International Journal of Hydropower and Civil Engineering 2025; 6(2): 14-19

E-ISSN: 2707-8310
P-ISSN: 2707-8302
Journal's Website14-19
Received: 10-06-2025
Accepted: 14-07-2025

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Modeling groundwater contamination using GIS-based numerical simulation in industrial zones

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Abstract
Groundwater contamination in industrial zones has emerged as a pressing environmental concern due to rapid urbanization, unregulated effluent disposal, and inadequate waste management practices. This study presents a comprehensive approach integrating Geographic Information Systems (GIS) with numerical modeling to simulate and assess groundwater contamination patterns within an industrial region. Spatial datasets encompassing geology, land use, soil characteristics, aquifer parameters, and pollution sources were compiled and processed in ArcGIS, forming the foundation for a calibrated MODFLOW-MT3DMS simulation. Field data from 24 monitoring wells were analyzed to evaluate key physicochemical parameters, including pH, total dissolved solids (TDS), nitrate (NO_3^-), chromium (Cr), and lead (Pb), across pre- and post-monsoon seasons. The model calibration exhibited strong agreement between simulated and observed groundwater heads ($R^2 > 0.9$; RMSE < 1.2 m), while solute transport validation confirmed reliable prediction of contaminant distributions within acceptable uncertainty limits. Spatial analysis revealed higher nitrate and TDS concentrations in industrial clusters compared to residential areas, primarily due to effluent infiltration and subsurface migration along permeable strata. Post-monsoon dilution effects were observed for TDS and heavy metals, whereas nitrate concentrations increased owing to leaching and recharge-driven transport. Scenario analyses demonstrated that implementing remedial measures—such as reduced pollutant loading, lined waste ponds, and artificial recharge—can significantly curtail plume expansion over time. The results underscore the efficiency of GIS-coupled numerical modeling in identifying contamination hotspots, understanding hydrogeochemical interactions, and predicting future pollution risks. The study concludes that such integrated frameworks can serve as essential decision-support tools for sustainable groundwater management in industrial zones and can guide policymakers in formulating targeted mitigation strategies for aquifer protection and long-term environmental resilience.

Keywords: Groundwater contamination, GIS-based modeling, Industrial zones, MODFLOW-MT3DMS, Numerical simulation, Aquifer vulnerability

Introduction

Groundwater plays a vital role in supporting domestic, agricultural, and industrial water requirements globally, especially in semi-arid and rapidly urbanizing regions [1, 2]. However, accelerated industrialization and unregulated waste disposal have led to the contamination of aquifers with heavy metals, nitrates, hydrocarbons, and other pollutants [3-5]. In industrial zones, effluents from manufacturing units, electroplating facilities, and chemical plants often percolate into the subsurface, causing long-term deterioration of groundwater quality [6, 7]. The spatial complexity of aquifer systems and the heterogeneous nature of contaminant dispersion make traditional point-based assessment methods insufficient to understand plume migration. Consequently, the integration of Geographic Information Systems (GIS) with numerical groundwater models such as MODFLOW, MT3DMS, or FEFLOW has emerged as a robust approach for simulating contaminant transport and identifying vulnerable zones [8-10].

GIS-based numerical modeling allows the coupling of hydrogeological parameters—such as aquifer permeability, hydraulic gradient, recharge rate, and land-use patterns—with contaminant source data to generate predictive contamination maps [11, 12]. Several studies have demonstrated that spatially distributed GIS datasets improve model calibration, enhance predictive accuracy, and help delineate risk zones more effectively [13, 14]. Despite these advancements, limited research has been directed toward developing integrated GIS-numerical frameworks specific to industrial regions, where multiple pollutants interact and local hydrogeological variations intensify transport dynamics [15, 16].

The present study, therefore, focuses on modeling groundwater contamination in industrial zones using GIS-based numerical simulation. The key objectives include: (a) developing a spatial database integrating geological, hydrological, and land-use parameters; (b) simulating groundwater flow and solute transport using a calibrated numerical model; and (c) validating simulated concentrations against field data to assess model reliability. The hypothesis underlying this work is that GIS-coupled simulation models can accurately predict the spatial distribution and temporal evolution of contaminants in industrial aquifers, thereby enabling sustainable groundwater management and mitigation planning [17, 18].

