# NUMERICAL SIMULATION OF GROUNDWATER POLLUTION IN HILLY AREAS WITH COMPLEX TERRAIN BASED ON GMS

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**Abstract.** Groundwater resources are an important source of drinking water and are of strategic importance. Leakage of storage materials or wastewater may occur during petrochemical production, leading to groundwater pollution. Taking a petrochemical construction project in complex hilly region of Hunan Province, China as an example, a groundwater flow and solute transport model was established by using groundwater simulation system GMS according to engineering analysis and investigation. According to the characteristics of hilly and plain areas, the precipitation infiltration recharge was calculated by using the hydrology method and precipitation infiltration coefficient method respectively to improve the simulation accuracy of the model. The model was established to simulate the solute transport of toluene, COD, ammonia nitrogen and petroleum on the 100th, 1000th day and 20th yearafter leakage of a tank farm and sewage treatment plant under abnormal working conditions. The results show that organic pollutants are mainly controlled by convection, and inorganic pollutants are controlled by convection and dispersion, and the pollution halos would all move out of the construction area after 20 years, but not out of the simulation area. In order to prevent and respond to and deal with pollution incidents in a timely manner and minimize the impact, zoning and categorization of seepage control measures should be taken, and a groundwater monitoring plan and an emergency plan for pollution treatment should be formulated.

**Keywords:** groundwater in hilly region; GMS; petrochemical pollution; numerical simulation.

## 1. Introduction

In addition to being a vital supply of drinking water, groundwater resources are strategically significant for the development of the local economy, society, and ecological civilization [1]. Groundwater has lower flow rates, a slower rate of renewal, a weaker capacity for self-purification [2; 3], and it is more difficult to treat and restore pollutants than for surface water [4]. Furthermore, the effects of groundwater pollution may extend beyond the groundwater itself and have a lasting impact on ecosystems and surface water [5; 6].

In recent years, petrochemical and other industries have developed to varying degrees in different countries and regions around the world, which has caused varying degrees of groundwater pollution while promoting economic development [7; 8]. Petrochemical products have a lengthy natural restoration period and are difficult to break down. If they leak into the ground and contaminate groundwater, there could be disastrous repercussions due to the complexity of the pollutants and the challenge of remediating the groundwater [9; 10]. Therefore, it is of great significance to simulate and predict the regional groundwater flow and possible pollution conditions before putting into production, and to propose effective preventive and control measures to protect the ecological environment and water safety [11].

Currently, numerical models are extensively utilized to simulate groundwater flow and contamination [12-14]; nevertheless, the majority of the time, the model source and sink terms are calculated using a single calculation approach, which ignores topographical variations. The hilly, complicated terrain area has different topography and features than the plains [15], therefore, when simulating and parameterizing groundwater numerically, it is important to take these differences into account to make the simulation more accurate. In this paper, a chemical park construction project in Yueyang City, Hunan Province is used as the research object. A variety of methods are used to calculate the source and sink terms of the model according to the characteristics of the hills and plains in the area, so improving the simulation accuracy of the groundwater flow numerical model of the hilly area in the complex terrain after the groundwater flow numerical model is established using GMS software. The model simulates and predicts the solute transport of four pollutants – toluene, COD, ammonia and petroleum – on the 100th, 1000th day and 20th year following the tank farm and wastewater treatment plant leaks under abnormal operating conditions. Pollution prevention and control measures are then suggested.

The terrain and landscape of the research area are dominated by hills, with an overall elevation of 21.4~588.1 m and undulating topography that is high in the east and low in the west. There is a year-

DOI: 10.22616/ERDev.2024.23.TF234

round stream that runs from east to west, which eventually joins the Yangtze River via the skimming channel. The research area simple stratigraphic structure is mostly made up of Lengjiaxi Group ($P_{tln}$) slate, pulverized clay ($Q_4^{al}$), and Quaternary fill ($Q_4^{ml}$). There are two types of groundwater: loose pore water of the Quaternary System and weathered fissure water of the whole/medium weathered slate of the Lengjiaxi Group. These two types of groundwater are closely related to each other.

## 2. Materials and methods

### 2.1. Conceptual model

Pore water and fissure water can be combined into a single submersible aquifer based on the hydrogeological investigation of the study region. The research object is situated in a region with complicated topography that is hilly and includes both plains and hills. Because of the varying topography, the atmospheric precipitation recharge in the plain region is determined using the precipitation infiltration coefficient method, and in the hilly region, it is determined using the base-flow splitting method in the hydrological method, where the groundwater storage recession coefficient is assumed to be 0.9 times that of the base-flow recession coefficient [16]. In the research region, evapotranspiration is minimal and is combined with precipitation replenishment. Darcy's law was used to calculate the groundwater discharge to streams.

