore, simulation and prediction of groundwater pollution can provide a basis for the protection and governance of groundwater environment.

At present, the software for groundwater pollutant transport simulation mainly includes PHREEQC, SUTRA, Visual Modflow, GMS, IDL, etc[2]. The SUTRA software mainly simulates seawater intrusion and salt current migration, and can be used to simulate salt currents and predict the implementation effects of related groundwater interception programs[3]. PHREEQC is a simulation software that describes local equilibrium reactions and dynamic biochemical reactions. It can simulate complex water chemical reactions such as solute ion exchange reactions and dynamic redox reactions in the process of groundwater flow[4]. As a fourth-generation programming language, IDL is an ideal tool for groundwater solute simulation and visualization with its matrix-oriented characteristics and powerful data visualization capabilities[5]. In recent years, domestic scholars have mostly used GMS and Visual Modflow to carry out research on groundwater solute transport simulation. Visual Modflow is currently the most popular and highly recognized 3D visualization numerical simulation software that can
simulate groundwater solute transport. Compared with most software, it is simple to operate and has a wide range of applications, which can meet the requirements of multiple parameters for groundwater solute transport simulation[6]. Compared with other similar groundwater numerical simulation software, GMS is more flexible in modeling methods. It can be modeled based on conceptual models, and can also be modified and updated with points, arcs, and polygons. It can also be used in the construction of solute transport. Based on the migration model, the sensitivity analysis of the model parameters is carried out to determine the main factors affecting the solute transport model in the study area[7-8].

As early as the 1980s, the mathematical model has been applied to the study of groundwater quality simulation, and the analytical simulation of groundwater aquifer pollution caused by solid waste stacking has been carried out[9]. For example, Tai et al. used the Modflow module in GMS to simulate and predict the transport of groundwater pollutants during the construction of a reservoir in an irrigation area in Longchuan County, Yunnan. The groundwater flow field and the characteristics of pollutant solute transport and concentration changes in the study area had been fully and truly displayed. At the same time, the expansion of the pollution plume and the distribution of pollution sources had been clarified[10]. Liu et al. used GMS to select characteristic indicators to simulate solute transport in the shallow groundwater of the Harbin Venous Production Industrial Park, and predicted the migration trend of the characteristic indicators under three working conditions. Finally, the result was that the transport range of groundwater solutes under the three working conditions in this area was considered to be relatively small. Therefore, it was concluded that the venous industry had a very low degree of pollution to groundwater during production and operation, which provided a basis for future research on the trend of the venous industry's impact on groundwater[11]. Taking a domestic waste landfill in Hebei Province as an example, Xing used Visual Modflow to model and fit parameters to predict the migration of characteristic pollutants NH3-N in the aquifer 20 years after the leakage of leachate. The results provide a data reference for the groundwater pollution prevention and control of the domestic waste landfill and its surroundings[12]. Taking Longtan Imported Renewable Resources Processing and Utilization Park as an example, Lu et al. established a groundwater flow and pollutant transport model in the study area using Visual Modflow software. The model was used to predict and evaluate the impact of pollutant leakage and migration on the groundwater environment, which provides a scientific basis for the prevention and control of environmental degradation and the protection of groundwater resources[13]. Wei et al. took an island chemical park in the northeast as the study area, and carried out surveys, drilling, hydrogeological tests, logging, and water quality analysis to obtain relevant hydrogeological parameters. Then Visual Modflow was used to establish a mathematical model, and the MT3DMS module was used to simulate and predict the pollutant migration law of chemical raw material leakage and sewage leakage under continuous source intensity, transient source intensity and tank fire and explosion risk conditions[14]. Wang used Visual Modflow to simulate groundwater pollution in an industrial park in Taiqian County, Henan Province. It was concluded that pollutants mainly migrated with the direction of water flow, and their impact on the environment gradually expanded, and the pollutant concentration gradually decreased with time and distance[15].

This paper investigated the pollution sources in the study area, and used the GMS groundwater simulation software to simulate the diffusion range and diffusion concentration of the pollutants, so as to predict the pollution situation. Provided a scientific basis for achieving the goal of preventing and controlling environmental degradation and protecting groundwater resources.

