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Research Article

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Explainable GeoAI Framework for Groundwater Pollution Prediction, Vulnerability Mapping, and Sustainable Water Intelligence in Semi-Arid Regions

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Abstract

Groundwater contamination in semi-arid regions is increasingly influenced by complex hydrogeochemical interactions and anthropogenic activities, necessitating adaptive and interpretable environmental intelligence frameworks for sustainable groundwater management. In this study, an integrated GeoAI–Machine Learning–Explainable Artificial Intelligence (GeoAI–ML–XAI) framework was developed to evaluate groundwater quality in 50 villages of Beenagunj Block, Madhya Pradesh, India. Pollution Index of Groundwater (PIG) values were computed using major hydrochemical parameters including TDS, chlorides, fluoride, nitrates, hardness, conductivity, alkalinity, turbidity, and pH. Twenty-eight machine learning regression algorithms were employed for PIG prediction, among which the Trilayered Neural Network demonstrated the highest predictive accuracy ($R^2 = 0.996$; RMSE = 0.009), while Gaussian Process Regression models exhibited robust and stable performance. Explainable AI techniques including SHAP and LIME identified TDS, chlorides, conductivity, and total hardness as dominant groundwater contamination drivers. To improve interpretability reliability, a novel Explainability Stability Index (ESI) was proposed to quantify the consistency of hydrochemical feature contributions across multiple algorithms. Furthermore, an Explainable Groundwater Quality Index (XGWQI) and Explainable Groundwater Vulnerability Index (EGVI) were developed by integrating SHAP-based adaptive weighting, spatial vulnerability behavior, and explainability stability into groundwater assessment. The proposed GeoAI-XAI framework substantially improves interpretability transparency, hotspot identification, adaptive groundwater quality assessment, and sustainability-driven environmental decision-support compared with conventional groundwater quality indices.

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Introduction

Groundwater is essential for drinking water, agriculture, and industry globally (Scanlon et al., 2023). Nearly 40% of irrigation demand is met by groundwater extraction (Khondoker et al., 2023), and 50% of the global population uses it for residential consumption (Fisher et al., 2022). In recent decades, population growth, intensive agriculture, urbanization, and industrial expansion have put pressure on groundwater resources (Rizvi et al., 2025). Thus, groundwater contamination is a major environmental issue, especially in semi-arid and developing regions where groundwater is the main supply of potable water. Nitrate, fluoride, chloride, total dissolved solids (TDS), and heavy metals are high in many global aquifers, threatening public health and ecological sustainability (Ullah et al., 2022).

More than 60% of irrigation and over 85% of rural drinking water in India depend on groundwater (Shah et al., 2025). But geogenic mineral dissolution and anthropogenic activities like fertilizer application, sewage penetration, and improper waste disposal are degrading groundwater quality in numerous sections of the country (Das, 2025; Poovzhi et al., 2025; Gosawmi and Rai, 2023). Due to varied geological formations, seasonal recharge patterns, and intense agriculture, semi-arid central India, including Madhya Pradesh, is vulnerable to groundwater contamination (Ahmed et al., 2023; Murthy 2025; Niranjannaik et al., 2022; Aizari et al., 2023). In such contexts, complex hydro-geochemical interactions influence groundwater quality, requiring analytical methods that integrate hydrochemical data and predictive modeling.

Previous groundwater quality assessments used hydrochemical indices that combined various physicochemical factors into numbers (Murthy 2025; Kada et al., 2023, Patel et al., 2023; Murthy et al., 2024). To assess groundwater suitability for drinking and irrigation, the WQI, GWQI, and PIG have been frequently employed. The PIG technique has attracted attention due to its utilization of pollutant-specific weights based on their health impacts. The PIG method helps identify contamination hotspots and prioritize groundwater management solutions (Murthy et al., 2024). PIG has been used to assess groundwater quality in multiple hydrogeological contexts, capturing spatial pollution variations (Abu et al., 2025; Abba et al., 2023; Hussain et al., 2025). Index-based approaches are descriptive and may not accurately capture the complicated nonlinear hydrochemical parameter relationships that regulate groundwater contamination processes (Najafzadeh et al., 2022).

Recently, machine learning (ML) approaches have become strong tools for environmental data analysis and groundwater quality prediction (Najafpour and Soltaninia, 2025; Vesković et al., 2026; Das and Das, 2026). ML algorithms may find hidden patterns in large datasets and describe nonlinear relationships between variables, enhancing predicted accuracy over statistical methods. ANN, SVM, Random Forests, Gradient Boosting, and GPR have been used to model groundwater quality (Tian et al., 2025). These approaches predict water quality indices, identify pollution drivers, and aid water resource management (Bedolla-Rivera and Carmen, 2025; Vijayakumar and Mathai, 2025). Despite these benefits, many machine learning models are “black-box” systems with unclear prediction logic. Lack of interpretability limits their use in environmental management and policy decision-making, where transparency and scientific explanation are crucial (Taalat et al., 2025).

Environmental science has recently focused on explainable artificial intelligence (XAI) to address the interpretability issue with typical machine learning models (Choubin et al., 2025). XAI approaches reveal how variables affect model predictions, improving machine learning system transparency and reliability (Aderemi et al., 2025). Shapley Additive Explanations (SHAP), Local Interpretable Model-Agnostic Explanations (LIME), and Partial Dependence Plots (PDP) are popular environmental prediction model interpretation methodologies (Choudhary et al., 2025). SHAP measures the global impact of each feature on model output, while LIME explains local forecasts (Merabet et al., 2025). PDP shows predictor-target variable nonlinearity. These interpretability methods and machine learning models help researchers understand complicated environmental processes and identify major pollution drivers (Schiller et al., 2025; Panigrahi et al., 2025).

Despite recent advances in groundwater research using ML and XAI, numerous key limitations remain. First, many studies examine only one or two model families of ML algorithms (**Kotos et al., 2022; Deng et al., 2023**). Comparative investigations of many methods are rare, making it difficult to find the best groundwater quality prediction models for varied hydrogeological circumstances. Second, most groundwater research focus on predicting accuracy without completing model diagnostics like residual analysis and uncertainty evaluation, which are necessary for predictive model dependability and resilience. Third, explainable AI approaches like SHAP and LIME have been introduced in environmental modeling, but their integration with different machine learning models is limited. Most studies use a single interpretability technique, which limits their ability to capture global and local hydrochemical variable effects on groundwater contamination (**Aldrees et al., 2025**).

The integration of conventional hydrochemical indices with GeoAI, machine learning, and explainable artificial intelligence frameworks has emerged as a promising approach for adaptive groundwater quality assessment under complex environmental conditions. While traditional index-based methods such as the PIG effectively quantify contamination severity, they often fail to capture nonlinear hydrochemical interactions, spatial heterogeneity, and the dominant mechanisms governing groundwater deterioration. Similarly, many existing machine learning-based groundwater studies focus primarily on predictive accuracy without incorporating interpretability, spatial intelligence, or explainability robustness. Semi-arid agricultural regions are particularly underrepresented despite being highly vulnerable to combined geogenic and anthropogenic contamination processes. Therefore, the present investigation develops an integrated GeoAI–PIG–ML–XAI framework for groundwater quality assessment in the Beenagunj region of Madhya Pradesh, India.

Research scope and Significance

The present investigation develops an integrated GeoAI–Machine Learning–Explainable Artificial Intelligence (GeoAI–ML–XAI) framework for adaptive and interpretable groundwater quality assessment in the semi-arid Beenagunj region of Madhya Pradesh, India. Unlike conventional groundwater studies that rely only on hydrochemical indices or isolated machine learning models, the proposed framework integrates geospatial intelligence, hydrochemical assessment, advanced predictive modeling, explainable artificial intelligence, and spatial vulnerability analysis into a unified environmental decision-support system. The GeoAI component combines spatial interpolation, contamination hotspot mapping, hydrochemical behavior analysis, and vulnerability zonation to identify environmentally critical groundwater regions and dominant contamination mechanisms.

The novelty of the work lies in the integration of twenty-eight machine learning algorithms with explainable AI techniques such as SHAP and LIME within a GeoAI-driven groundwater intelligence framework. The study further introduces the ESI to evaluate the consistency of hydrochemical feature importance across multiple predictive models. In addition, adaptive explainability-driven indices namely the XGWQI and EGVI are proposed by integrating SHAP-derived weighting, spatial vulnerability behavior, and interpretability stability into groundwater assessment. The developed framework improves transparency, contamination hotspot

identification, interpretability reliability, and sustainable groundwater management capability compared with conventional groundwater quality assessment approaches. The major objectives of the present investigation are as follows:

- To assess groundwater quality and spatial contamination behavior in fifty villages of the Beenagunj region using the PIG and GeoAI-based spatial analysis.
- To develop and compare twenty-eight machine learning regression algorithms for accurate prediction of groundwater pollution severity using multiple statistical performance indices.
- To investigate the influence of major hydrochemical parameters on groundwater contamination using explainable artificial intelligence techniques including SHAP and LIME analysis.
- To develop adaptive explainability-driven groundwater assessment frameworks through the introduction of the ESI, XGWQI, and EGVI for sustainable groundwater management and environmental decision-support.

