Visualizing Ammonia Nitrogen Transport in Groundwater Using MODFLOW and MT3DMS: A Case Study from Xinxu, Xiamen, China

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Abstract：In response to the increasing risk of groundwater pollution in rapidly urbanizing coastal environments, this study develops a high‐resolution three‐dimensional model to simulate the transport of ammonia nitrogen (NH_4^+) in Xinxu Town, Xiamen, China. Integrating 148 borehole datasets, multi‐source monitoring data, and a 5 m resolution digital elevation model, we constructed a heterogeneous groundwater flow model with a 50×50 ×5 m grid using MODFLOW. Boundary conditions reflect regional recharge–discharge patterns and continuous leachate input from a municipal solid waste treatment facility. The subsequent MT3DMS-based solute transport simulation examines NH_4^+ migration under varying hydrological scenarios over a six‐year period. Model results reveal predominant southeastward contaminant migration aligned with hydraulic gradients, with shallow layers exhibiting faster transport velocities than deeper strata. Critical discharge zones were identified in low‐lying northeastern areas, highlighting potential risks to downstream water users. The model provides a robust tool for visualizing pollutant plumes, assessing long‐term impacts of waste facility leachate, and informing targeted management strategies.

Keywords：Groundwater flow field; Numerical simulation; MODFLOW; MT3DMS; Ammonia nitrogen transport

DOI：10.69979/3041-0843.26.01.006

1 Introduction

Groundwater is the planet's largest store of liquid freshwater and underpins social-economic development, food security and ecosystem resilience. Globally, it supplies about 50 % of drinking water, 40 % of agricultural irrigation and 30 % of industrial demand, but these benefits are jeopardized by over-extraction, pollution and climate stressors. Satellite and well data show that groundwater-level declines have accelerated in 30 % of the world's aquifers since 1980, with losses most pronounced in dry cropland regions and densely populated deltas [1]. Nitrogen species are among the most pervasive pollutants driving this deterioration. A recent global assessment found that legacy nitrogen stored in aquifers now delivers up to 65 % of total nitrogen loads to major river basins, prolonging eutrophication decades after surface inputs fall [2]. In drinking-water supplies, excess ammonium (NH_4^+) and nitrate pose acute risks ranging from methemoglobinemia in infants to elevated cancer incidence, prompting stringent regulatory limits [3].

Landfill leachate is a leading point source of ammonia nitrogen. Case studies from China's karst and alluvial settings report NH_4^+ concentrations 3–5 times higher than regulatory thresholds in downgradient wells, with plume lengths exceeding 1 km when hydrogeological barriers are weak[4, 5]. Xiamen—a subtropical coastal megacity—has seen reactive-nitrogen emissions more than triple since the 1990s, and monitoring shows upward NH_4^+ trends near the Eastern Waste Treatment Center, the city's largest solid-waste facility[6]. Yet quantitative understanding of subsurface transport processes in this terrain remains limited.

Process-based numerical models provide a powerful framework for disentangling coupled flow and transport mechanisms, evaluating management scenarios and designing monitoring networks. The U.S. Geological Survey's MODFLOW has become the international standard for simulating groundwater dynamics, with recent versions supporting parallel computation and variable-density flow. Its companion code MT3DMS (and the enhanced MT3D-USGS) extends these capabilities to multispecies solute transport, including advection, dispersion and complex reactions. Numerous regional studies have leveraged the MODFLOW-MT3DMS suite to reproduce nitrate and ammonia plumes in heterogeneous aquifers, demonstrating good agreement with field observations and informing remediation design. However, no high-resolution model has yet been applied to the fractured-granite–alluvium system of Xinxu, where steep hydraulic gradients intersect anthropogenic recharge and tidal influences.