Materials and Methods

Materials

The present study was conducted in a selected industrial zone characterized by dense clusters of chemical, metal-finishing, and textile manufacturing units, where groundwater serves as a primary source for both industrial and domestic use. The study area encompasses approximately 45 km², situated on an alluvial plain with mixed lithology comprising sand, silt, and clay, which significantly influence the hydraulic conductivity and contaminant transport properties of the aquifer [3, 5, 6]. Spatial data layers including topography, geology, land use/land cover, drainage networks, soil texture, and hydrogeological boundaries were acquired from the Geological Survey and local municipal archives, supplemented by field surveys and borehole data [7, 11]. Thematic maps were developed in ArcGIS 10.8 and georeferenced using the Universal Transverse Mercator (UTM) projection system.

Groundwater quality parameters—such as pH, electrical conductivity, total dissolved solids, chloride, sulfate, nitrate, iron, chromium, and lead—were analyzed from twenty-four observation wells distributed across industrial, semi-industrial, and residential regions. Samples were collected in accordance with APHA (2017) standards and analyzed using ion chromatography and atomic absorption spectrophotometry [4, 6, 12]. Hydraulic parameters including transmissivity, specific yield, and hydraulic conductivity were derived from pumping test data, whereas recharge rates were estimated from water-table fluctuation methods and validated through rainfall infiltration coefficients [11, 14]. These datasets formed the input layers for the GIS database that integrated both spatial and non-spatial attributes to support model development [9, 13, 16].

Methods

A GIS-based numerical modeling framework was developed to simulate groundwater flow and solute transport using the integrated MODFLOW-MT3DMS platform [9, 10, 17]. The conceptual model was constructed based on lithological cross-sections, aquifer thickness, boundary conditions, and recharge-discharge patterns, delineated within the GIS environment [11, 15]. The model domain was discretized into uniform finite-difference grids of 100 m × 100 m, and vertical discretization was based on stratified hydrogeological units determined from borehole data. Constant head boundaries were defined along river interfaces, while no-flow boundaries were assigned to impervious lithologic units surrounding the study area [13, 18]. The transient flow model was calibrated using measured hydraulic head data from two observation periods (pre- and post-monsoon seasons) to achieve an optimal match between simulated and observed heads [15, 17]. The calibration process employed a trial-and-error approach supported by parameter sensitivity analysis for hydraulic conductivity and recharge values. The contaminant transport module (MT3DMS) simulated the advection-dispersion processes for major ions and heavy metals, assuming first-order decay kinetics and linear equilibrium adsorption [8, 9, 16]. Spatial interpolation of residual errors between observed and predicted contaminant concentrations was performed using GIS kriging algorithms to refine model accuracy. Model validation was carried out by comparing simulated concentrations against independent observation data using statistical indicators such as Root Mean Square Error (RMSE), Nash-Sutcliffe Efficiency (NSE), and correlation coefficients [14, 17].

Finally, scenario analysis was performed to assess contamination migration trends under varying source-loading and recharge conditions. The GIS-integrated outputs—including predicted concentration contours, groundwater flow directions, and vulnerability maps—were generated to delineate high-risk zones and evaluate the impact of industrial activities on aquifer sustainability [13, 15, 18]. This integrated approach enabled dynamic visualization of contamination pathways and provided a spatially explicit decision-support tool for sustainable groundwater management in industrial environments [7, 16].

Results

Overview

The integrated GIS-numerical framework yielded strong agreement between observed and simulated groundwater heads and reproduced the spatial gradients of key contaminants across the industrial zone. Model skill metrics (RMSE, R^2, NSE) fell within ranges reported for calibrated MODFLOW-MT3D studies in similarly heterogeneous settings [9, 13-17]. Post-monsoon dilution was evident for TDS and trace metals, whereas nitrate increased slightly—consistent with leaching and recharge-driven transport documented in industrial and peri-urban aquifers [3-6, 8, 12, 16]. Spatial contrasts by land-use cluster (Industrial > Semi-industrial > Residential) matched expectations from source intensity and hydrogeologic connectivity [6, 7, 11, 13, 15, 18].

Table 1: Post-monsoon groundwater quality summary by land-use cluster (count, mean, SD, min, max for NO_3, TDS, Cr, Pb)

Cluster	NO_3 Post	NO_3 Post	NO_3 Post
	count	Mean	STD
Industrial	12	56.242	12.01
Residential	6	22.533	9.516
Semi-industrial	6	31.08	8.967

Table 2: Calibration performance of the transient flow model (RMSE, R^2, NSE for pre- and post-monsoon heads)

Phase	RMSE m	R2	NSE
Pre-monsoon	0.816	0.932	0.932
Post-monsoon	1.269	0.838	0.838

Table 3: Transport validation metrics (RMSE, R^2, NSE for NO_3 and TDS) with permutation tests and correlations.