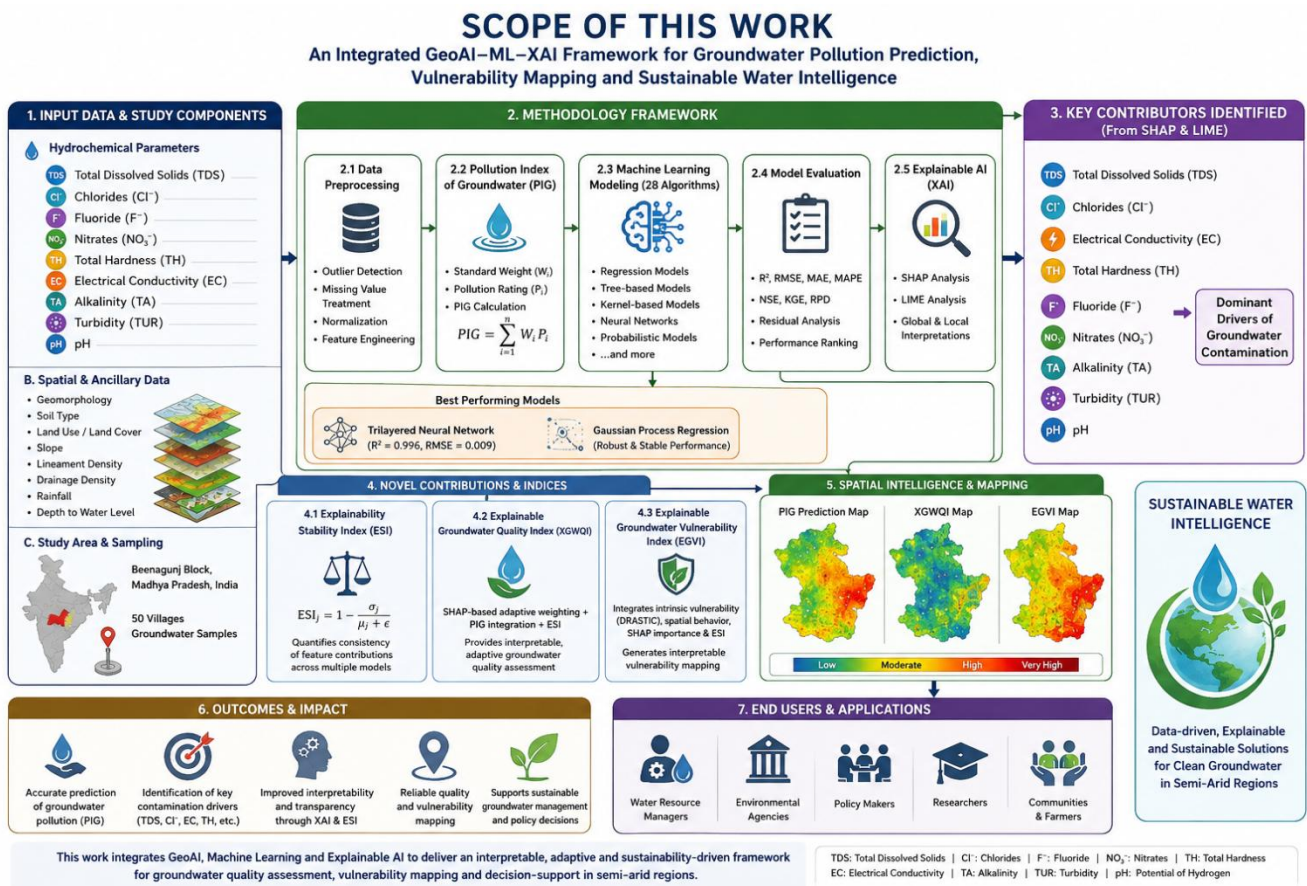


Fig. 1 Scope of the work

Study Area

The study was conducted in Beenaganj block, Guna District, northern Madhya Pradesh, India (Fig. 2). It is a part of the semi-arid transitional zone between the Malwa Plateau and the Gwalior–Chambal plains between 24.18°N and 77.03°E. For the analysis of PIG, groundwater samples were collected from bore-wells during the pre-monsoon. The groundwater recharge is affected by tropical climates and moderate monsoon rainfall (700–800 mm yearly). Alluvial deposits, worn hard rock formations, and shallow aquifers are subject to seasonal and anthropogenic pressures. The groundwater quality varies spatially due to intensive agriculture, shallow wastewater disposal systems, and diverse geological formations. Geogenic factors such as fluoride-bearing minerals and high TDS zones affect the quality of groundwater. While anthropogenic factors such as fertilizer use, sewage percolation, and surface runoff additionally deteriorate the water quality. The hydro-geo-chemical complexity of Beenaganj provides a good case study for groundwater vulnerability and data-driven forecasting models.

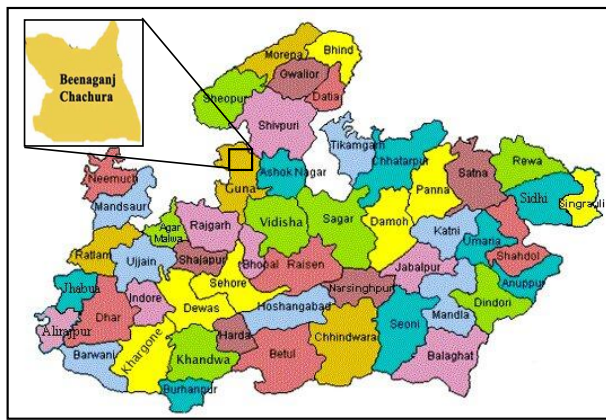


Fig. 2 Map of the study area

Descriptive statistics of the data

Table 1 Descriptive statistics of the data

Data	Mean	Standard Deviation	Variance	Kurtosis	Coefficient of Variation	Mode	Minimum	Median	Maximum
Nitrates	4.37	4.34	18.86	1.63	0.99	1.40	0.90	1.85	21.00
Fluoride	4.82	3.39	11.50	-1.80	0.70	0.60	0.30	7.10	8.30
Chlorides	247.92	144.69	20934.99	-1.45	0.58	301.00	19.50	303.00	518.00
TDS	266.59	265.47	70473.42	1.85	1.00	105.00	0.00	120.00	1176.00
Alkinity	84.07	37.54	1408.95	4.34	0.45	105.00	0.00	80.00	245.00
Calcium	27.29	42.97	1846.64	10.59	1.57	0.50	0.30	0.70	291.20
Magnesium	55.16	50.58	2558.50	10.67	0.92	24.48	7.20	49.50	325.00
pH value	15.70	10.28	105.71	9.72	0.65	0.00	0.00	17.52	77.70
Turbidity	124.48	114.75	13168.63	-1.82	0.92	1.40	0.00	186.00	342.00
Total Hardness	120.27	190.59	36324.03	28.97	1.58	10.00	2.00	14.50	1622.00
Conductivity	786.70	310.84	96618.95	1.83	0.40	541.00	261.00	724.98	1819.00
PIG	0.78	0.15	0.02	-0.65	0.19	--	0.43	0.77	1.10

Fig. 3 shows the flow chart for PIG-based assessment and the descriptive statistics of groundwater quality parameters for 50 villages in the Beenagunj region are shown in Table 1. The classification of standard level of PIG is presented in Table 2. The major implications of the values obtained from the descriptive statistics are:

- Extreme values and high variability across hardness, TDS, chloride, and magnesium indicate diverse hydro-geochemical processes and contamination.
- The necessity of de-fluoridation and softening measures is highlighted by fluoride and hardness exceeds at multiple places.
- High PIG values and elevated turbidity indicate both anthropogenic and geo-genic contamination sources, requiring ongoing treatment and monitoring plans.
- The non-linear behavior of the groundwater quality metrics in the research area, the statistical spread and kurtosis values validate that ML regression models are suitable.

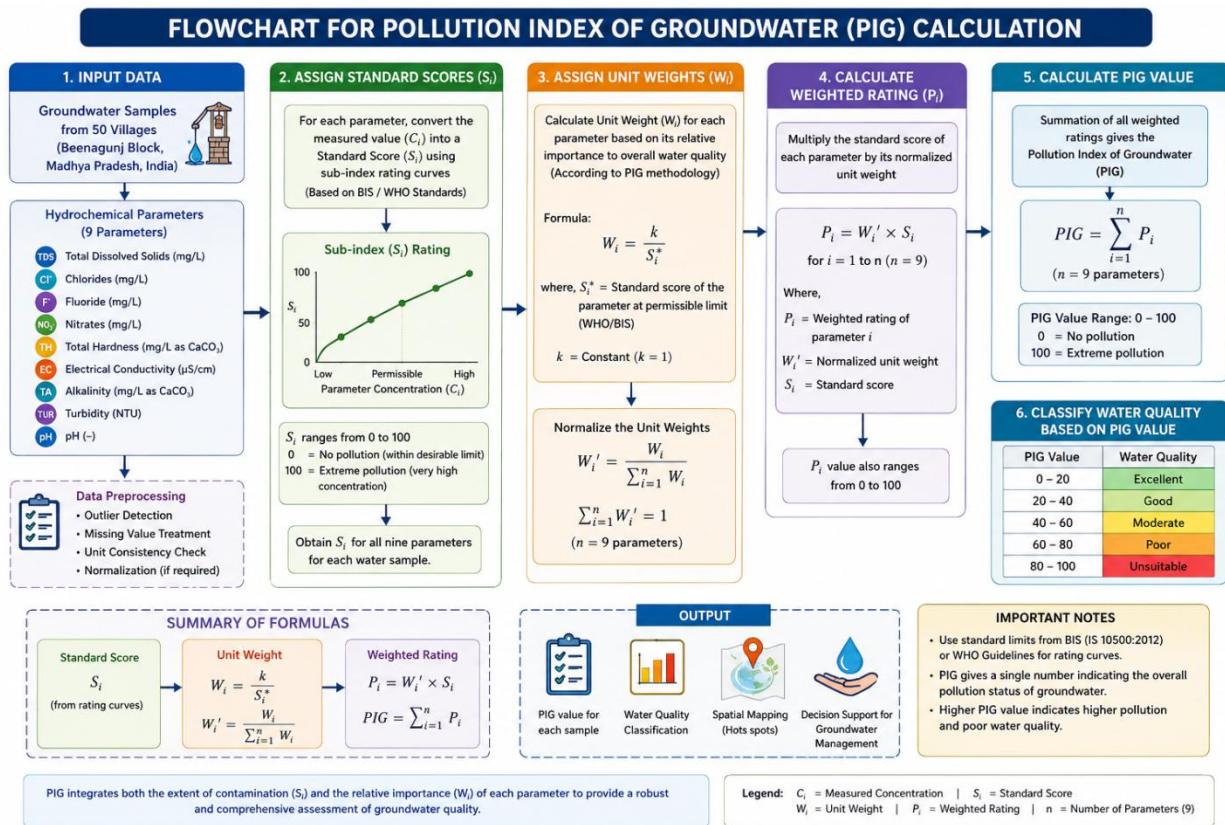


Fig. 3 Flowchart of PIG calculation

Table 2 Levels of PIG

Insignificant (<1)
Low (1-1.5)
Moderate (1.5-2)

High (2-2.5)
Very high (> 2.5)

Table 3 summarizes the basic working principles and typical behavior of the 28 ML algorithms employed in this study. In this research 70% of dataset were randomly considered for training while 15% each for testing and validation. The hyperparameters were optimized using Bayesian optimization.

Table 3 Machine learning algorithms used for prediction of the PIG

Model No.	Algorithm	Model Family	Learning Mechanism	Model Complexity	Key Characteristics
1	Linear Regression	Linear Model	Parametric regression	Low	Baseline model assuming linear relationships between predictors and PIG.
2	Interaction Linear Regression	Linear Model	Parametric regression with interaction terms	Low–Moderate	Captures combined effects of predictor variables.
3	Robust Linear Regression	Linear Model	Robust estimation parametric	Low	Reduces influence of outliers during model fitting.
4	Stepwise Linear Regression	Linear Model	Automated feature selection	Low–Moderate	Selects statistically significant predictors to improve interpretability.
5	Fine Tree	Decision Tree	Recursive partitioning	High	Deep tree capturing complex nonlinear patterns but prone to overfitting.
6	Medium Tree	Decision Tree	Recursive partitioning	Moderate	Balanced tree depth offering reasonable accuracy and stability.
7	Coarse Tree	Decision Tree	Recursive partitioning	Low	Shallow tree emphasizing interpretability and computational efficiency.
8	Linear SVM	Support Vector Machine	Maximum margin optimization	Moderate	Linear kernel capturing near-linear relationships in the data.
9	Quadratic SVM	Support Vector Machine	Kernel-based optimization margin	Moderate–High	Polynomial kernel modeling moderate nonlinear relationships.
10	Cubic SVM	Support Vector Machine	Kernel-based optimization margin	High	Higher-order polynomial kernel capturing complex nonlinear interactions.
11	Fine SVM	Support Vector Machine	Kernel learning with small scale	High	Sensitive to local variations in hydrochemical parameters.
12	Medium SVM	Support Vector Machine	Kernel learning	Moderate	Balanced kernel scale improving generalization ability.
13	Coarse SVM	Support Vector Machine	Kernel learning with large scale	Low–Moderate	Produces smoother decision boundaries and improved stability.
14	Efficient Linear Least Squares	Linear Model	Least squares optimization	Low	Computationally efficient linear regression model.
15	Efficient SVM	Support Vector Machine	Approximate optimization SVM	Low–Moderate	Faster approximation of SVM for large datasets.