2 Study Area

2.1 Geographical Location

A certain area in the northeast of Xiamen integrates residential, industrial, agricultural, and reservoir functions, where production, living, and ecological functions are intertwined. Located in this area, the Xiamen East Garbage Disposal Center processes over 3,700 tons of domestic waste and over 200 tons of kitchen waste daily, making it the main potential pollution source in the region. Monitoring shows that the ammonia nitrogen concentration in the wells on the site has reached a maximum of 3.76 mg/L, exceeding the standard and showing an upward trend. The pollutants are spreading southeast along the groundwater flow direction. Although the ammonia nitrogen concentration in the downstream areas (0.027–0.409 mg/L) still meets the Class III standard for groundwater, the continuously rising pollution trend warns that preventive measures need to be taken to strengthen pollution prevention and control and source blocking to ensure the long-term safety of regional groundwater.

2.2 Geological and Hydrogeological Condition

2.2.1 Geological Condition

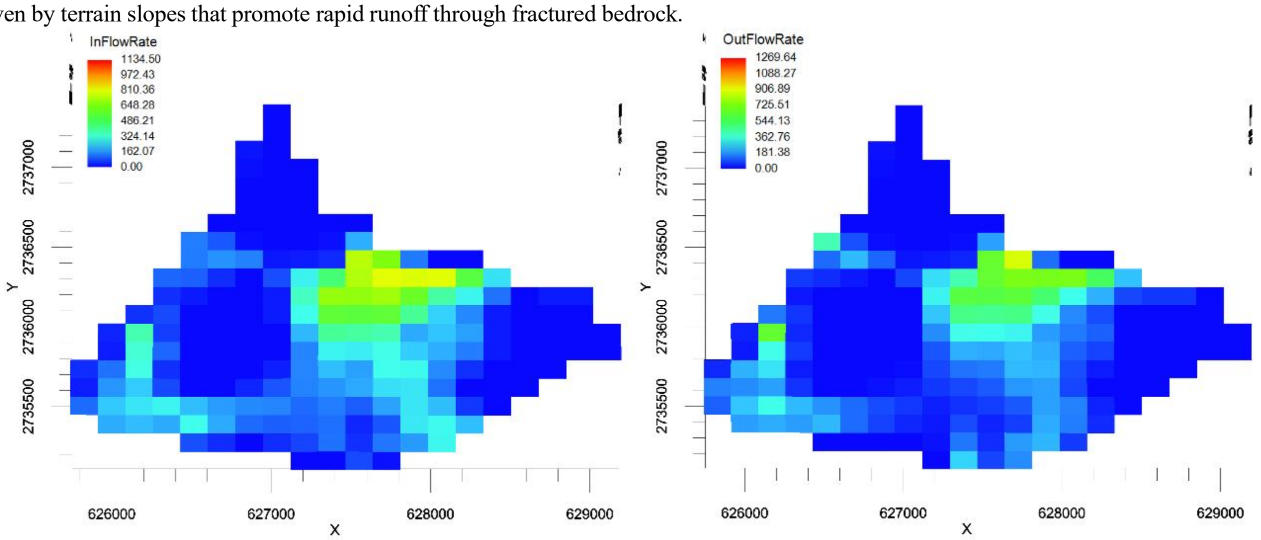
The geomorphology of Xinxu Town is defined by Late Pleistocene alluvial–proluvial fans and erosion–denudation terraces. The former appear as fan-shaped accumulations at foothills formed by flood deposition, while the latter represent fluvial erosion terraces reflecting the combined effects of intermittent tectonic uplift and surface denudation. the major stratigraphic units include Jurassic to Early Cretaceous formations such as muscovite-altered syenogranite (γmuJ_3), granitic porphyry ($\gamma\pi$), and monzogranite ($\eta\gamma K_1$). The central and western portions of the study area are predominantly composed of sedimentary rocks, mainly consisting of clay, fine to medium sand, and gravelly sand, which are the result of long-term depositional processes. In contrast, the eastern region is characterized by volcanic rocks and granitic intrusive bodies, reflecting a geological history marked by volcanic activity and magmatic intrusions. These lithological differences highlight the region's tectonic complexity and past geological dynamism. Fault zones in the eastern and southern areas have shaped the stratigraphic pattern, with later geological processes partially concealing them and adding to the structural complexity.