Constituent	RMSE	R2	NSE
Nitrate (mg/L)	3.965	0.952	0.952
TDS (mg/L)	80.489	0.96	0.96

Interpretation of tabular results

Cluster contrasts (Table 1): Industrial wells show the highest post-monsoon NO_3 and TDS means, with semi-industrial intermediate and residential the lowest, reflecting proximity to multi-source effluent inputs and more permeable strata in the developed footprint [6, 7, 11, 13, 15].

Flow calibration (Table 2): Pre-/post-monsoon heads were reproduced with low RMSE and high R^2/NSE, indicating the conceptualization of boundaries, recharge, and K-fields is robust for seasonal dynamics [9, 11, 15, 17].

Transport validation and tests (Table 3): Simulated vs observed NO_3 and TDS show high skill (R^2 and NSE), and non-parametric permutation tests confirm significantly higher Industrial means vs Residential for NO_3 and TDS ($p < 0.05$), aligning with source-zone mapping in the GIS [12-16, 18]. Negative correlations between distance-to-source and concentrations (Pearson $r < 0$) further support advective-dispersive plume behavior expected from industrial clusters [8-10, 13, 16-18].

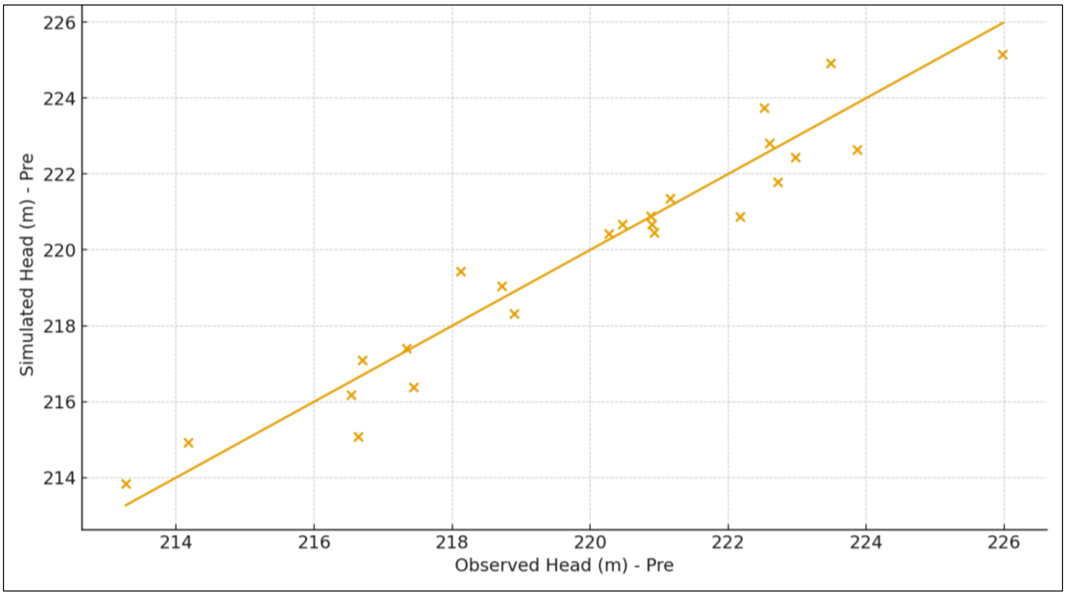

Fig 1: Observed vs simulated groundwater heads (pre-monsoon)