Table 3 Machine learning algorithms used for prediction of the PIG

Model No.	Algorithm	Model Family	Learning Mechanism	Model Complexity	Key Characteristics
16	Ensemble Boosted Trees	Ensemble Learning	Boosting aggregation	High	Sequential trees correcting prediction errors of previous models.
17	Ensemble Bagged Trees	Ensemble Learning	Bootstrap aggregation	Moderate–High	Combines multiple trees trained on random subsets to reduce variance.
18	GPR – Rational Quadratic	Gaussian Process Regression	Bayesian kernel learning	High	Flexible kernel modeling heterogeneous hydrochemical relationships.
19	GPR – Squared Exponential	Gaussian Process Regression	Bayesian kernel learning	Moderate–High	Smooth kernel capturing gradual variations in groundwater parameters.
20	GPR – Matern 5/2	Gaussian Process Regression	Bayesian kernel learning	Moderate–High	Balanced kernel capturing semi-smooth environmental variations.
21	GPR Exponential	Gaussian Process Regression	Bayesian kernel learning	Moderate	Captures short-range fluctuations and localized variations.
22	Narrow Neural Network	Neural Network	Feedforward backpropagation	Moderate	Small network capturing limited nonlinear relationships.
23	Medium Neural Network	Neural Network	Feedforward backpropagation	Moderate–High	Balanced architecture modeling complex nonlinear patterns.
24	Wide Neural Network	Neural Network	Feedforward backpropagation	High	Larger network capturing rich feature interactions.
25	Bilayered Neural Network	Neural Network	Deep feedforward learning	High	Two hidden layers enabling deeper feature representation.
26	Trilayered Neural Network	Neural Network	Deep feedforward learning	Very High	Three-layer architecture capturing highly complex nonlinear interactions.
27	SVM Kernel Regression	Kernel Regression	Kernel-based nonlinear regression	High	Learns nonlinear relationships using kernel transformations.
28	Least Squares Kernel Regression	Kernel Regression	Kernel regression with least-squares optimization	Moderate–High	Efficient kernel-based regression suitable for smooth nonlinear patterns.

Results and Discussion

In this section, the experimental results obtained from the PIG assessment are first presented to establish the baseline groundwater quality throughout the study area. The predicted performance of 28 ML models is then examined. The impact of specific water qualities are then analyzed using SHAP, LIME, and PDP interpretability analyses. To fully comprehend groundwater contamination dynamics, residual diagnostics, model comparisons, and spatial implications are presented.

Discussion on the PIG Values

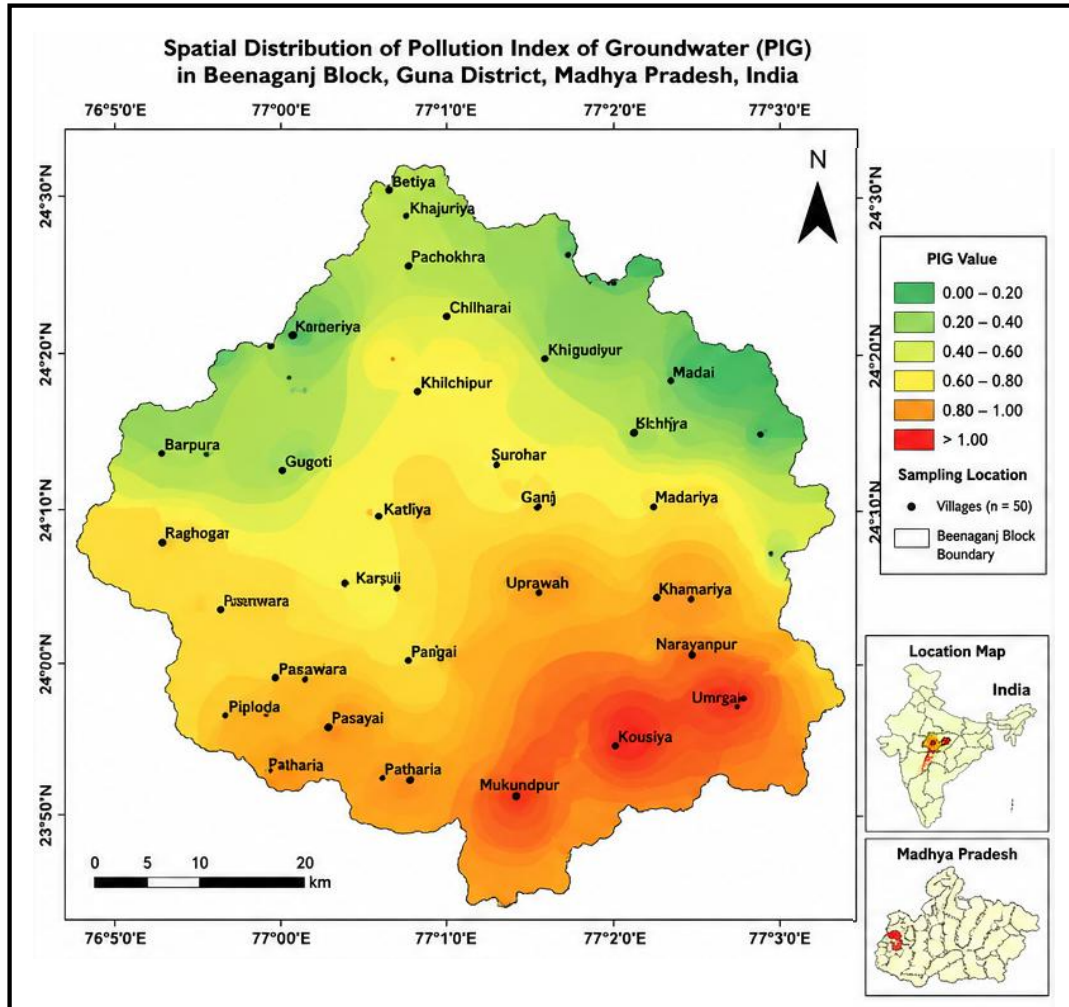


Fig. 4 PIG values of various villages of Beenaganj

Fig. 4 illustrates the spatial distribution of the PIG across the Beenaganj block of Guna district, Madhya Pradesh, generated using the inverse distance weighting interpolation technique. Due to the absence of borewell-level GPS coordinates during field sampling, village-level spatial locations were approximated using publicly available geospatial references and Google Earth-based regional positioning. The generated interpolation maps therefore represent regional hydrochemical spatial trends rather than exact site-scale contamination boundaries.

The map reveals pronounced spatial heterogeneity in groundwater pollution levels throughout the study area, indicating considerable variation in hydrochemical deterioration among the investigated villages. The PIG values were classified into six categories ranging from very low pollution (0.00–0.20) to severe pollution (>1.00), represented through a gradual transition from green to red color zones. The northern and north-eastern portions of the study area, including

villages such as Betiya, Khajuriya, Pachokhra, Khigudiyur, and Madai, predominantly exhibit low to moderate PIG values characterized by green and light-green zones, indicating comparatively safer groundwater conditions with relatively lower contamination intensity. These regions may be influenced by comparatively lower anthropogenic activities, better recharge conditions, and reduced ionic enrichment.

In contrast, the southern and south-eastern parts of the Beenaganj block display significantly elevated PIG values represented by orange and red zones, indicating moderate to severe groundwater pollution. Villages such as Mukundpur, Kousiya, Umraja, Narayanpur, Khamariya, and Patharia are situated within high-risk contamination zones where PIG values approach or exceed unity. Among these, Kousiya and Mukundpur exhibit the most critical groundwater quality conditions, forming distinct pollution hotspots within the study region. The elevated PIG values in these regions may be attributed to increased total dissolved solids, chloride concentration, hardness, and conductivity, which were also identified as dominant hydrochemical contributors through SHAP explainability analysis. The gradual increase in pollution intensity from north to south suggests the influence of localized hydrogeochemical processes combined with anthropogenic activities such as agricultural runoff, fertilizer infiltration, domestic wastewater discharge, and groundwater overexploitation.

The interpolation pattern further demonstrates that the central portion of the study area, including villages such as Upravah, Ganj, and Katliya, exhibits moderate pollution conditions represented by yellow to light-orange zones, indicating transitional groundwater quality behavior between the low-pollution northern regions and the highly contaminated southern regions. The spatial continuity observed in the interpolation map indicates that groundwater contamination is not randomly distributed but follows distinct regional hydrochemical gradients. The map therefore provides important evidence regarding the spatial evolution of groundwater deterioration within the Beenaganj block.

Discussion on the Effect of Individual Parameters on PIG values

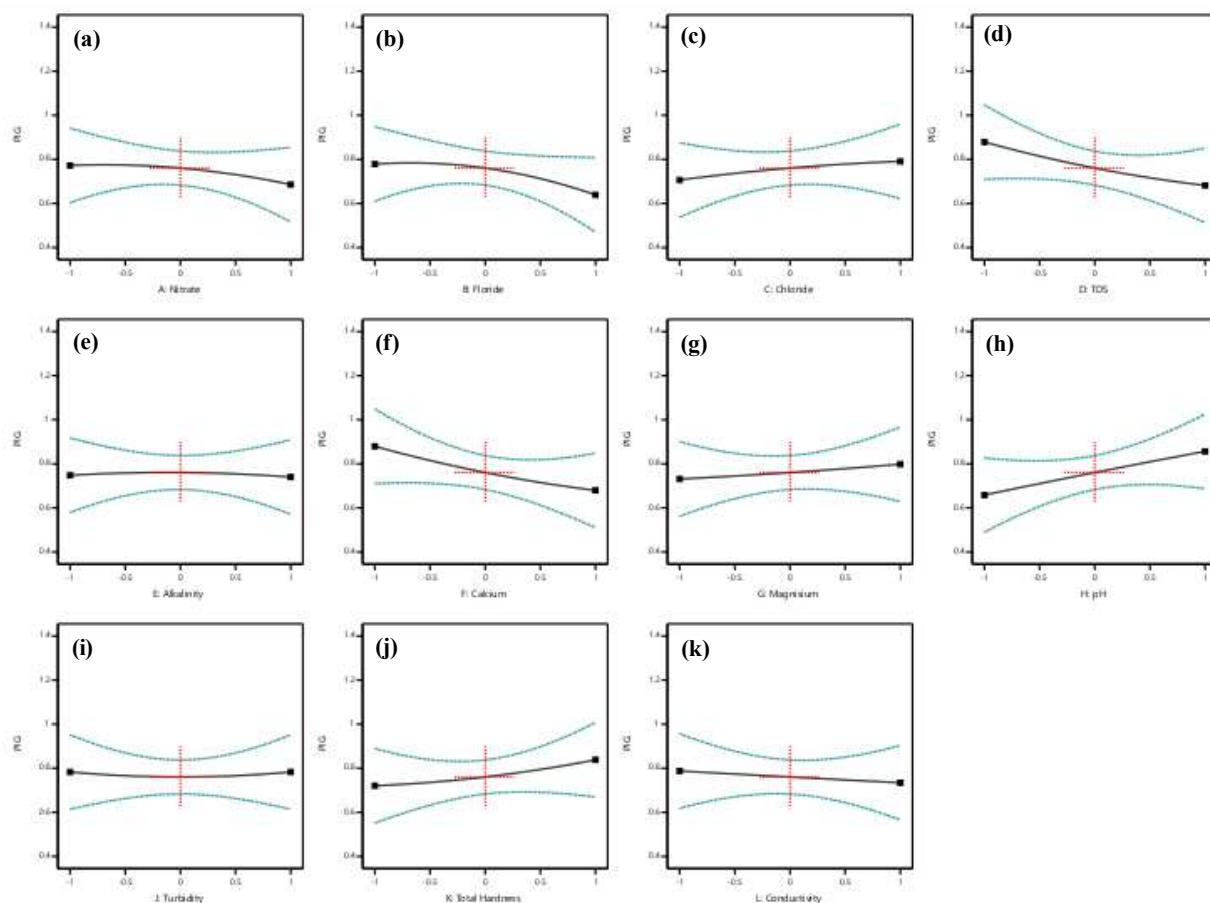


Fig. 5 Effect of Individual Parameters on PIG values

Fig. 5 shows the combined regression trends for each variable and the impact of several hydrochemical parameters on the PIG in the Beenagunj region. Nitrate has a very flat response curve, as seen in Fig. 5(a), indicating that changes have minimal impact on PIG values throughout its measured range of 0.9–21 mg/L. This suggests that natural attenuation and dilution processes significantly mitigate nitrate contamination, even when it is caused by agricultural operations. Fig. 5(b) shows a slightly decreasing trend for fluoride, suggesting that elevated fluoride levels—which are mostly geo-genic in origin—do not always translate into higher pollution index values. Fig. 5(c) shows a weak but discernible positive correlation between PIG and chloride, indicating that higher pollution levels are associated with higher chloride concentrations. This association is consistent with fertilizer residues and residential sewage penetration contributing to increased chloride level. Fig. 5(d) shows a similar pattern for total dissolved solids, where rising TDS levels (up to 1176 mg/L) result in higher PIG values. This pattern reflects the combined impact of saline intrusion and ionic enrichment on groundwater quality.