Based on data collected from 33 geotechnical investigation projects conducted within and around the study area, the shallow strata are primarily composed of relatively loose sandy soils and strongly weathered granite, with thicknesses ranging from 9.7 to 14.33 meters. In some sections, mineral components have undergone weathering into clay minerals. The middle stratum consists mainly of blocky, strongly weathered granite and feldspar that has transformed into clay minerals, typically found at depths between 6.79 and 11.72 meters. The deep stratum is characterized by residual gravelly cohesive soils and sandy cohesive soils, derived from the weathering of granitic bedrock. In this layer, feldspar has largely altered into secondary minerals such as kaolinite, with thicknesses varying from 1.43 to 17.42 meters. The bottom layer comprises unweathered to slightly weathered hard granite, which exhibits low permeability and thus can serve as a natural barrier to vertical groundwater migration.

2.2.2 Hydrogeological Condition

The study area exhibits a hydrogeological regime marked by limited recharge and storage capacity, abbreviated flow paths, and predominantly shallow groundwater circulation. Within this context, three principal aquifer types are identified: unconsolidated porous deposits, weathered residual porous–fractured horizons, and fractured bedrock formations. These aquifers chiefly occupy residual pediment and piedmont landscapes, where groundwater movement is relatively rapid yet spatially constrained . Surface water bodies are discontinuous, and unconfined aquifers prevail throughout the region. Surface water bodies are discontinuous, and unconfined aquifers prevail throughout the region. Except in the southeastern sector, where yields are moderately higher, the study area as a whole may be regarded as deficient in groundwater resources.

As shown in Figure 1a, areas with high groundwater inflow rates are mainly located in the low-lying northeast, where rainfall tends to accumulate, forming key recharge zones. In Xinyu Town, intensive agriculture relies on well-extracted groundwater for irrigation. Most of the water is lost through runoff or evapotranspiration, with only a small portion recharging the aquifer. The Dongxi River and its tributaries serve as the main groundwater discharge channels. As shown in Figure 1b, zones with high outflow rates are mainly in the northeast and west, driven by terrain slopes that promote rapid runoff through fractured bedrock.



(a) Groundwater Inflow Rate **(b) Groundwater Outflow Rate**

Figure1 Inflow and Outflow Rate of Groundwater

3 Methods

3.1 Conceptual Model

The development of a conceptual model, as a prerequisite for numerical simulation, involves the generalization of stratigraphic structure, analysis of hydrogeological conditions, and assessment of hydraulic properties. In this study, we integrated multiple data sources, including a digital elevation model (DEM) of the study area and its surroundings, engineering borehole data, and geological maps, to develop a detailed model of the subsurface geological structure. This approach aligns with the fusion technology of multi-source data, which comprehensively utilizes geology, drilling, geography, and other data sources to build a 3D geological model, thereby compensating for the limitations of single data sources and making the model more consistent with actual geological conditions.

The southeast of the study area lies the boundary between the aquifer and the aquiclude. The northern boundary is primarily a constant - head boundary determined by surface runoff. The southwestern boundary is a flow - boundary demarcated based on the divide of precipitation. To effectively reduce the uncertainty of model parameters and to ensure high accuracy and reliability in simulating the hydraulic characteristics and solute transport behavior during numerical analysis, we assumed that the porous medium was in a state of full saturation when constructing the flow field model.