The unified submersible aquifer in the research area that is reproduced by the model is generalized by fissure water and loose pore water of the Quaternary system. The watershed serves as the watertight barrier on the research area's north, east, and south sides, while the river serves as the fixed-head boundary on the southwest side, defining the simulation region for the groundwater model (Fig. 1.).

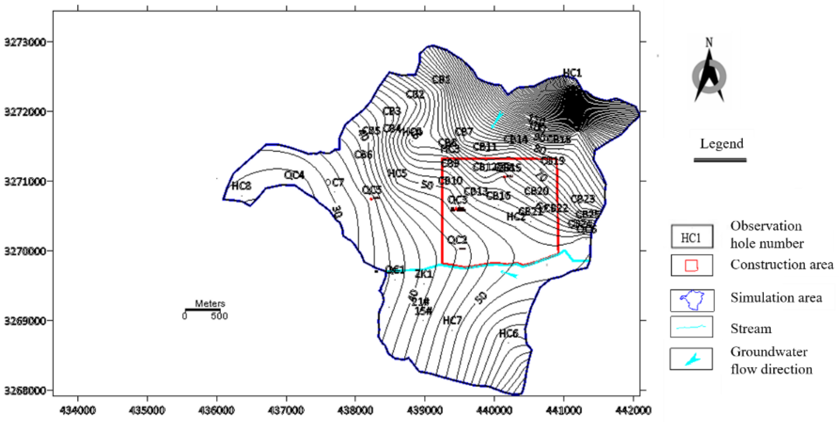

Fig. 1. **Simulation area diagram**

### 2.2. Mathematical model

Since the generalized submersible aquifer conforms to the seepage in porous media described by the MODFLOW model in GMS, a two-dimensional groundwater flow model with non-homogeneous (fractional homogeneous), isotropic, and non-stationary distribution parameters is adopted in the groundwater flow simulation. This model can be expressed mathematically as follows:

$$\begin{aligned}
&\frac{\partial}{\partial x}\ T_{xx}\frac{\partial H}{\partial x} + \frac{\partial}{\partial y}\left(T_{yy}\frac{\partial H}{\partial y}\right) + W = \mu^{*}\frac{\partial H}{\partial t} \quad (x,y)\in\Omega, t > 0\\
&H(x,y,0) = H_0(x,y) \qquad (x,y)\in\Omega\\
&H(x,y,t)|_{\Gamma_1} = H_1(x,y,t) \quad (x,y)\in\mathit{\Gamma}_1, t > 0 \text{ (1st type of boundary )}\\
&T\frac{\partial H}{\partial n}_{\Gamma_2} = q_0(x,y,t) \qquad (x,y)\in\Gamma_2, t > 0) \text{ (2nd type of boundary)} ,
\end{aligned} \tag{1}$$

where $H(x,y,t)$ – head value at any point $(x,y)$ at any moment t ($m$);
$\Omega$ – groundwater seepage area;
$\Gamma_1$, $\Gamma_2$ – first and second type of boundary, respectively;
$T_{xx}$, $T_{yy}$ – hydraulic conductivity in the main direction of $x$ and $y$, respectively, $m \cdot d^{-1}$;

$W$ – source-sink terms;
$\mu^*$ – specific yield.

Leaks from the wastewater treatment plant and storage tank locations in chemical parks could contaminate groundwater. Using the MT3DMS module in the GMS software and the groundwater flow model previously constructed, potential pollution can be simulated by solute transport using the following mathematical model:

$$\begin{aligned}
&\frac{\partial C}{\partial t} = D_{xx}\frac{\partial^2 C}{\partial x^2} + D_{yy}\frac{\partial^2 C}{\partial y^2} - \frac{u_x}{n_e}\frac{\partial C}{\partial x} - \frac{u_y}{n_e}\frac{\partial C}{\partial y} + f\,(x,y) \in \Gamma_1, t > 0 \\
&C(x,y,0) = C_0(x,y) \qquad (x,y) \in \Omega \\
&C(x,y,t)|_{\Gamma_1} = C_1(x,y,t) \qquad (x,y) \in \Gamma_1, t > 0 \\
&(Cu - D\mathrm{grad}C) \cdot \vec{n}|_{\Gamma_2} = \varphi(x,y,t)\,(x,y) \in \Gamma_2, t \geq 0 \qquad ,
\end{aligned} \tag{2}$$