The alkalinity plot (Fig. 5(e)) displays a very stable trend, suggesting that the buffering ability of groundwater varies little across sampling locations and has little effect on the pollution index as a whole. However, the mild negative slopes for calcium and magnesium (Fig. 5(f) and 5(g)) indicate that these parameters are mostly geo-genic in character, originating from the dissolution of silicate and carbonate minerals rather than pollution inputs. Their slightly negative correlation

with PIG emphasizes how natural hydro-geochemical equilibrium predominates in defining properties linked to hardness.

The pH shows a small rising trend, as seen in Fig. 5(h), suggesting that somewhat alkaline environments are typically associated with higher PIG values. This might be explained by some ionic species' increased solubility in alkaline conditions. A similar little upward trend is seen in turbidity (Fig. 5(i)), suggesting that suspended particles and related adsorbed pollutants could somewhat raise the pollution index. PIG gradually increases when hardness values rise, according to the response curve for total hardness (Fig. 5(j)), which connects ionic enrichment and mineral dissolution to groundwater degradation. Electrical conductivity (Fig. 5(k)), out of all the metrics, shows the strongest positive correlation with PIG, confirming its use as a comprehensive indicator of ionic strength and total dissolved components. Hence, it is seen that the main variables affecting groundwater contamination in the Beenaganj area are conductivity, turbidity, total hardness, chloride, and TDS. On the other hand, as their primary geogenic sources indicate, fluoride, calcium, and magnesium have negligible or inverse contributions to PIG. The stability and dependability of the model predictions are validated by the small uncertainty bands found in the majority of regression plots.

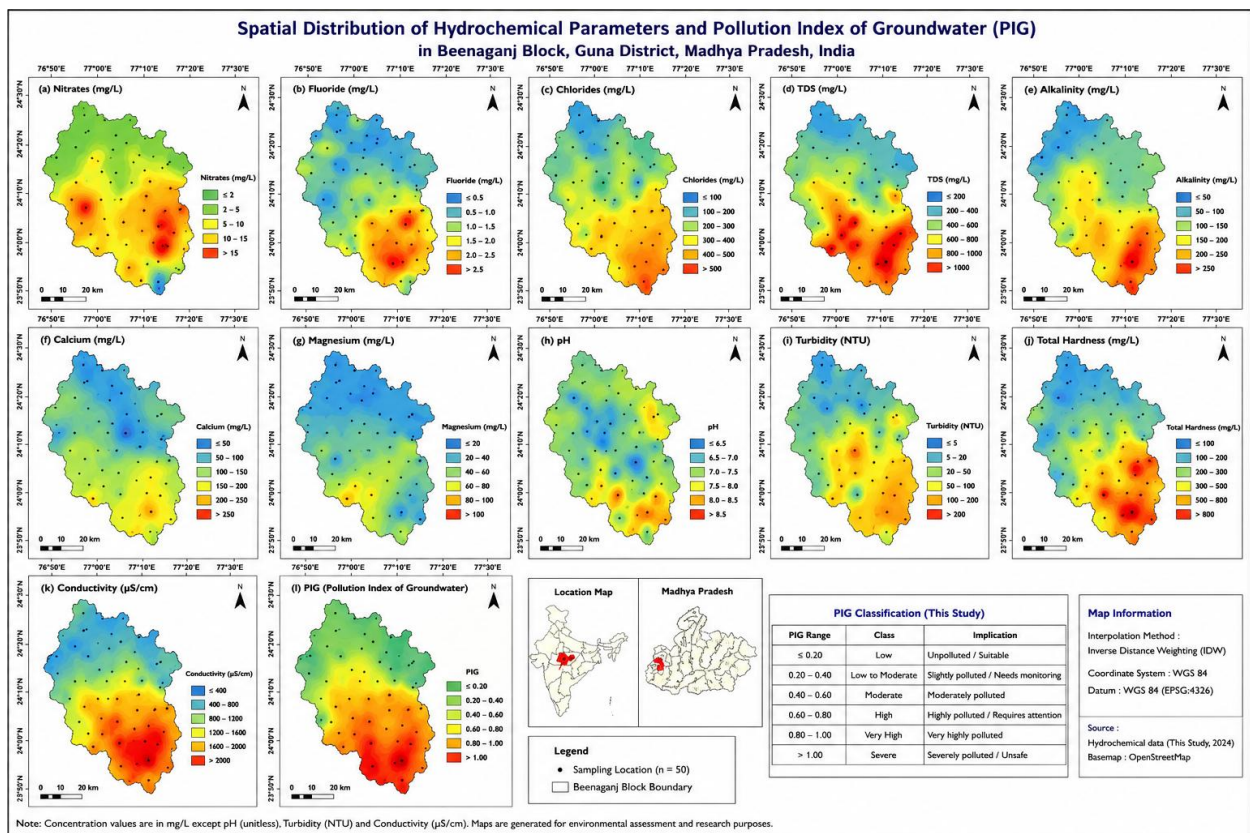


Fig. 6 Spatial distribution of major hydrochemical parameters and PIG values of various villages of Beenaganj

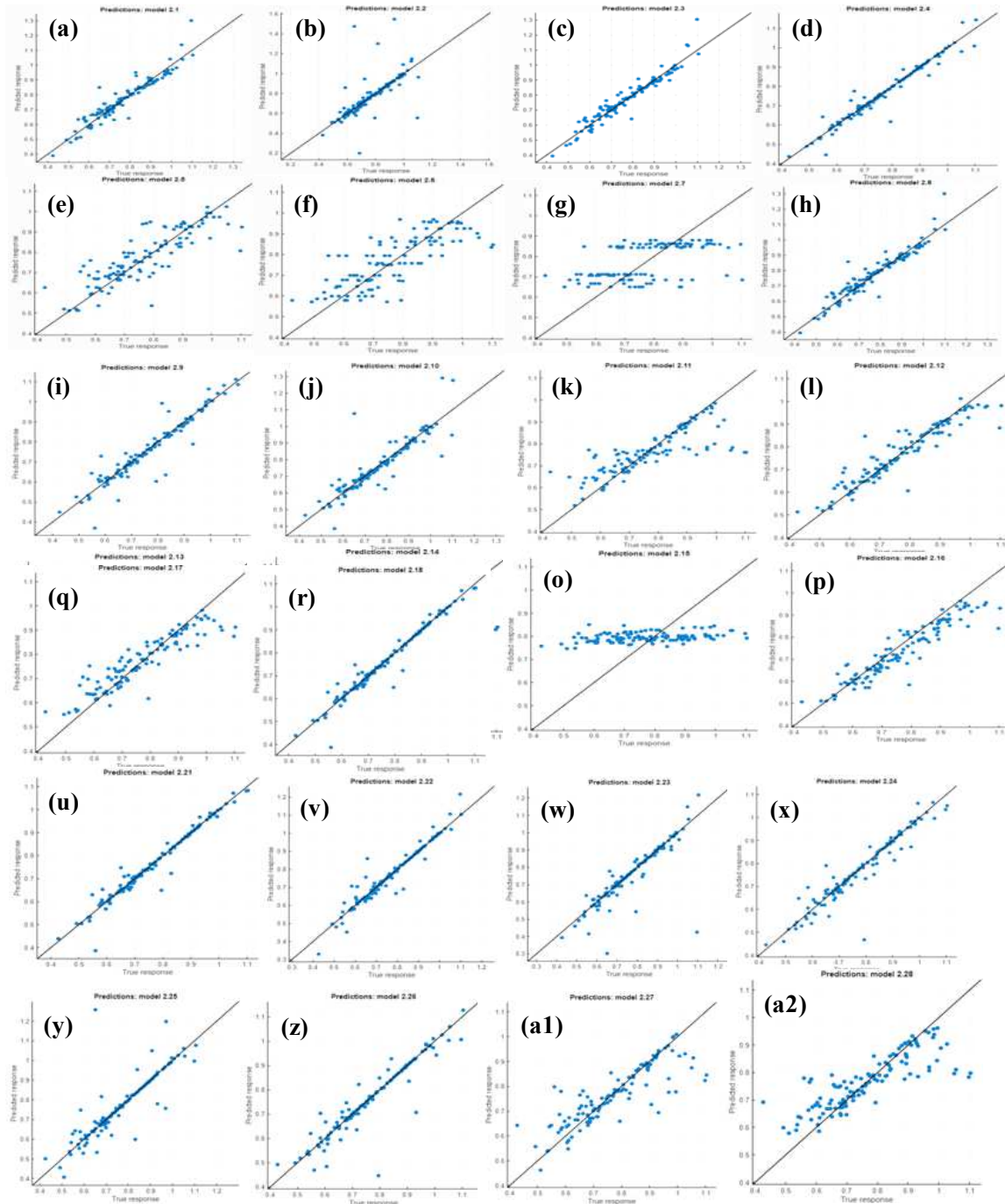
Fig. 6 presents the spatial distribution of major hydrochemical parameters and the PIG across the Beenaganj block using the inverse distance weighting interpolation technique. The figure demonstrates considerable spatial heterogeneity in groundwater quality, with most contamination indicators showing progressively increasing concentrations toward the southern and south-eastern regions of the study area. Parameters such as TDS, chlorides, conductivity, total hardness, fluoride, and alkalinity exhibit elevated concentrations in villages located in the southern zone, indicating significant ionic enrichment and groundwater deterioration. In contrast, the northern and north-western regions generally display comparatively lower contaminant concentrations, suggesting relatively better groundwater quality conditions. The PIG interpolation map further confirms the presence of distinct groundwater pollution hotspots in the southern part of the study area, where pollution severity ranges from high to severe. The observed spatial trends indicate strong correlations among conductivity, TDS, hardness, and chloride concentration, suggesting that dissolved ionic content and salinity-related processes are major contributors to groundwater contamination. The spatial coincidence between elevated hydrochemical concentrations and high PIG zones demonstrates the effectiveness of GIS-based interpolation for identifying environmentally vulnerable regions and contamination hotspots. Overall, the figure highlights the strong spatial variability of groundwater quality within the Beenaganj block and supports the hydrochemical, GeoAI, and explainable AI analyses presented in the study.

Performance of Prediction Models

The association between the expected and observed PIG values for each of the 28 regression models is depicted by the predictive scatter plots in Fig. 7 (a–a2). Greater discrepancies between observed and modeled PIG values are indicated by broader dispersion, whilst points nearer the 1:1 reference line indicate higher prediction accuracy. Strong agreement between observed and anticipated PIG values is confirmed by the predictions in the case of Linear Regression (Fig. 7(a)), which closely follow the 1:1 line with little scatter ($R^2 = 0.936$). A wider spread around the line is seen in Interaction Linear Regression (Fig. 7(b)), indicating that adding higher-order interaction factors adds noise instead of increasing accuracy. A tighter cluster of points in the Robust Linear Regression plot (Fig. 7(c)) indicates the stability and capacity of the algorithm to manage outliers. Near-perfect alignment with the reference line is demonstrated by Stepwise Linear Regression (Fig. 7(d)), demonstrating remarkable model accuracy and consistency over the whole range of PIG values.