3.2 Groundwater Flow Model

Darcy's Law, a fundamental principle describing fluid flow in porous media, states that fluid velocity is proportional to the hydraulic gradient and inversely proportional to the medium's permeability. In practice, groundwater flow shows clear directional features due to anisotropic media's varying permeability coefficients. Thus, the fundamental groundwater flow equation must integrate mass conservation and Darcy's Law to accurately describe flow patterns in three - dimensional space. Based on the three-dimensional governing equation, the finite difference method is used to discretize the flow domain and solve the equations numerically, thereby simulating the dynamic changes of the groundwater system. The mathematical expression for this is:

$$\frac{\partial}{\partial x}\left(K_x\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial h}{\partial z}\right)+W=S_s\frac{\partial h}{\partial t}$$

Where K_x, K_y and K_z are the permeabilities in the x, y and z directions; h is the groundwater hydraulic pressure head; W is the recharge/discharge rate per unit volume; S_s is the specific storage coefficient; and t is time.

3.3 Ammonia Nitrogen Transport Simulation

MT3DMS, built on MODFLOW, is a modular 3D transport model. It's designed to simulate convection, dispersion, and chemical reactions of dissolved constituents in groundwater systems. This model not only comprehensively accounts for these processes of various pollutants but also flexibly handles complex source/sink terms and boundary conditions, enabling accurate simulation of pollutant transport in aquifers. The three-dimensional solute transport equation for groundwater is as follows:

$$R\frac{\partial C}{\partial t}=\frac{\partial C}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_i}\right)-\frac{\partial}{\partial x_i}(v_iC)+\frac{q_s}{\theta}C_s-\lambda(C+\frac{q_b}{\theta}\overline{C})$$

Where, C is the concentration of the pollutant dissolved in water; R is the retardation factor; t represents time in days; x_i denotes the spatial coordinate in meters; D_{ij} is the hydrodynamic dispersion coefficient tensor; v_i is the groundwater seepage velocity in the i direction; q_s signifies the source (positive) or sink (negative) term; θ is the porosity; C_s is the concentration of the pollutant adsorbed onto the medium; λ stands for the reaction rate constant; q_b refers to the sink term flow rate; $\overline{C}$ is the average concentration of the pollutant.

4 Results

4.1 Stratigraphic Structure

The geological structure of the study area was modeled using digital elevation models (DEMs), engineering borehole data, and geological maps. As shown in Figures 2 triangulated irregular networks (TINs) were used to generate stratigraphic horizons based on the distribution of borehole data within the study area. The distribution pattern of the strata in the study area is shown in Figure 2.

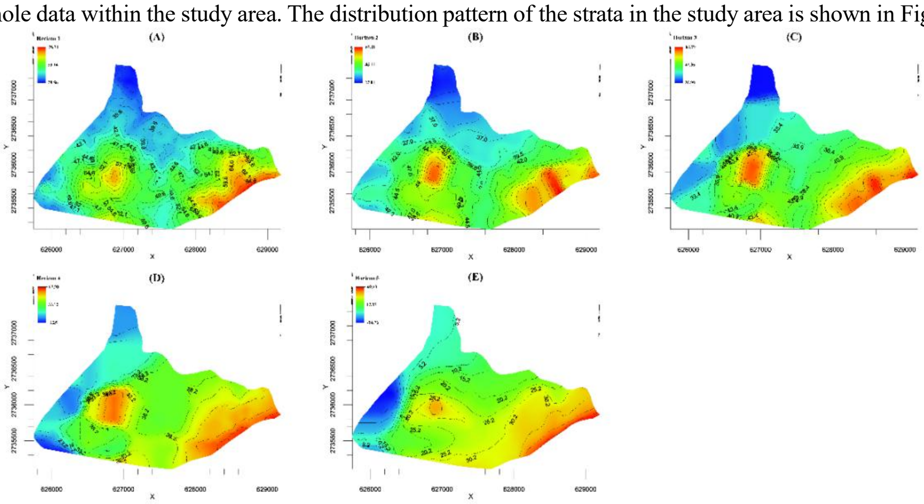


Figure 2 The stratigraphic distribution pattern of the study area.with (A) Ground Surface, (B) Bottom of Fill Layer, (C) Bottom of Residual Layer, (D) Bottom of Fractured Bedrock Zone, (E) Top of Unweathered Bedrock.