where $D_{xx}\frac{\partial^2 C}{\partial x^2}$ and $D_{yy}\frac{\partial^2 C}{\partial y^2}$ – dispersion terms;
$\frac{u_x}{n_e}\frac{\partial C}{\partial x}$ and $\frac{u_y}{n_e}\frac{\partial C}{\partial y}$ – convective terms;
$f$ – solute increment due to chemical reaction or adsorptive degradation;
$C$ – solute concentration;
$T_{xx}$， $T_{yy}$ – hydraulic conductivity in the main direction of $x$ and $y$, respectively, $\mathrm{m \cdot d^{-1}}$;
$\varphi$ – solute flux at the boundary;
$u$ – seepage velocity;
grad$C$ – concentration gradient;
$n_e$ – effective porosity, which is equal to specific yield;
$D_{xx}$, $D_{yy}$ – main vector of x and y, respectively.

### 2.3. Model identification and validation

The simulation is numerically simulated using the finite difference method, and the simulation region is divided into square grids spaced 100 meters apart in a Cartesian coordinate system. A total of 5673 grid cells are split in the plane, of which 1470 are effective cells.

The test-estimate-correction approach was employed in this simulation to identify and validate the model parameters. The initial flow field for the model identification in the 2022 flat water period was the submerged isohaline line; the model was validated using the submerged isohaline line in the 2023 dry water period. The submerged aquifer was separated into 15 parameter zones in accordance with the complex topography and hydrogeological circumstances of the study area. Fig. 2a and Table 1 display the calibrated hydrogeological parameter zone divisions and values. The groundwater flow field fitting is shown in Fig. 2b. The simulated groundwater flow field fits well with the measured flow field, indicating that the numerical model developed in this study can portray the groundwater in the simulated area.

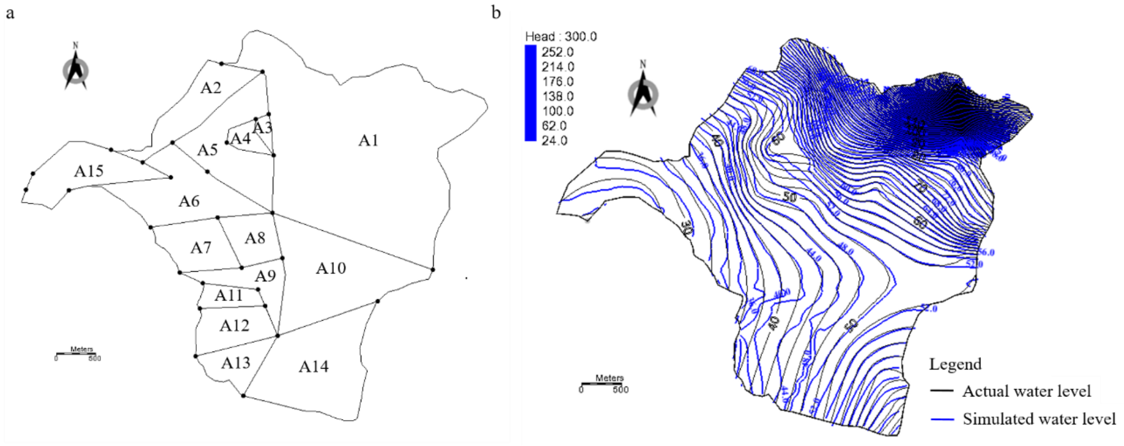

Fig. 2. **Fitted flow field plots and parametric zoning results**

Table 1

**Values of hydrogeological parameters for each zone**

| Zone | Hydraulic conductivity, $m \cdot d^{-1}$ | Specific yield | Zone | Hydraulic conductivity, $m \cdot d^{-1}$ | Specific yield | Specific yield | Zone | Hydraulic conductivity, $m \cdot d^{-1}$ |
|---|---|---|---|---|---|---|---|---|
| A1 | 0.08 | 0.1 | A6 | 0.08 | 0.15 | A11 | 10 | 0.1 |
| A2 | 0.04 | 0.1 | A7 | 0.01 | 0.15 | A12 | 8 | 0.1 |
| A3 | 0.08 | 0.1 | A8 | 0.12 | 0.1 | A13 | 10 | 0.1 |
| A4 | 10 | 0.1 | A9 | 2.5 | 0.1 | A14 | 0.04 | 0.1 |
| A5 | 0.04 | 0.1 | A10 | 0.4 | 0.15 | A15 | 0.01 | 0.15 |

## 3. Results and discussion

There is little chance of pollution from the chemical park while everything is running smoothly. Only in unusual circumstances could leaks from malfunctioning wastewater treatment plant and storage tanks affect groundwater. Toluene is the primary pollutant seeping from the tank farm, whereas COD, ammonia, nitrogen, and petroleum are the primary pollutants leaking from the wastewater treatment plant. The source strength of each pollutant into the groundwater under unusual circumstances is shown in Table 2.