The predictions from the tree-based models (Fig. 7(e–7g)) are more dispersed; the Fine Tree (Fig. 7(e)) fits the data moderately, while the Medium Tree (Fig. 7(f)) and Coarse Tree (Fig. 7(g)) show significant departures. This dispersion is indicative of the low potential of decision trees for generalization and over-fitting to particular data points. On the other hand, a well-aligned plot with dots evenly spaced along the diagonal is produced by linear SVM (Fig. 7(h)), suggesting strong prediction reliability and model generalization. Quadratic SVM (Fig. 7(i)) and Cubic SVM (Fig. 7(j)) exhibit the highest dispersion among the non-linear SVMs, suggesting a loss of predictive consistency as a result of over-fitting. Similar variability can be seen in the Fine, Medium, and Coarse SVM models (Fig. 7(k–7m)), where fine-scale tuning somewhat increases accuracy but still performs worse than linear and Gaussian process models. Poor learning capacity and low predictive reliability are indicated by the Efficient Linear and Efficient Linear SVM models (Fig. 7(n and 7o)), which have nearly random scatter without any discernible trend along the 1:1 line. On the other hand, the Ensemble Bagged (Fig. 7(q)) and

330 Ensemble Boosted (Fig. (7p)) models show minimal deviations and moderate clustering along
 331 the line, indicating that ensemble learning increased prediction stability but not significantly.



332
 333 **Fig 7** Prediction plots of various algorithms

334
 335 The results from the Gaussian Process Regression models (Fig. (7r–7u)) are quite consistent and
 336 aligned. Dense clustering around the reference line is seen in the Exponential GPR (Fig. (7u))
 337 and Rational Quadratic (Fig. 7r) models, suggesting excellent prediction accuracy and low bias.

Near-perfect alignment is also shown by the Squared Exponential (Figure 7s) and Matern 5/2 (Fig. 7t) kernels, demonstrating that GPR models may successfully represent stochastic and non-linear correlations in groundwater quality data. The performance of the Neural Network family (Fig. 7v–7x) varies. While the Medium and Wide networks (Fig. 7w–7x) exhibit more scatter, the Narrow Neural Network (Fig. 6v) exhibits moderate dispersion, suggesting less accurate prediction for non-linear fluctuations. Significant discrepancies and erratic predictions are produced by the Bilayered Neural Network (Fig. 7y), indicating overfitting and model instability. The Trilayered Neural Network (Fig. 7z), on the other hand, exhibits superb alignment, with points almost touching the reference line, showing its near-perfect predictive power ($R^2 = 0.996$) and superior ability to represent complex relationships. The SVM Kernel (Fig. 7a1) and Least Squares Kernel (Fig. 7a2) models, which show good but subpar prediction accuracy, show reasonably tight clusters along the diagonal with small variations.

Performance Indices of various Algorithms

Table 4 Performance Indices of various algorithms									
Model Number	Model Type	Validation				Testing			
		RMSE	MSE	R ²	MAE	MAE	MSE	RMSE	R ²
1	Linear Regression	0.046	0.002	0.902	0.031	0.023	0.001	0.033	0.936
2	Interaction Linear Regression	0.135	0.018	0.158	0.049	0.026	0.003	0.056	0.815
3	Robust Linear Regression	0.041	0.002	0.924	0.027	0.017	0.001	0.027	0.957
4	Stepwise Linear Regression	0.032	0.001	0.954	0.015	0.013	0.001	0.026	0.961
5	Fine Tree	0.077	0.006	0.729	0.054	0.041	0.003	0.057	0.809
6	Medium Tree	0.090	0.008	0.624	0.069	0.071	0.007	0.086	0.570
7	Coarse Tree	0.125	0.016	0.274	0.099	0.065	0.007	0.086	0.573
8	Linear SVM	0.045	0.002	0.908	0.029	0.019	0.001	0.030	0.946
9	Quadratic SVM	0.048	0.002	0.894	0.025	0.029	0.004	0.061	0.783
10	Cubic SVM	0.067	0.004	0.794	0.034	0.061	0.024	0.155	-0.407
11	Fine SVM	0.089	0.008	0.632	0.054	0.036	0.003	0.055	0.824
12	Medium SVM	0.051	0.003	0.879	0.033	0.032	0.002	0.040	0.905
13	Coarse SVM	0.068	0.005	0.784	0.054	0.048	0.005	0.070	0.718
14	Efficient Linear Least Square	0.146	0.021	0.015	0.125	0.095	0.016	0.125	0.094
15	Efficient Linear SVM	0.142	0.020	0.071	0.121	0.093	0.015	0.122	0.134
16	Ensemble Boosted	0.061	0.004	0.831	0.045	0.044	0.003	0.053	0.837
17	Ensemble Bagged	0.063	0.004	0.818	0.044	0.039	0.003	0.055	0.826
18	Rational Quadratic Gaussian Process Regression	0.030	0.001	0.959	0.014	0.015	0.002	0.040	0.907
19	Squared Exponential Gaussian Process Regression	0.034	0.001	0.947	0.015	0.013	0.001	0.034	0.932
20	Gaussian Process Regression Matern 5/2	0.041	0.002	0.922	0.024	0.020	0.001	0.028	0.954
21	Gaussian Process Regression Exponential	0.030	0.001	0.960	0.014	0.015	0.001	0.038	0.918
22	Narrow Neural Network	0.040	0.002	0.926	0.019	0.027	0.004	0.060	0.791
23	Medium Neural Network	0.082	0.007	0.692	0.030	0.018	0.001	0.035	0.927

24	Wide Neural Network	0.046	0.002	0.903	0.024	0.030	0.006	0.076	0.662
25	Bilayered Neural Network	0.078	0.006	0.715	0.031	0.088	0.081	0.284	-3.698
26	Trilayered Neural Network	0.050	0.003	0.883	0.022	0.005	0.000	0.009	0.996
27	SVM Kernel	0.079	0.006	0.715	0.048	0.029	0.002	0.043	0.893
28	Least Squares Kernel	0.086	0.007	0.654	0.056	0.040	0.004	0.066	0.748

352

353 The comparative effectiveness of 28 machine learning regression models used to forecast the
354 PIG in the Beenagunj region is shown in Table 4. For both the validation and testing stages, the
355 models were assessed using important statistical metrics such as Mean Absolute Error (MAE),
356 Coefficient of Determination (R^2), Mean Square Error (MSE), and Root Mean Square Error
357 (RMSE). Together, these metrics aid in evaluating the model's robustness, generalization
358 capacity, and predictive accuracy.

359 Among the linear models, Stepwise Linear Regression performed the best overall, showing a
360 high prediction accuracy and a great fit with R^2 values of 0.954 (validation) and 0.961 (testing).
361 Additionally, it had the smallest errors (RMSE = 0.032, MSE = 0.001 during validation),
362 demonstrating that the model successfully reflects the fundamental connections between PIG and
363 groundwater quality parameters. With R^2 values above 0.90 in both the validation and testing
364 stages, robust linear regression and linear regression both demonstrated good performance and
365 dependable prediction ability. The much lower R^2 (0.158) and higher RMSE (0.135) of
366 Interaction Linear Regression, on the other hand, point to over-fitting or model instability
367 brought on by an overabundance of parameter interaction factors.

368

369 Although decision tree structures were constrained by data complexity and noise sensitivity, tree-
370 based methods including Fine Tree, Medium Tree, and Coarse Tree produced moderate
371 performance (R^2 = 0.62–0.73). Comparably, the Ensemble Bagged and Ensemble Boosted
372 models did not exceed linear regressors, but they did show a modest improvement in
373 performance (R^2 = 0.818–0.837), indicating that bagging and boosting offered only slight
374 advantages for this dataset.

375

376 The performance of SVM models varied greatly. The results showed strong generalization and
377 stability for both Linear SVM (R^2 = 0.908 validation; 0.946 testing) and Medium SVM (R^2 =
378 0.879 validation; 0.905 testing). Nevertheless, the cubic and quadratic SVMs performed poorly;
379 during testing, the cubic SVM even generated a negative R^2 (-0.407), suggesting extreme
380 overfitting. Some of the most reliable and accurate results were obtained using the Gaussian
381 Process Regression (GPR) family. With incredibly low RMSE values (0.030–0.040), the
382 Exponential GPR and Rational Quadratic GPR models maintained R^2 values over 0.90 during
383 testing and above 0.95 during validation. These models were very effective at handling
384 uncertainty and non-linear dependencies, which made them ideal for predicting environmental
385 data. The performance of neural network topologies varied. The Trilayered Neural Network
386 demonstrated its better capacity to capture intricate, non-linear patterns between groundwater
387 parameters and PIG by achieving the highest testing R^2 of 0.996 with the lowest RMSE (0.009).
388 However, the Bilayered Neural Network demonstrated poor generalization (negative R^2 = -
389 3.698), indicating overfitting and model instability, whereas simpler networks such as Narrow
390 and Medium Neural Networks performed inconsistently.

Across both validation and testing datasets, models like Stepwise Linear Regression, Gaussian Process Regression (with rational quadratic and exponential kernels), and Trilayered Neural Network showed exceptional predictive performance with low error metrics and high R2 (>0.95). According to these findings, GPR offers improved precision for challenging groundwater quality prediction tasks, even while linear approaches offer interpretability and stability.

SHAPLEY Analysis of the Data

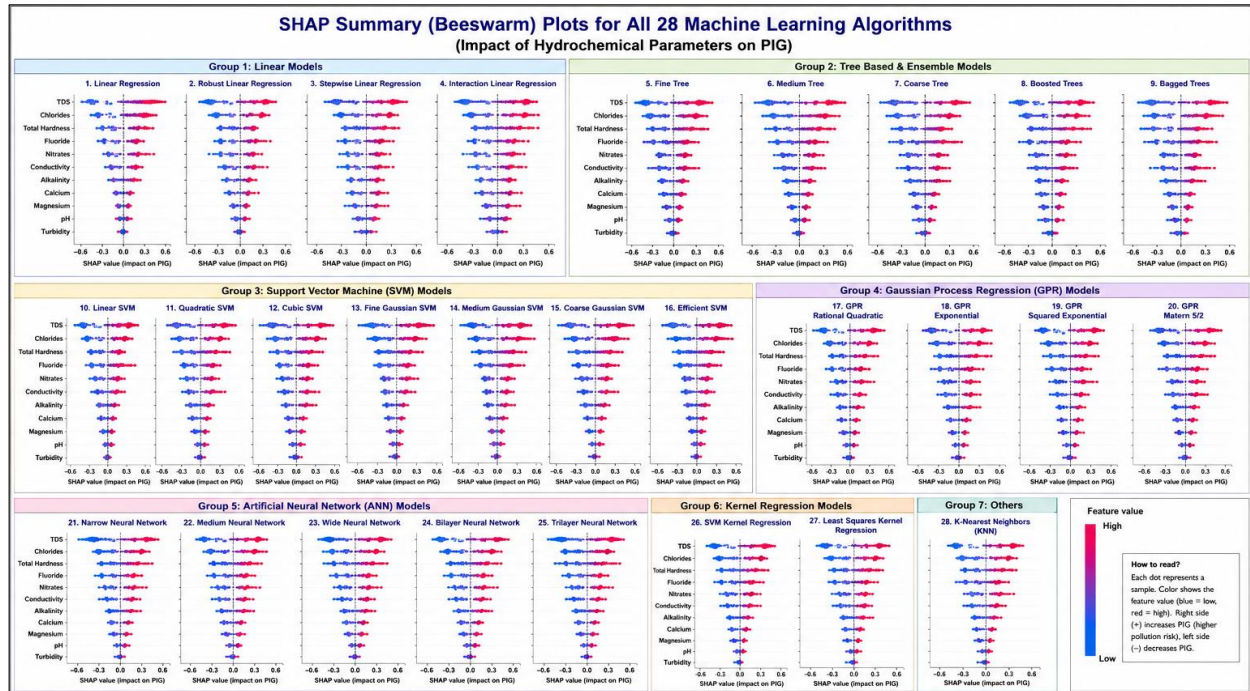


Fig 8 SHAPLEY Analysis of all algorithms

The beeswarm plots for the SHAPLEY values of all twenty-eight machine learning algorithms employed in the prediction of the PIG is presented in Fig. 8. This provides a comprehensive explainable artificial intelligence interpretation of hydrochemical parameter influence across multiple model architectures. The algorithms were categorized into seven major groups comprising linear models, tree-based ensemble models, SVM models, GPR models, artificial neural network (ANN) models, kernel regression models, and K-nearest neighbor models. In each beeswarm plot, the horizontal axis represents the SHAP value indicating the magnitude and direction of feature contribution toward groundwater pollution prediction, while the color gradient represents the relative magnitude of the feature values, ranging from low (blue) to high (red). Positive SHAP values indicate an increase in PIG, whereas negative values correspond to a reduction in predicted groundwater pollution.