By integrating the generated horizons with stratigraphic thickness data, the vertical geological structure of the study area was generalized into four main layers: fill, residual soil, fractured zone, and bedrock, forming the basis for constructing a complete solid model . This generalization process involves simplifying the complex geological information obtained from the borehole data and DEMs into a more manageable form that can be effectively used in numerical simulations. The fill layer consists of artificial deposits, while the residual soil layer is derived from the weathering of parent rocks. The fractured zone represents the intensely fractured granite, and the bedrock is the unweathered granite that serves as the base of the geological structure. The solid model provides a comprehensive 3D representation of the subsurface geology, which is essential for understanding groundwater flow and solute transport processes in the study area.

To further enhance the accuracy of the model, the spatial distribution of horizontal and vertical hydraulic conductivity was determined based on permeability data obtained from geotechnical tests on borehole samples within the site. This information was used to construct corresponding 3D conductivity grids (Figure 3), which are critical for simulating the anisotropic flow characteristics of groundwater in the different geological layers. The horizontal and vertical variations in hydraulic conductivity reflect the inherent heterogeneity of the subsurface materials and their impact on groundwater movement and pollutant transport.

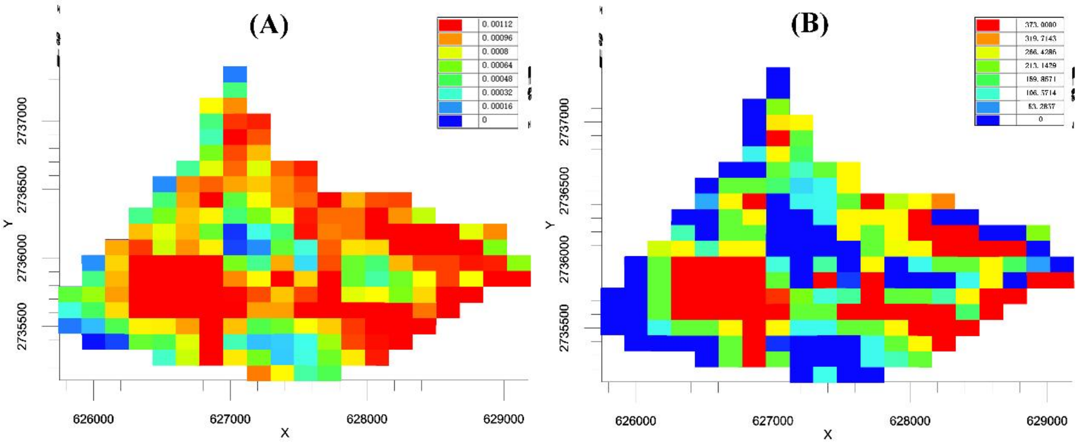


Figure 3. Hydraulic conductivity grids: (A) horizontal hydraulic conductivity; (B) vertical hydraulic conductivity.

4.2 Groundwater Flow Velocity Model

To effectively minimize parameter uncertainty and enhance the accuracy and reliability of hydraulic and solute transport simulations, the aquifer medium was assumed to be fully saturated during flow model development. In this study, the MODFLOW software was employed to simulate groundwater flow based on Darcy's law and the groundwater continuity equation. The flow domain was discretized into grid cells, and a three-dimensional groundwater velocity model was developed (Figures 4). As shown in the figures, red zones indicate groundwater discharge areas, typically located in low-lying terrain or zones with high hydraulic gradients or elevated permeability, often associated with strong recharge or transmissive formations. Blue zones represent recharge areas, generally situated in higher elevations or in lithologically compact strata. Groundwater flow directions are closely aligned with the hydraulic gradient, showing a clear trend of movement from blue (inflow) zones toward red (outflow) zones. The model also reveals that shallow groundwater exhibits higher flow velocities than deeper layers , reflecting the influence of depth-dependent variations in permeability and hydraulic gradient.