Table 2

**Calculation list of pollution source strength under abnormal working condition**

| Location of pollution sources | Stockpile, $m^3$ | Contaminant | Density, $kg \cdot m^{-3}$ | Limits, $mg \cdot L^{-1}$ | Mass entering groundwater, kg |
|---|---|---|---|---|---|
| Tank farm | 1700 | Toluene | 900 | 0.7 | 1153.2 |
| Wastewater treatment plant | $1.42 \cdot 10^6$ | COD | 0.09 | 3 | 15.7 |
| | $1.42 \cdot 10^6$ | Ammonia | 0.0046 | 0.5 | 0.8 |
| | $1.42 \cdot 10^6$ | Petroleum | 0.017 | 0.05 | 3.0 |

### 3.1. Results

The tank farm is situated in the southeast corner of the project construction area. Fig. 3a provides information on the pollution plume transmission on the 100th, 1000th day and 20th year following the simulated incidence of contamination. On the 100th day, the organic pollutant toluene centre concentration of contamination plume reached 33,596.15 $mg \cdot L^{-1}$ impacting groundwater. Due to the insoluble nature of toluene, the contamination plume is mostly carried to the southwest by groundwater flow under the influence of groundwater convection. The area gradually grows, and after 1,000 days, the leading edge of the contamination halo is moved beyond the southern boundary of the construction area, and after 20 years, the boundary is moved out of the boundary by 42.73 m. The area that exceeds the standard is 0.24 $km^2$, but it has not gone beyond the simulation area boundary.

The wastewater treatment plant is situated in the southwest corner of the project construction area. Groundwater is impacted by the concentration of COD, ammonia, and petroleum in the centre of the pollution plume on day 100, which is higher than the limit value. The organic pollutants petroleums were primarily transported to the southwest with the groundwater flow under groundwater convection (Fig. 3b). The non-organic pollutants COD and ammonia nitrogen were primarily transported to the southwest and around the groundwater flow under convection and dispersion (Fig. 3c-d). Following the leak, the pollution plume area progressively grew. After 100 days, the leading edge of the pollution plume moved beyond the western boundary of the construction area, and after 20 years, the boundaries of COD, petroleum, and ammonia nitrogen moved by 8.6, 1.41, and 15.56 meters, respectively, with exceedance areas of 0.06 $km^2$, 0.05 $km^2$, and 0.04 $km^2$, but none of them crossed the simulation area boundary.

### 3.2. Discussion

Under unusual working conditions, the contaminants moved convectively and diffusely under the influence of groundwater dynamics after leaking from the wastewater treatment plant and the tank farm, and the contaminated area progressively grew. The leading edge of the contamination halo moves out of the southern boundary of the construction area on the 1000th day after the leak. The pollutant toluene contamination plume in the tank farm is primarily transported to the southwest with groundwater flow under the action of groundwater convection. Petroleum organic pollutants are primarily in the groundwater convection with the groundwater flow to the southwest direction, following the leakage of the 100th day of the leading edge of the pollution plume that is moved out of the construction area west boundary. COD and ammonia nitrogen in the wastewater treatment plant in the convection and dispersion effect the groundwater flow to the southwest and around the transport. The simulated area border was not crossed by the plume of any contaminants.

It is evident from the pollution characteristics of the various pollutants discussed above that different hydrodynamic effects are experienced by organic and non-organic pollutants during groundwater migration, leading to irregularities in the distribution of pollution in space and time as well as varying levels of pollution produced. Non-organic pollutants dissolve in water through the process of movement caused by convection and dispersion of numerous effects of the role of the impact of transport faster; organic matter is not soluble in water, mostly due to groundwater convection movement. Thus, it is recommended that anti-seepage measures be taken during project construction by classification and zoning, and that corresponding pollution treatment measures be formulated by classification and zoning. Additionally, a groundwater monitoring plan should be set up to guarantee that, in the event of a leak during abnormal working conditions, prompt action will be taken to minimize the impact.