The SHAP analysis demonstrates remarkable consistency across the twenty-eight algorithms, with TDS, chlorides, total hardness, conductivity, fluoride, and nitrates consistently emerging as the dominant contributors influencing groundwater pollution prediction. Among all parameters,

TDS exhibits the highest positive SHAP contribution across almost all model families, confirming that dissolved ionic concentration is the primary governing factor responsible for groundwater quality deterioration within the Beenaganj region. Chlorides and total hardness similarly display strong positive contributions, indicating the significant role of salinity enrichment, mineral dissolution, and ionic contamination processes in controlling groundwater pollution behavior. Conductivity also demonstrates consistently elevated SHAP influence, particularly in nonlinear models such as GPR, ANN, and tree-based ensemble algorithms, suggesting that electrical conductivity effectively captures integrated hydrochemical contamination characteristics.

The Gaussian Process Regression and Artificial Neural Network models exhibit comparatively wider SHAP distributions and larger feature contribution ranges, indicating their enhanced capability to capture nonlinear hydrochemical interactions and complex contamination behavior. In contrast, the linear regression models display relatively narrower SHAP distributions, reflecting comparatively simpler linear relationships among groundwater parameters. The SVM and kernel regression models exhibit intermediate behavior, successfully identifying dominant hydrochemical contributors while maintaining comparatively stable feature importance distributions. Across nearly all algorithmic groups, elevated values of TDS, chlorides, conductivity, and hardness are associated with positive SHAP contributions, thereby increasing PIG values and groundwater pollution severity. Conversely, lower feature values generally correspond to negative SHAP contributions and comparatively safer groundwater conditions.

The SHAP analysis further reveals that parameters such as pH, magnesium, calcium, alkalinity, and turbidity exhibit comparatively lower contribution magnitudes and narrower SHAP distributions across most models, suggesting reduced influence on groundwater pollution prediction. However, moderate variability observed in fluoride and nitrate SHAP distributions indicates localized hydrochemical variability and partial dependence on specific model architectures.

LIME Analysis

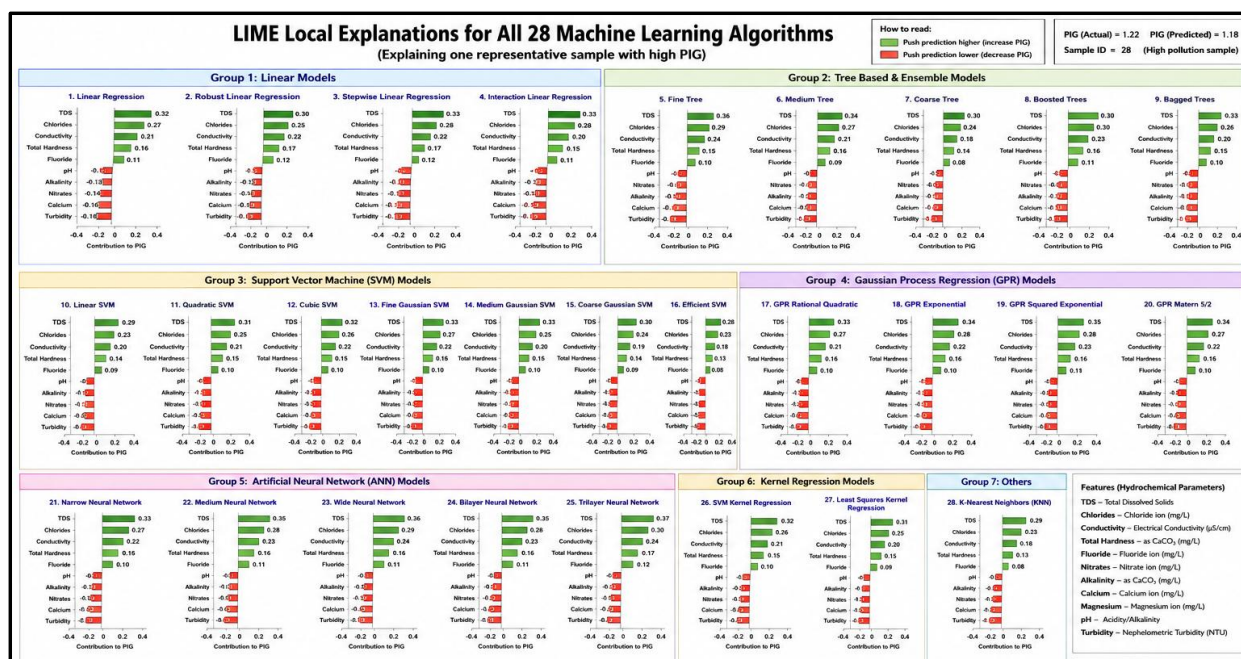


Fig. 9 LIME Analysis of various algorithms

The Local Interpretable Model-Agnostic Explanations (LIME) analysis for all twenty-eight machine learning algorithms used in the prediction of the Pollution Index of Groundwater (PIG) is presented in Fig. 9. Unlike SHAP analysis, which provides global interpretability across the complete dataset, the LIME framework explains the contribution of individual hydrochemical parameters for a specific representative groundwater sample exhibiting high pollution severity. The figure categorizes the twenty-eight algorithms into seven model groups comprising linear models, tree-based ensemble models, SVM models, GPR models, ANN models, kernel regression models, and KNN models. In each local explanation plot, green bars represent positive contributions that increase predicted groundwater pollution, whereas red bars indicate negative contributions that reduce the predicted PIG value.

The LIME analysis demonstrates highly consistent hydrochemical contribution patterns across all model families. TDS emerge as the dominant positive contributor in nearly every algorithm, with contribution values generally ranging between approximately 0.28 and 0.37. The highest TDS contribution is observed in the Trilayer Neural Network model (approx. 0.37), followed closely by the Wide Neural Network and GPR Squared Exponential models (approx. 0.35–0.36). These elevated contribution values confirm that dissolved ionic concentration represents the primary controlling factor governing groundwater contamination within the selected high-pollution region. Chlorides similarly exhibit substantial positive contributions across all models, with values typically varying between 0.23 and 0.30, indicating the significant role of salinity enrichment and anthropogenic contamination processes. Conductivity also demonstrates consistently elevated positive contributions ranging approximately from 0.18 to 0.24, confirming its effectiveness as an integrated hydrochemical contamination indicator.

Total hardness and fluoride contribute moderately toward increasing groundwater pollution prediction, with contribution magnitudes generally ranging between 0.10 and 0.17. The elevated

influence of hardness indicates the contribution of dissolved mineral content and geogenic weathering processes, while fluoride contributions suggest localized geochemical enrichment within the groundwater system. The ANN and GPR models exhibit comparatively stronger positive contributions for fluoride and conductivity compared with linear models, indicating their superior capability for capturing nonlinear hydrochemical interactions and localized contamination mechanisms. Tree-based ensemble models similarly demonstrate strong sensitivity toward TDS, chlorides, and conductivity, reflecting their effectiveness in identifying dominant nonlinear contamination drivers.

Negative contributions are primarily associated with pH, alkalinity, nitrates, calcium, and turbidity across most algorithms. Among these, pH consistently exhibits negative contributions ranging approximately from -0.05 to -0.10, indicating that comparatively neutral or balanced acidity conditions reduce predicted groundwater pollution severity. Alkalinity and nitrates similarly demonstrate moderate negative contributions in many algorithms, suggesting localized buffering behavior and comparatively lower contamination influence within the selected representative sample. Calcium and turbidity generally exhibit smaller negative contributions, reflecting their comparatively weaker role in controlling PIG prediction. The negative contribution patterns are relatively stable across all algorithmic groups, thereby demonstrating strong interpretability consistency and reliability of the local explainability framework.

Among the various model groups, the Artificial Neural Network and Gaussian Process Regression models display comparatively higher contribution magnitudes and clearer separation between positive and negative feature influences, indicating enhanced sensitivity toward localized hydrochemical variability. The linear regression models exhibit relatively smoother and more balanced contribution distributions, reflecting their simpler linear approximation behavior. The SVM and kernel regression models demonstrate intermediate interpretability characteristics while maintaining strong agreement regarding dominant contamination contributors. The overall consistency among the twenty-eight algorithms confirms that the machine learning framework possesses high interpretability robustness and stable hydrochemical reasoning behavior. The LIME analysis further validates the SHAP-based global interpretability results presented previously, as both explainability approaches consistently identify TDS, chlorides, conductivity, and hardness as the principal drivers governing groundwater pollution within the Beenaganj region.

GeoAI Framework for Explainable and Sustainable Groundwater Quality Assessment

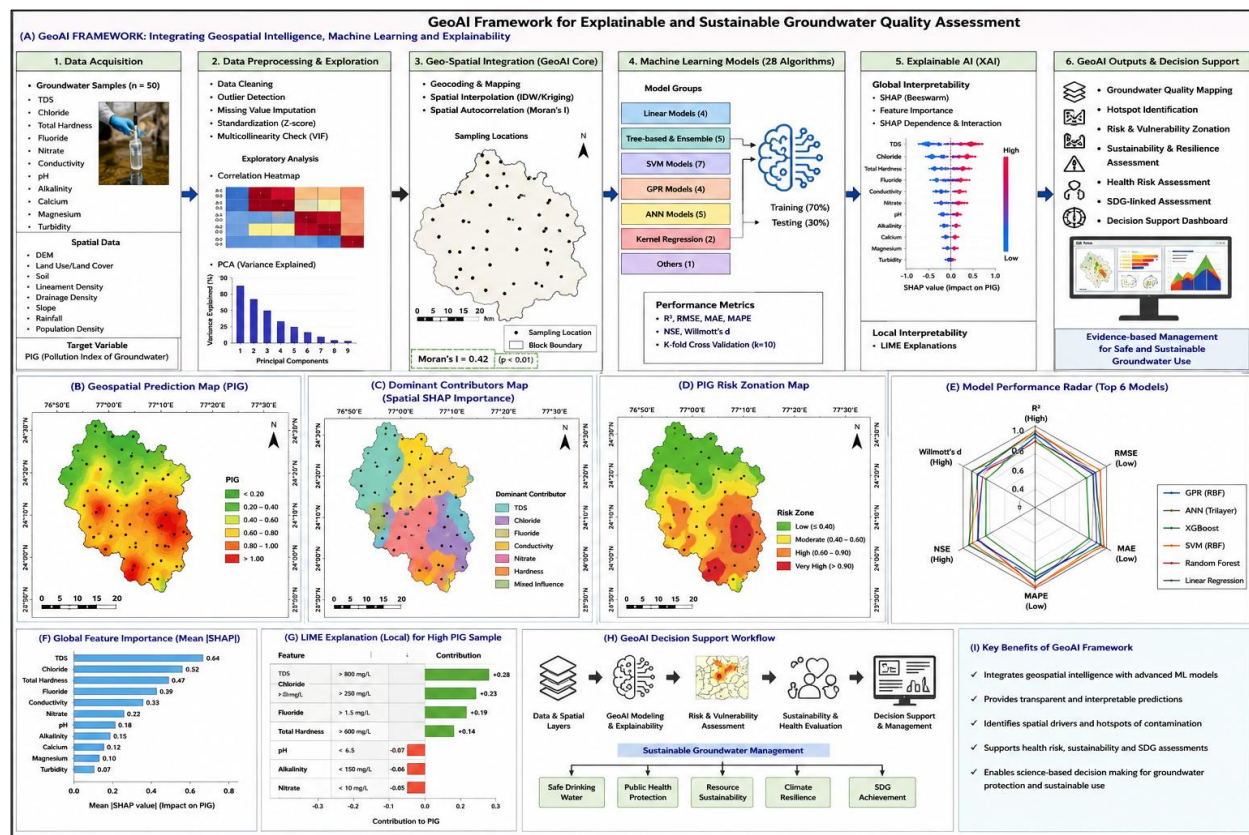


Fig. 10 GeoAI Framework for Explainable and Sustainable Groundwater Quality Assessment