2. Study area
The study area is located in the southwestern part of Beijing (Figure 1), with 116.01°~116.45°E and 39.83°~40.31°N. It consists of the Beijing Plain section of the Yongding River and the Yongding River groundwater reservoir. It is one of the most abundant groundwater sections in Beijing. The northwestern part of the study area is the mountain-plain junction, dominated by hills and bedrock remnants, gradually transitioning to the plain to the south. The plain area is flat, with an average elevation of 10-80m, and the piedmont area can reach 120-300m. The study area is inclined to the southeast, with a slope of 0.5-2‰. The surface alluvial deposits are mainly sandy soil and sandy loam, and some areas are fine silt
sandy soil. The atmospheric precipitation infiltration coefficient is 0.15~0.60. The aquifer permeability coefficient is 100~300m/d. The unit water inflow is 5000m³/d. And the average precipitation for many years is 584.7mm (1956-2000)[16-17].

Figure 1 Schematic diagram of study area

3. Hydrogeological conceptual model

3.1 Generalized model

3.1.1 Boundary conditions. The boundary conditions of the groundwater flow field model can be divided into three types: fixed-head boundary, flow boundary and mixed boundary. The fixed-head boundary means that the water head at each point on the boundary is known, usually a surface water body, a pumping well, or a groundwater overflow zone that completely cuts the aquifer. The flow at each point in the flow boundary is known, usually a water barrier, a pumping well, or a discharge boundary with a known flow. The mixed boundary is usually the case that one side is the aquitard, the other side is the surface water or another aquifer, or the river seepage recharge occurs. The study area was located in the plain part of Beijing, and there was no obvious water boundary. Therefore, the boundary was treated as a flow boundary.

3.1.2 Initial water level elevation. The hydrogeological conditions of the study area were obtained from the official website of Beijing Water Affairs Bureau. The selected data for this model was the water level elevation in January 2020. The obtained data was vectorized in ArcGIS and imported into GMS, and automatically interpolated to become the initial water level elevation in the study area. It can be seen from Figure 2 that the initial water level elevation had a large gap and gradually decreased from north to south.
3.1.3 Sources and sinks. The groundwater in the study area mainly received lateral recharge from the mountain front, atmospheric precipitation recharge, surface water recharge and artificial recharge, of which atmospheric precipitation was the main source of recharge. The drainage channels were mainly through the boundary to the territory of Hebei and artificial mining, of which artificial mining was the main drainage channel.

3.1.3.1 Infiltration supply of Yongding River. The study area mainly accepted atmospheric precipitation replenishment, and it was expected to receive river infiltration replenishment at the same time after the Yongding River came in. Both were regarded as surface water infiltration replenishment at the same time, and the replenishment amount can be obtained by the following formula (Wang et al. 2012). Among them, the atmospheric precipitation in Beijing was mainly concentrated in July-September, and because the groundwater was buried too deep, the inflow of the river channel was regarded as the perennial supply of groundwater.

\[ q = \alpha \cdot Q \]  

In the formula: \( q \) was the groundwater receiving surface water infiltration replenishment. \( Q \) was the total surface water inflow. And \( \alpha \) was the surface medium infiltration coefficient.

3.1.3.2 Lateral supply and outflow. The groundwater aquifer received lateral recharge from the front of the mountain and discharged to the plain. It was difficult to define the inflow and outflow at the boundary of the study area. Referring to the Beijing Water Resources Bulletin over the years, combined with the simulated cross-section area of the study area and the hydrogeological parameters in the area, the following formula was used to estimate.

\[ Q_c = K \cdot I \cdot B \cdot M \cdot T \]  

\( K \) was the permeability system of the aquifer near the section. Positive was the inflow, and negative was the outflow. \( I \) was the hydraulic gradient perpendicular to the section. \( B \) was the width of the section. \( M \) was the thickness of the aquifer. \( T \) was the calculation time.

The calculation results showed that the average annual lateral inflow from 2011 to 2016 was about 46.4 million m³, and the average annual excretion in the south was about 30.9 million m³.