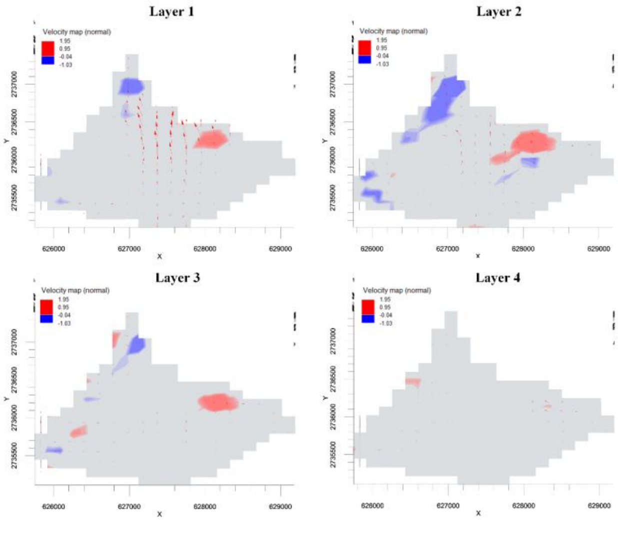


Figure 4 The groundwater flow field

4.3 Ammonia Nitrogen Transport Simulation

The groundwater flow model constructed using MODFLOW was imported into GMS for further processing. Using the established boundary conditions and initial hydraulic head distribution (Figure 5), the MT3DMS model was initialized to simulate solute transport under consistent flow conditions.

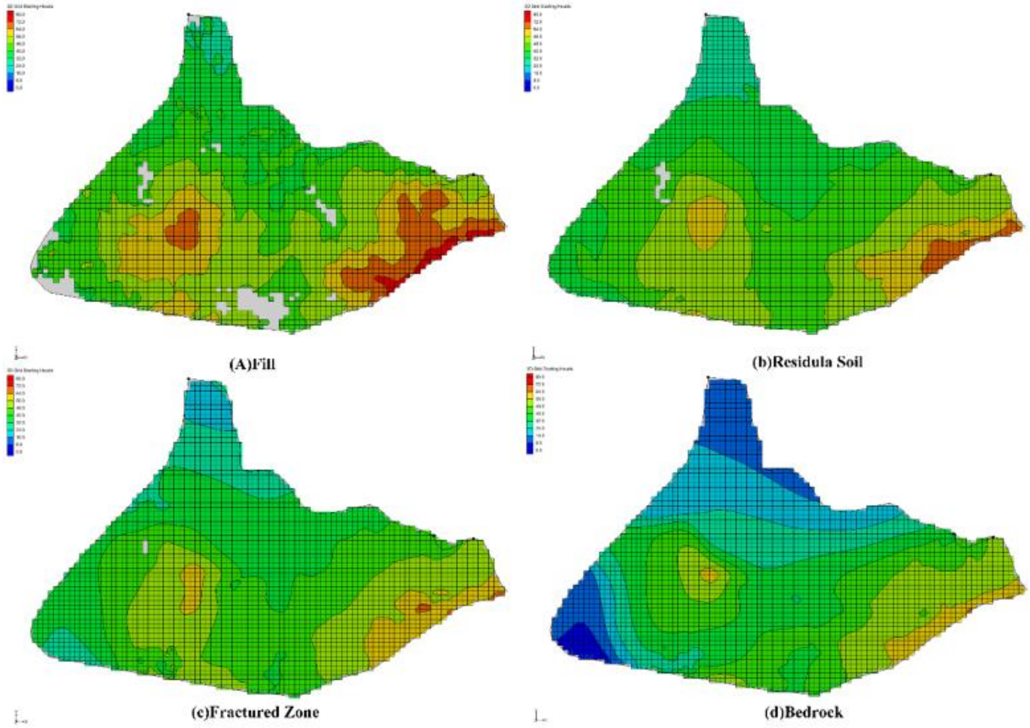


Figure5 Initial hydraulic conditions

Meteorological data from the Xiamen Gaoqi Weather Station, part of the Integrated Surface Database (ISD) provided by the National Oceanic and Atmospheric Administration (NOAA), were used to define the recharge boundary conditions for simulating groundwater contaminant transport. The eastern solid waste treatment facility was assumed to act as a continuous source of leachate. Initial background concentrations of ammonia nitrogen were assigned based on monitoring data from the national groundwater monitoring well XM09 and supporting environmental investigation reports. The MT3DMS model was used to simulate the temporal evolution of ammonia nitrogen concentrations over a six-year period. The simulation results are presented in Figure 6.