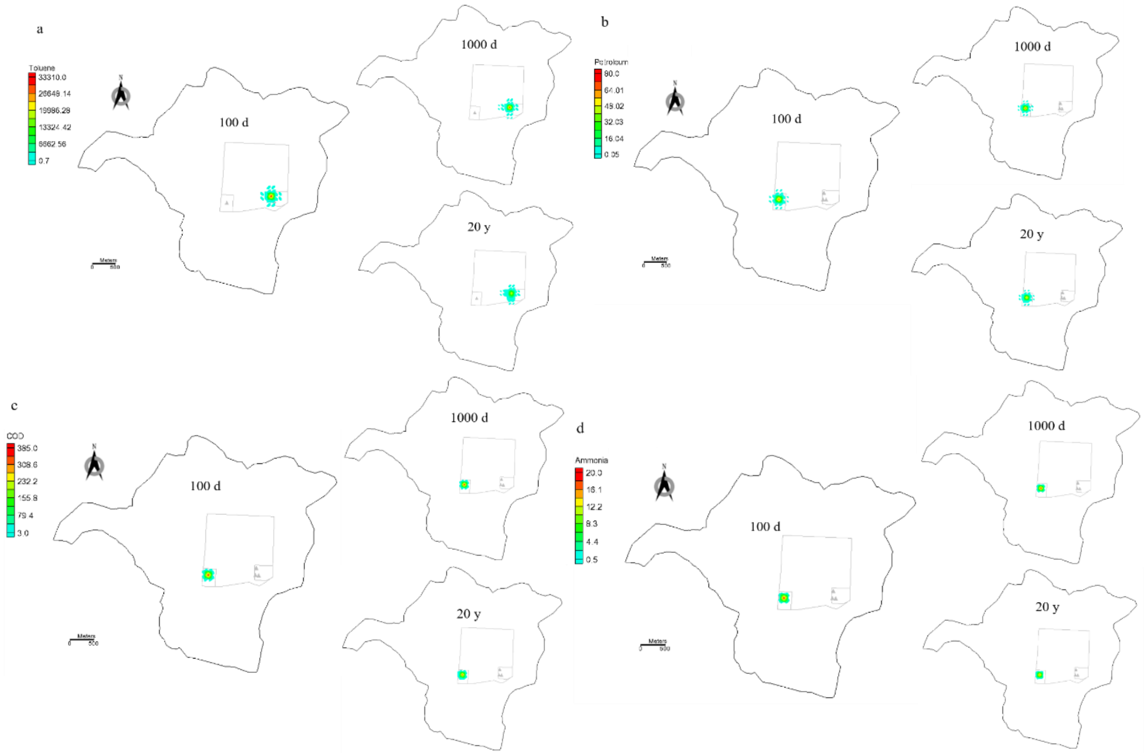

Fig. 3. **Schematic diagram of toluene contamination plume over time in a leaking tank farm**

## Conclusions

1. Using GMS, a groundwater flow and solute transport model was created in this study to mimic the leaking of a petrochemical construction project under unusual working conditions in a hilly, complex environment of Yueyang City, Hunan Province. A combination of field exploration and hydrogeological investigation is required to adjust the reference due to the large topographic relief and elevation difference in the hilly area with complex terrain, which differs from the plain area in the simulation process. Different calculation methods are used in the model to calculate the source and sink terms.
2. Hydrodynamic effects on the migration of pollutants in groundwater vary depending on the solubility of organic and non-organic substances; organic pollutants are primarily subject to convection and migrate with groundwater flow, whereas non-organic pollutants are also subject to

dispersion and migrate in all directions. Toluene and petroleum species are less subject to dispersion and less diluted, so the maximum transport distances after 20 years (toluene: 555.73 m, petroleum species 444.88 m) are greater than for COD (321.8 m) and ammonia nitrogen (326.67 m). Both anti-seepage and pollution treatment measures must be arranged in a zoned and classed manner since this difference results in uneven pollution levels and temporal and spatial distribution.

3. Since precipitation infiltration is the primary method of recharging groundwater in hilly regions and baseflow is the mode of discharge, the baseflow partitioning method – as opposed to the precipitation infiltration coefficient method – is typically employed to compute the recharge of groundwater from atmospheric precipitation. Owing to the limitations of the survey conditions, this study solely examined the differences in the atmospheric precipitation recharge calculation method between plain and hilly areas during the model adjustment process. In the future, it can be further refined in other areas to distinguish between them, such as grid dissection and encryption, evapotranspiration calculation, etc. to bring the simulation closer to reality.

## Author contributions

Conceptualization, J.L. and Y.L.; methodology, G.L.; software, Y.L.; validation, Y.L. and Q.S.; investigation, J.L., Y.L., Q.S. and G.L.; data curation, Y.L; writing – original draft preparation, Y.L.; writing – review and editing, J.L and V.B. All authors have read and agreed to the published version of the manuscript.

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