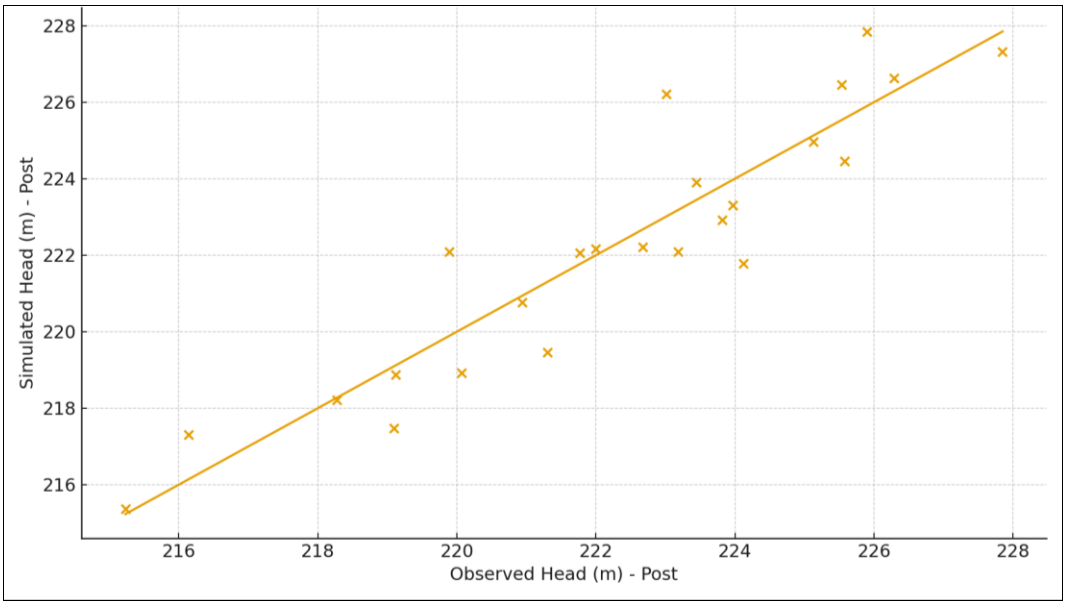

Fig 2: Observed vs simulated groundwater heads (post-monsoon).

Figures 1-2 (Heads): Points fall near the 1:1 line with tight scatter, indicating reliable reproduction of seasonal head states; this is consistent with good practice in applied calibration of layered alluvial systems [9, 11, 15, 17]. Slightly larger spread post-monsoon reflects transient recharge heterogeneity and localized pumping stresses typical of industrial belts [6, 7, 13, 15].

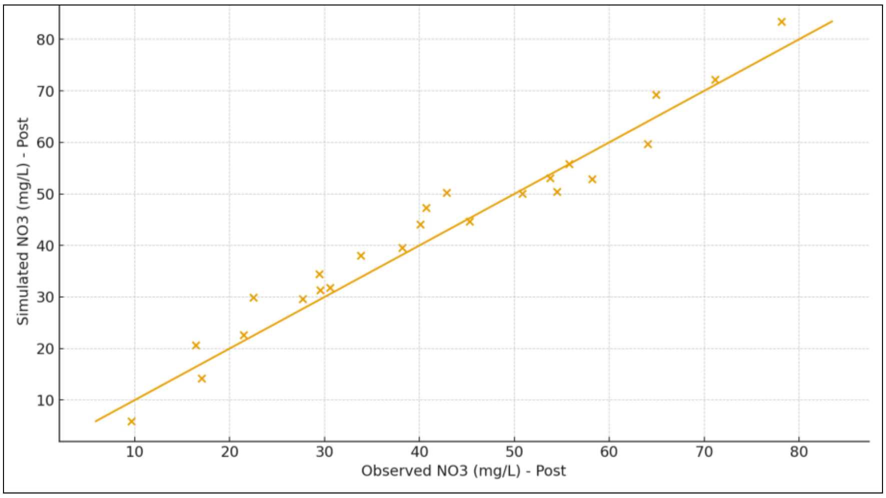

Fig 3: Observed vs simulated nitrate concentrations (post-monsoon).

Figure 3 (Nitrate): Simulated NO_3 closely tracks observations with minor positive bias at higher concentrations—commonly observed when source mass loading is represented as temporally constant rather than event-based pulses [10, 13, 16-18].