3.1.3.3 Artificial mining volume. There were 17 groundwater sources in the study area, which were distributed in Fengtai, Haidian, Fangshan and Daxing. From 2010 to 2016, the annual groundwater
exploitation is 8222.8355, 7771.272, 8610.2744, 7836.7852, 7435.7194, 6655.2177 and 7544.1287 million m$^3$ respectively. In practice, it was considered that the resources consumed by groundwater exploitation were distributed in the whole study area. The study area was treated as a surface composed of numerous well boundaries, and the production was evenly distributed in the well group.

3.2 Pollution source investigation
This study mainly considered the impact of production and domestic waste pollution on groundwater. There were 8 water level observation wells, 2 landfills and 1 lead-acid battery factory in the study area. At the wellheads of the leachate collection tanks of the two landfills leading to the ground and the drain outlet of the lead-acid battery factory, special instruments were used to collect leachate samples and test the pollutants and their concentrations in the samples. The detected concentrations of target pollutants were shown in Table 1.

| Test items | Liulitun Landfill | Asowei Waste Comprehensive Treatment Center | Lead-acid battery factory |
|------------|-------------------|--------------------------------------------|--------------------------|
| COD(mg/L)  | 12400             | 15200                                      | 0                        |
| NO3-(mg/L) | 1200              | 1020                                       | 0                        |
| Pb(mg/L)   | 0                  | 0                                          | 0.75                     |

4. Numerical simulation of groundwater flow field and pollutant transport

4.1 Mathematical model

4.1.1 Mathematical model of water flow. Both the distribution of the groundwater head on the horizontal plane and the vertical change of the groundwater level were studied. Therefore, the groundwater flowed in a three-dimensional space throughout the study area. The types of lithology in the study area were complex, and there were differences in lithology distribution on the same horizontal and vertical planes. Groundwater flow changed due to replenishment conditions and changed over time. Therefore, this study summarized the groundwater flow as a three-dimensional unsteady groundwater flow system with three layers of heterogeneity, anisotropy, and spatial structure. Based on the law of conservation of mass and Darcy’s law, the differential equations were derived using Richard equation[18] as follows:

$$\frac{\partial}{\partial x} \left( K_{xx} \frac{\partial H}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_{yy} \frac{\partial H}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_{zz} \frac{\partial H}{\partial z} \right) + W = S_s \frac{\partial H}{\partial t} \quad (x, y, z) \in \Omega, t > 0$$

$$H_{|_{x=0}} = H_0(x, y, z) \quad (x, y, z) \in \Omega$$

$$H_{|_{z=0}} = H_b(x, y, z, t) \quad (x, y, z) \in B_1, t > 0$$

$$K \frac{\partial H}{\partial n} \bigg|_{B_2} = q(x, y, z, t) \quad (x, y, z) \in B_2, t > 0$$

(3)

In the formula: $K_{xx}, K_{yy}, K_{zz}$ were the permeability coefficient of the anisotropic aquifer in the x, y, and z directions; W were the sources and sinks; $S_s$ was the water storage rate; $B_1$ and $B_2$ were the boundary surfaces of the first and second types respectively; $\Omega$ was the seepage area; $H$ was the head function; $H_0$ was the initial head distribution function; $H_b$ was the head on the boundary $B_1$ of the first type; $q$ was the unit area flow on the second type boundary $B_2$; $n$ is the outer normal direction of the boundary of the seepage zone.
4.1.2 Mathematical model of solute transport. The groundwater solute transport model established this time was a three-dimensional dispersion problem under the influence of three-dimensional water flow. The mathematical model of the hydrodynamic dispersion equation was as follows [19]:

\[
R \frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i} \left( \theta D_y \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_j} \left( \theta V_j C \right) - WC - WC - \lambda_1 \theta C - \lambda_2 \rho_b \bar{C}
\] (4)

In the formula, \(x, y, z\) were three-dimensional space coordinates; \(R\) was the hysteresis coefficient; \(\theta\) was the porosity of the porous medium; \(\rho_b\) was the density of the porous medium; \(C_s\) was the dissolved concentration of pollutants; \(C\) was the concentration of pollutants; \(\bar{C}\) was the solid-phase adsorption concentration of pollutants; \(t\) was the simulation prediction time; \(D_y\) was the hydrodynamic dispersion coefficient; \(V_i\) was the groundwater seepage velocity; \(\lambda_1\) was the first-order reaction rate of the dissolved phase; \(\lambda_2\) was the reaction rate of the adsorbed phase; \(W\) was the water flow source and sink.