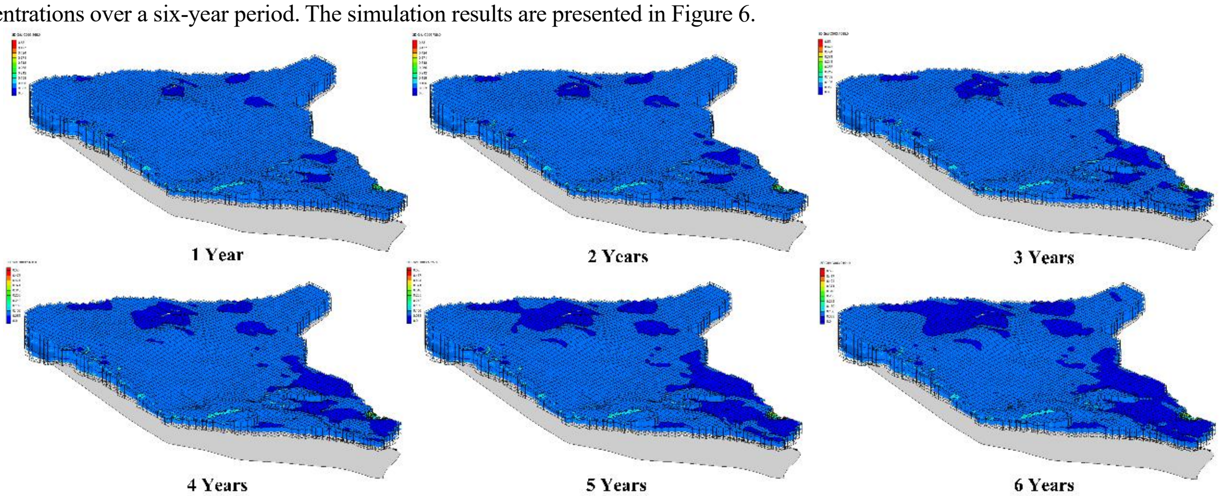


Figure 6 Ammonia Nitrogen Diffusion Simulation

5 Conclusion

Based on data from 148 boreholes, years of monitoring data (2019 – 2023), and a 5-meter resolution DEM, this study constructed a high-precision three-dimensional groundwater flow and solute transport model in Modflow to simulate the migration pattern of ammonia nitrogen (NH_4^+) in Xinxiu Town, Xiamen. The model adopts a 50-meter × 50-meter × 5-meter heterogeneous aquifer discretization framework, combining actual recharge and discharge conditions with continuous infiltration boundaries. Through coupled simulation using MT3DMS, it was found that pollutants generally migrate southeastward, consistent with the regional hydraulic gradient; the migration speed of shallow pollution is significantly higher than that of deep pollution, and the low-lying areas in the northeast are the main accumulation zones. The results confirm the model's ability to capture complex flow paths and identify high-risk pollution areas in groundwater.

This model provides a reliable decision-making tool for local water resource management and environmental planning. It is recommended to prioritize the restoration and monitoring of the discharge areas in the northeast and downstream water supply wells to address the threat posed by elevated NH_4^+ concentrations to water safety. Furthermore, this modeling framework supports multi-scenario simulation analysis, which is helpful for developing adaptive management strategies. Future research can introduce reactive solute transport mechanisms and long-term data assimilation techniques to further enhance the model's predictive ability and support the sustainable protection of groundwater in rapidly urbanizing coastal areas.

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