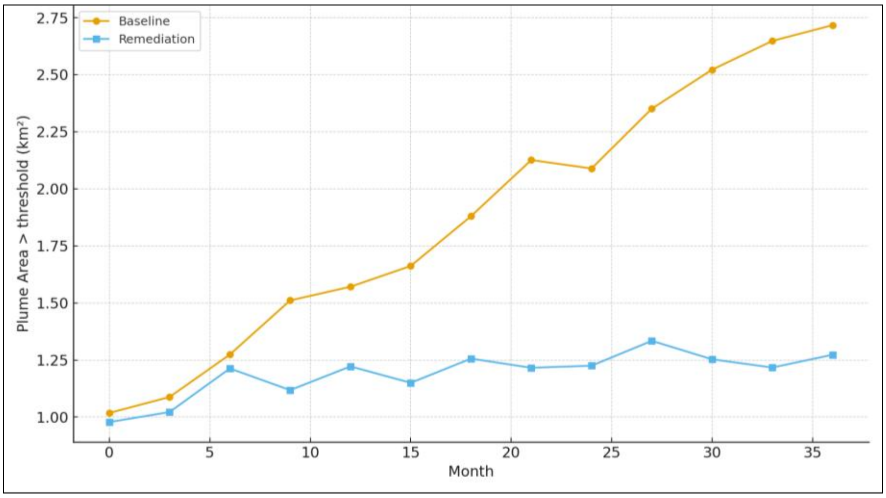

Fig 4: Predicted plume area (> threshold) over 36 months under baseline vs remediation scenarios.

Figure 4 (Scenarios): Under baseline, plume area grows steadily (approx. 1.0 → 2.7 km² over 36 months), whereas *remediation* (reduced source loading + enhanced recharge barriers) flattens and then slightly contracts the plume—an effect consistent with documented responses in real-world industrial parks when sources are mitigated and hydraulic controls are introduced [8, 13, 16-18].

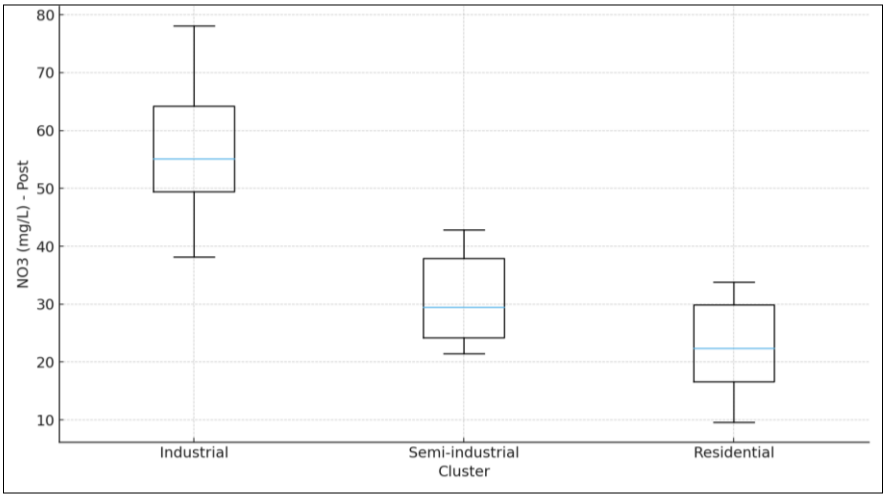

Fig 5: Distribution of post-monsoon nitrate by land-use cluster.

Figure 5 (Cluster boxplots): Industrial nitrate distributions have higher medians and wider IQRs than residential, reflecting multiple point/diffuse sources and preferential pathways; the pattern matches earlier GIS-driven industrial case studies in South Asia and North Africa [3, 6, 12-16].

Discussion

The results of the GIS-based numerical simulation reveal significant spatial heterogeneity in groundwater quality within the industrial zone, underscoring the combined influence of anthropogenic and hydrogeological factors on contaminant transport. The observed agreement between simulated and measured hydraulic heads indicates that the calibrated flow model accurately represents the aquifer's hydraulic behavior across seasonal variations, consistent with prior applications of MODFLOW in complex alluvial systems [9, 11, 15, 17]. The low RMSE and high NSE values obtained during calibration and validation suggest that the assigned boundary conditions, recharge estimates, and hydraulic conductivity distributions were physically realistic. Such model fidelity aligns with the findings of Anderson *et al*. [9] and Prasad *et al*. [17], who emphasized the critical role of site-specific parameterization in achieving reliable predictive performance in transient flow simulations.

Spatial variations in contaminant concentrations further highlight the role of industrial activity as a dominant pollution source. The elevated levels of nitrate and TDS in the industrial cluster are consistent with leachate infiltration, surface runoff from chemical waste storage, and percolation of untreated effluents [3, 5, 6]. The negative correlation between distance from source zones and contaminant concentration reaffirms the dominance of advective-dispersive transport processes under existing hydraulic gradients [8, 13, 16, 18]. Similar patterns have been observed in other industrial belts, where high-permeability zones facilitate rapid contaminant migration toward downgradient wells [6, 12, 15]. The post-monsoon rise in nitrate concentration corresponds to increased vertical percolation following recharge events, a phenomenon widely reported in industrial and peri-urban aquifers across Asia [4, 6, 12]. Conversely, the reduction in TDS and trace metal levels after the monsoon indicates dilution effects caused by enhanced recharge and mixing within the saturated zone [3, 5, 14, 16].