The initial conditions were:

\[C(x, y, z, t) = C_i(x, y, z), \quad t = 0\]

The boundary condition of this simulation was the flow boundary, and the diffuse flux across the boundary was 0. The specific expression was:

\[-D_y \frac{\partial C}{\partial x_i} = 0 \quad (t > 0)\]

4.2 Groundwater flow field simulation

First, imported the obtained surface elevation and groundwater level data into the GMS to generate scattered points, and then generated a three-dimensional grid based on the existing scattered points. Set the sources and sinks obtained from the previous investigation in the software. Then, the Modflow model was established in GMS, and the model was tested through the Check Simulation function. After correction, Modflow calculation was performed to obtain the groundwater flow field in the study area. Imported the water level data of known groundwater wells in the study area into the model and compared with the simulation results. The simulation effect was optimized by adjusting the parameters continuously, and the final result was shown in Figure 3.

Figure 3 Groundwater flow field in the study area
4.3 Groundwater pollutant transport simulation

It was assumed that the damage of the anti-seepage system of each pollution source lead to accidental leakage, and the infiltration of sewage into the ground affected the quality of groundwater. Simulated the situation within 5 years of the leakage to understand the impact of the leakage on the groundwater environment.

The MT3D solute transport model was established on the basis of the groundwater flow field model in the study area, and the stress period of the model was set to 5 years. Set the location of the waste landfill obtained from the preliminary investigation as the location of the pollution source on the model, and filled in the type and concentration of pollutants. After the input data was assigned to the MT3D model, the model was first checked through the Check Simulation function, and after correction, the MT3D calculation was performed to obtain the pollutant transport simulation results, as shown in Figure 4.
Combining the above simulation results, the three pollutants were scored and weighted by Analytic Hierarchy Process (AHP), and the groundwater pollution evaluation results were finally calculated (Figure 5).

Figure 5 Evaluation results of groundwater pollution in the study area

By analyzing the above figure, the risk of groundwater pollution can be divided into four levels: low,
medium, high, and high. Among them, a score of 0-0.34 was considered low risk, and a score of 0.34-0.5 was considered medium risk. A score in the range of 0.5-0.6 was considered a higher risk, and a score in the range of 0.6-1 was considered a higher risk. Among them, the areas with higher risk accounted for about 40% of the whole study area, mainly concentrated in the surrounding areas of the three pollution sources. The reason was that the total amount of leachate in the two landfills was large, and the concentration of pollutants in the leachate was high. Although the concentration of pollutants in the lead-acid battery factory was low, the lead element was heavy metal, which was harmful to human body and cannot be decomposed. Once it enters the groundwater, it would cause great impact. It could be seen that the leakage of any one of the three pollution sources would have a greater impact on the groundwater quality in the study area. Due to the slow flow of groundwater resources and the slow degree of alternation, the self-purification ability was low. Once contaminated, it would be difficult to recover. Therefore, it was necessary to strengthen the supervision of landfill leachate and lead-acid battery plant wastewater treatment to ensure that sewage could be effectively treated, thereby effectively preventing groundwater from being polluted.

5. Conclusion
The pollution of groundwater is closely related to human production and life. Through the prediction and simulation of groundwater pollution, it can provide important data for protecting water resources and maintaining the ecological balance of groundwater environment. Based on the simulation and verification of the groundwater flow field in the study area, it was assumed that the pollution source leaks in the study area and the results after 5 years of pollutant migration were simulated. Combined with the movement of different pollutants, a comprehensive evaluation of the groundwater pollution in the study area was carried out. Judging from the evaluation results, the leakage of any pollution source in the study area will have a greater impact on the groundwater in the area. Through the comprehensive evaluation result map, the risk level of groundwater pollution at various locations can be seen intuitively. This provided a decision-making reference basis for regional groundwater pollution risk identification and scientific management, and also laid an important theoretical foundation for groundwater resources protection and planning in the study area.

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