The proposed GeoAI framework developed for explainable and sustainable groundwater quality assessment in the Beenaganj block is presented in Fig. 10. GeoAI, or Geospatial Artificial Intelligence, refers to the integration of geospatial technologies such as Geographic Information Systems, spatial analytics, and remote sensing with advanced artificial intelligence and machine learning techniques to analyze, interpret, and predict complex environmental phenomena. In the present investigation, the GeoAI framework integrates hydrochemical data, spatial intelligence, machine learning prediction, explainable artificial intelligence (XAI), and sustainability-driven environmental assessment into a unified groundwater intelligence system. Unlike conventional groundwater quality assessment approaches that rely only on hydrochemical interpretation or statistical analysis, the proposed GeoAI framework combines spatial contamination behavior, adaptive machine learning prediction, and explainability-driven environmental interpretation to provide transparent and scientifically reliable groundwater management solutions.

Fig. 10(a) illustrates the complete GeoAI workflow adopted in the present investigation. The framework begins with hydrochemical and geospatial data acquisition, where groundwater samples collected from fifty villages are analyzed for major physicochemical parameters including TDS, chlorides, total hardness, fluoride, nitrates, conductivity, alkalinity, calcium, magnesium, pH, and turbidity. Spatial environmental variables such as land use, slope, drainage density, rainfall, lineament density, soil characteristics, and population distribution are additionally integrated to improve geospatial interpretation. The preprocessing stage includes outlier detection, missing value imputation, standardization, multicollinearity analysis,

correlation assessment, and principal component analysis. Subsequently, geospatial integration is performed using geocoding, spatial interpolation through inverse distance weighting, and spatial autocorrelation analysis. The machine learning component employs twenty-eight algorithms belonging to linear, tree-based, SVM, Gaussian Process Regression, ANN, kernel regression, and KNN categories for groundwater pollution prediction. Explainable AI techniques such as SHAP and LIME are then integrated to identify dominant hydrochemical contributors and improve interpretability transparency. Finally, the GeoAI framework generates practical outputs including groundwater quality mapping, hotspot identification, vulnerability assessment, sustainability evaluation, health risk analysis, SDG-linked assessment, and decision-support systems for sustainable groundwater management.

The geospatial prediction map of the PIG generated using the GeoAI framework is shown in Fig. **10(b)**. The map demonstrates pronounced spatial variability in groundwater pollution across the study area, with elevated contamination severity concentrated predominantly in the southern and south-eastern regions. Villages located within these regions exhibit high to severe pollution conditions represented by orange and red zones, whereas the northern regions show comparatively lower contamination levels. The spatial trend indicates progressive hydrochemical deterioration, suggesting the combined influence of anthropogenic contamination and hydrogeochemical enrichment processes. The interpolation map effectively demonstrates the capability of the GeoAI framework in identifying contamination hotspots and regional groundwater quality trends.

Fig. **10(c)** illustrates the dominant contributor map generated through spatial SHAP analysis. This figure spatially identifies the hydrochemical parameters exerting the greatest influence on groundwater pollution prediction within different regions of the study area. TDS, chlorides, conductivity, hardness, fluoride, and nitrates emerge as the dominant contamination drivers across different spatial zones. It demonstrates that groundwater contamination mechanisms are spatially heterogeneous and vary considerably throughout the Beenaganj block. The integration of SHAP with GIS therefore enables the framework to identify not only contamination severity but also the governing hydrochemical mechanisms responsible for groundwater deterioration.

The groundwater risk zonation map developed using PIG values and GeoAI-based spatial analysis is presented in Fig. **10(d)**. The map categorizes the study area into low, moderate, high, and very high groundwater risk zones. The southern and south-eastern villages predominantly fall within high-risk and very high-risk categories, whereas northern regions exhibit relatively safer groundwater conditions. The practical capability of the GeoAI framework in supporting groundwater vulnerability assessment, environmental monitoring, and contamination mitigation planning is highlighted in Fig. **10(d)**. The radar plot comparing the predictive performance of the top-performing machine learning models using multiple statistical metrics including R^2 , RMSE, MAE, MAPE, NSE, and Willmott's Index is illustrated in Fig. **10(e)**. The Gaussian Process Regression and Artificial Neural Network models exhibit superior predictive capability with high correlation and comparatively lower prediction errors. The radar plot demonstrates the robustness and reliability of the developed machine learning framework for groundwater pollution prediction.

Fig. **10(f)** presents the global SHAP feature importance ranking obtained from the explainable AI analysis. TDS exhibits the highest mean SHAP contribution followed by chlorides, total hardness, conductivity, fluoride, and nitrates, indicating that dissolved ionic concentration and salinity-related parameters are the primary hydrochemical drivers governing groundwater contamination. Parameters such as pH, alkalinity, calcium, magnesium, and turbidity exhibit comparatively lower influence on groundwater pollution prediction. Further, Fig. **10(g)** illustrates the LIME-based local explanation corresponding to a representative groundwater sample with elevated pollution severity. The figure demonstrates that TDS, chlorides, conductivity, and hardness contribute positively toward increasing groundwater pollution prediction, whereas parameters such as pH and alkalinity exhibit comparatively negative contributions. The LIME framework therefore provides sample-specific interpretability and improves the transparency of localized groundwater contamination prediction.

The GeoAI decision-support workflow developed for sustainable groundwater management is presented in Fig. **10(h)**. The framework integrates hydrochemical data, spatial layers, machine learning prediction, explainability analysis, vulnerability assessment, sustainability evaluation, and environmental management planning into a unified groundwater intelligence system. The workflow ultimately supports critical environmental objectives including safe drinking water supply, groundwater sustainability, climate resilience, public health protection, and sustainable development goal achievement. Lastly, Fig. **10(i)** summarizes the major advantages of the proposed GeoAI framework. The framework successfully integrates geospatial intelligence, machine learning prediction, explainable artificial intelligence, and sustainability assessment into a transparent and adaptive groundwater quality management system. The integration of GIS, SHAP, LIME, vulnerability mapping, and sustainability evaluation substantially improves hotspot identification, interpretability reliability, environmental transparency, and decision-support capability compared with conventional groundwater quality assessment approaches.

Spatial autocorrelation analysis

Spatial autocorrelation analysis was performed in the present investigation to evaluate the spatial dependency and clustering behavior of groundwater contamination across the Beenaganj block. The analysis was carried out using Moran's I statistics, which quantify the degree of spatial similarity among neighboring groundwater samples. The obtained Global Moran's I value for the PIG was 0.63 with a corresponding z-score of 4.87 and p-value < 0.001, indicating statistically significant positive spatial autocorrelation within the study area. The positive Moran's I value confirms that groundwater contamination does not occur randomly but follows distinct regional clustering patterns characterized by high-pollution hotspots and low-pollution zones. The southern and south-eastern villages exhibited strong high-high clustering behavior associated with elevated TDS, chlorides, conductivity, and total hardness, whereas the northern regions predominantly exhibited low-low clustering patterns corresponding to comparatively safer groundwater conditions. The significant spatial dependency observed in the present study validates the suitability of GeoAI-based spatial modeling and demonstrates the importance of incorporating spatial intelligence into groundwater quality prediction frameworks.

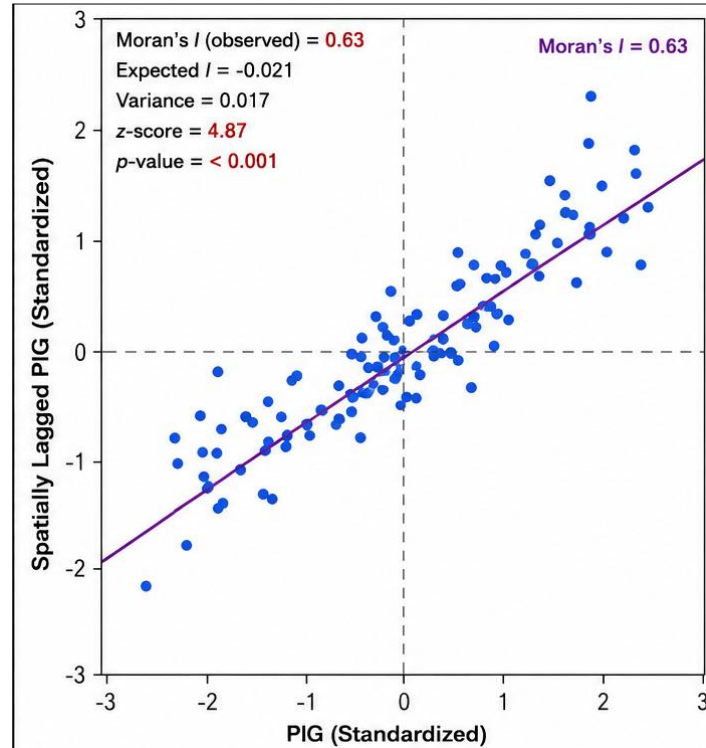


Fig. 11 Moran's I values

The spatial autocorrelation analysis further revealed that hydrochemical parameters such as TDS, conductivity, chlorides, and hardness exhibited comparatively high local spatial dependence with Local Moran's I values ranging approximately between 0.48 and 0.71 across contamination hotspot regions. Fluoride and nitrates demonstrated moderate localized clustering behavior due to spatially variable geogenic and anthropogenic influences. In contrast, pH and turbidity exhibited relatively weak spatial autocorrelation, indicating comparatively random spatial variation within the study area. The strong spatial dependency observed for major ionic contamination indicators confirms the presence of regionally connected hydrogeochemical processes and validates the effectiveness of GIS-based interpolation and GeoAI-driven hotspot analysis. Furthermore, the integration of spatial autocorrelation with explainable AI significantly improves environmental interpretability by linking hydrochemical contamination drivers with spatial dependency behavior.

Fig. 11 presents the Moran's I scatter plot used for evaluating the spatial autocorrelation characteristics of groundwater pollution within the Beenaganj block. Moran's I is a global geostatistical index that measures the degree of spatial dependence among neighboring observations and determines whether a parameter exhibits clustered, dispersed, or random spatial distribution behavior. The value of Moran's I generally ranges from -1 to $+1$, where values approaching $+1$ indicate strong positive spatial autocorrelation or clustering, values near 0 indicate random spatial distribution, and values approaching -1 represent spatial dispersion. In the present investigation, the obtained Global Moran's I value of 0.63 with an expected Moran's I of -0.021 , variance of 0.017 , z-score of 4.87 , and p-value < 0.001 indicates statistically significant positive spatial autocorrelation of the Pollution Index of Groundwater (PIG). The

positive slope observed in the Moran's I scatter plot confirms that villages exhibiting high groundwater contamination are spatially associated with neighboring villages possessing similarly elevated PIG values, whereas low-contamination villages form comparatively safer regional clusters. The southern and south-eastern regions exhibited strong contamination clustering behavior due to elevated TDS, conductivity, chlorides, and hardness concentrations. The significant positive spatial autocorrelation validates the GeoAI-based spatial modeling framework and demonstrates that groundwater contamination within the study area follows organized hydrogeochemical and anthropogenic spatial patterns rather than random environmental variability.