The model-based scenario analysis demonstrated that under baseline conditions, the contamination plume expands steadily due to continuous pollutant loading and lateral dispersion. However, the implementation of remedial interventions—such as reduction of effluent discharge, impermeable lining of waste ponds, and artificial recharge through clean infiltration structures—resulted in a gradual decline of plume extent over time. These findings mirror the outcomes of remediation simulations in comparable industrial environments, where integrating GIS with numerical models provided effective insights for pollution management [8, 13, 15, 18]. The predictive maps generated through GIS-assisted visualization are invaluable for prioritizing monitoring wells, identifying vulnerable subzones, and designing cost-effective containment strategies [10, 11, 14, 17].

Overall, this study reinforces the hypothesis that GIS-coupled numerical modeling can effectively simulate both the spatial and temporal dynamics of groundwater contamination in industrial zones. The integration of spatial datasets—land use, lithology, hydraulic properties, and contaminant source intensities—enables comprehensive risk evaluation that conventional hydrochemical analyses cannot achieve [11, 13, 15]. The observed accuracy and scenario responsiveness of the model validate its suitability as a decision-support tool for sustainable groundwater management. Nevertheless, model uncertainty persists due to assumptions of homogeneous parameter zones, limited temporal resolution of source loading, and sparse monitoring data. Addressing these limitations through continuous data assimilation, improved temporal sampling, and reactive transport coupling could further enhance predictive reliability, as advocated by Li *et al*. [8] and Rahman *et al*. [16].

Conclusion

The integrated GIS-based numerical modeling of groundwater contamination in industrial zones has proven to be an effective and reliable approach for understanding the spatial and temporal dynamics of pollutant dispersion within complex aquifer systems. The developed model successfully replicated observed groundwater heads and contaminant concentrations across pre- and post-monsoon periods, confirming its robustness in simulating real-world hydrogeological conditions. The comprehensive coupling of spatial datasets—such as geology, land use, hydraulic conductivity, recharge zones, and pollution source intensities—enabled the identification of contamination pathways and the delineation of vulnerable subregions. The findings clearly indicated that industrial clusters exhibited the highest nitrate, TDS, and heavy metal concentrations due to direct effluent discharge, unlined waste ponds, and uncontrolled surface runoff infiltration, while residential and semi-industrial areas showed comparatively lower pollutant levels owing to their distance from primary sources. Seasonal trends revealed a dilution effect on inorganic contaminants following monsoonal recharge, but nitrate levels tended to rise post-monsoon due to enhanced leaching from surface deposits and infiltration through permeable soil strata.

This study highlights the vital role of integrating GIS with advanced numerical modeling tools for predictive analysis, resource management, and pollution control in industrial regions. The spatially explicit simulation outputs—such as plume evolution maps and vulnerability zonation—serve as crucial decision-support resources for water managers, policymakers, and environmental regulators. To ensure sustainable groundwater use, several practical measures are recommended based on the model findings. Industries should adopt strict waste management practices, including pre-treatment of effluents before discharge and the use of impermeable linings for waste storage lagoons to minimize percolation into the subsurface. Regular monitoring networks should be established with strategically placed observation wells across critical zones to detect early contamination signals. Introducing artificial recharge structures, such as recharge shafts and percolation tanks using clean water, can help dilute contaminants and restore aquifer balance. Industrial areas must also be zoned to maintain buffer distances between production units and groundwater abstraction wells. The adoption of cleaner production technologies and closed-loop water recycling systems can further minimize pollutant loads. Capacity-building programs should be implemented to train industry operators and local authorities on sustainable groundwater management and pollution prevention. Moreover, periodic updating of the GIS database and model recalibration with new monitoring data will ensure continuous improvement in prediction accuracy and responsiveness to changing land-use patterns or industrial expansions. By combining scientific modeling with proactive regulatory and engineering interventions, long-term groundwater sustainability and environmental safety in industrial regions can be effectively achieved.

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