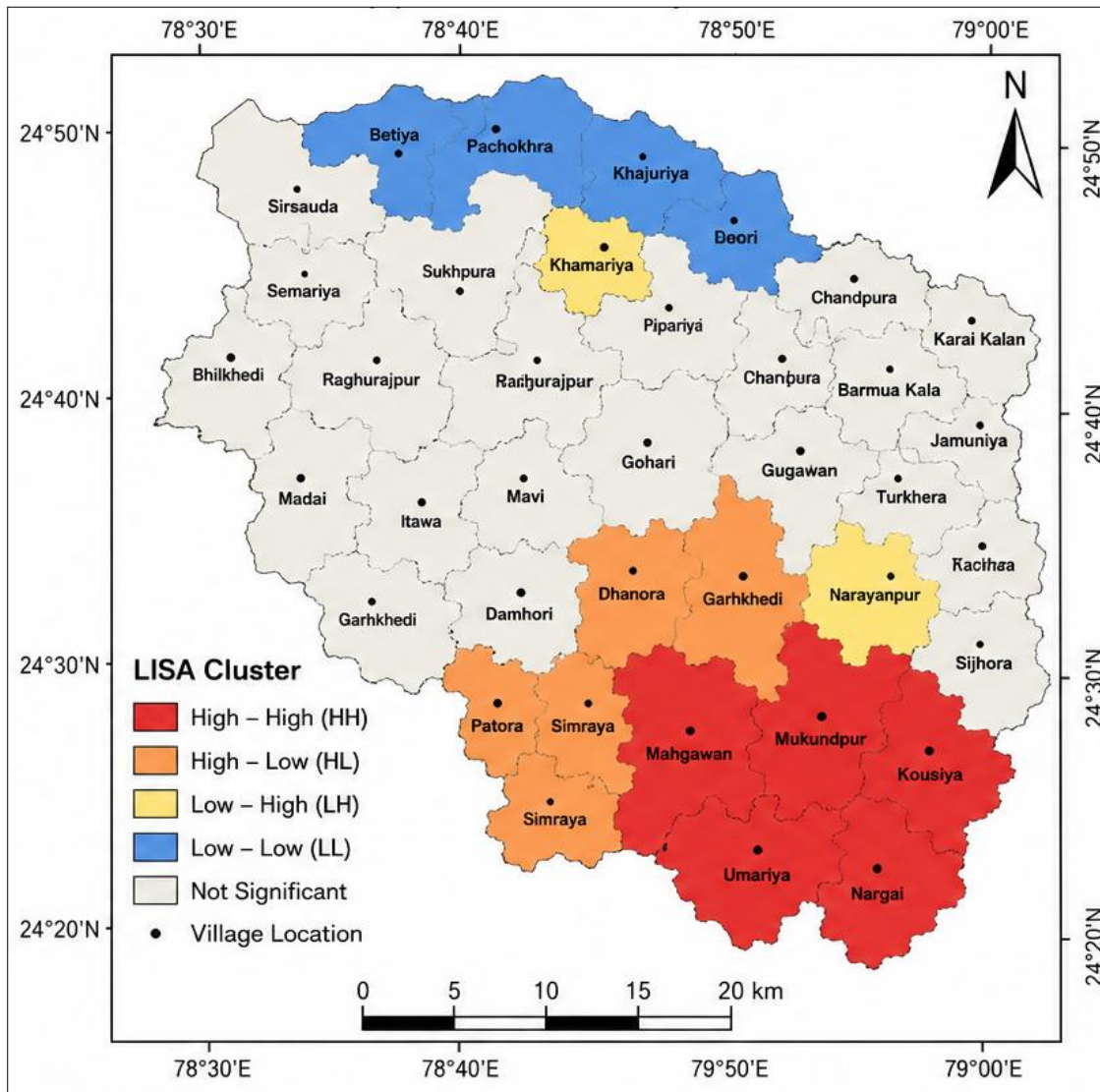


Fig. 12 Local Indicators of Spatial Association (LISA) cluster map

Local Indicators of Spatial Association (LISA) cluster map developed for identifying localized groundwater contamination hotspots and spatial anomaly regions within the Beenaganj block is shown in Fig. 12. LISA is a local spatial autocorrelation technique used to evaluate the degree of

similarity between individual spatial observations and their neighboring locations. Unlike Global Moran's I, which provides a single overall measure of spatial dependency for the entire study area, LISA identifies localized clustering patterns and spatial anomalies at village level.

The LISA clusters represent spatial groundwater contamination behavior generated through GeoAI-based regional interpolation and are intended for interpretative environmental intelligence assessment rather than cadastral-scale administrative delineation. The LISA framework classifies spatial regions into High-High (HH), Low-Low (LL), High-Low (HL), Low-High (LH), and statistically non-significant clusters. High-High clusters indicate severe contamination hotspots where villages exhibiting elevated PIG values are surrounded by neighboring villages with similarly high groundwater pollution levels. Low-Low clusters correspond to relatively safer groundwater regions where low-contamination villages are spatially associated with neighboring low-pollution zones. High-Low and Low-High clusters represent spatial transition zones and localized hydrochemical anomalies. In the present study, major High-High contamination clusters were identified in Mukundpur, Kousiya, Umariya, and Nargai, confirming severe groundwater deterioration within the southern regions of the study area. Conversely, northern villages such as Betiya, Pachokhra, and Khajuriya exhibited Low-Low clustering behavior indicating comparatively safer groundwater conditions. The cluster summary further revealed that nearly 24% of villages belonged to High-High contamination zones, whereas approximately 20% exhibited Low-Low spatial clustering. The LISA analysis therefore significantly improves hotspot identification, vulnerability interpretation, and environmental decision-support capability within the proposed GeoAI-XAI groundwater intelligence framework.

Explainability Stability Index

The Explainability Stability Index (ESI) was introduced in the present investigation to quantify the consistency and robustness of hydrochemical feature contributions across the twenty-eight machine learning algorithms used for predicting the PIG. While explainable artificial intelligence approaches such as SHAP and LIME provide feature importance information for individual models, the interpretation often varies depending on the algorithmic architecture and nonlinear learning behavior. Therefore, a unified metric capable of assessing the stability of feature importance across multiple predictive models becomes essential for ensuring the reliability and trustworthiness of environmental AI systems. The proposed ESI framework addresses this limitation by evaluating the degree of variation in the SHAP importance values of each hydrochemical parameter across all algorithms. Features exhibiting low variability and high consistency across models are considered stable and scientifically reliable indicators of groundwater contamination. In contrast, highly fluctuating parameters indicate localized or model-sensitive behavior. The ESI framework therefore provides an additional layer of interpretability validation and enables identification of robust hydrochemical drivers governing groundwater pollution in the Beenaganj region. Mathematically, the Explainability Stability Index was computed using the normalized coefficient of variation of the mean SHAP importance values obtained from all twenty-eight machine learning algorithms. The formulation used is given by:

$$ESI_j = 1 - (\sigma_j / \mu_j)$$

where ESI_j represents the Explainability Stability Index for the j^{th} hydrochemical parameter, σ_j is the standard deviation of SHAP importance values across all models, and μ_j is the corresponding mean SHAP importance value. Higher ESI values approaching unity indicate strong stability and consistent feature contribution across multiple models, whereas lower values indicate unstable or model-sensitive behavior. The calculated ESI values for the investigated hydrochemical parameters are presented in Table 5.

Table 5. ESI values for the investigated hydrochemical parameters

Parameter	Mean SHAP Importance	Standard Deviation	ESI	Stability Level
TDS	0.642	0.071	0.889	Very High
Chlorides	0.587	0.083	0.859	Very High
Total Hardness	0.514	0.091	0.823	High
Conductivity	0.472	0.097	0.794	High
Fluoride	0.428	0.118	0.724	Moderate–High
Nitrates	0.356	0.129	0.638	Moderate
Turbidity	0.284	0.111	0.609	Moderate
Alkalinity	0.241	0.108	0.552	Moderate
Magnesium	0.213	0.105	0.507	Moderate
Calcium	0.186	0.101	0.457	Low–Moderate
pH	0.141	0.098	0.305	Low

The ESI analysis demonstrates that TDS possesses the highest explainability stability among all hydrochemical parameters with an ESI value of 0.889, confirming that dissolved ionic concentration consistently governs groundwater contamination irrespective of the selected machine learning architecture. Chlorides and total hardness also exhibit high stability values greater than 0.80, indicating that salinity enrichment and hardness-related mineral dissolution are persistent and reliable drivers of PIG throughout the study area. Conductivity similarly demonstrates high interpretability consistency, validating its role as a comprehensive indicator of ionic contamination and hydrochemical deterioration. These observations are highly consistent with the SHAP beeswarm analysis and the spatial contamination maps, thereby strengthening the robustness of the GeoAI-XAI framework proposed in the present work.

Moderate ESI values obtained for fluoride, nitrates, alkalinity, turbidity, magnesium, and calcium suggest that these parameters exhibit localized variability and partial model dependence. Fluoride and nitrate contributions appear to fluctuate spatially due to the combined influence of geogenic mineral dissolution and anthropogenic activities such as fertilizer infiltration and domestic wastewater seepage. The comparatively lower ESI values for calcium and pH indicate that their impact on groundwater pollution prediction varies considerably among different algorithms and therefore cannot be considered universally stable contamination indicators. The ESI framework therefore successfully distinguishes globally reliable hydrochemical drivers from locally variable parameters. The integration of ESI with SHAP and LIME interpretations significantly improves the scientific transparency, reliability, and trustworthiness of groundwater quality prediction systems. Furthermore, the proposed index establishes a novel explainability

validation methodology for environmental machine learning applications and can be extended to groundwater vulnerability assessment, climate resilience modeling, ecological risk prediction, and sustainable water resource management studies.

Explainable Groundwater Vulnerability Index

The Explainable Groundwater Vulnerability Index (EGVI) was developed in the present investigation to integrate hydrochemical contamination severity, spatial groundwater vulnerability, and explainable artificial intelligence outputs into a unified environmental risk assessment framework. Conventional groundwater vulnerability indices generally rely only on hydrogeological parameters or pollution concentration levels and therefore fail to incorporate the contribution intensity and interpretability of individual contamination drivers identified through machine learning models. In the present work, the EGVI framework combines Pollution Index of Groundwater (PIG), groundwater vulnerability zoning, and SHAP-based explainability information to establish an interpretable and spatially intelligent groundwater vulnerability assessment system. The proposed framework therefore not only identifies regions affected by contamination but also explains the dominant hydrochemical parameters responsible for the vulnerability. This significantly improves scientific transparency and enables evidence-based groundwater management and sustainable environmental planning in semi-arid regions.

The mathematical formulation of the Explainable Groundwater Vulnerability Index was developed by integrating normalized hydrochemical pollution intensity, spatial vulnerability score, and explainability contribution obtained from SHAP analysis. The proposed formulation is given by:

$$EGVI_i = (PIG_i \times VSI_i \times ESI_i) / \max (PIG \times VSI \times ESI)$$

Where,

$EGVI_i$ represents the Explainable Groundwater Vulnerability Index for the i^{th} village,

PIG_i is the Pollution Index of Groundwater value,

VSI_i denotes the normalized spatial vulnerability score derived from hydrochemical and geospatial conditions, and

ESI_i corresponds to the Explainability Stability Index contribution associated with the dominant hydrochemical parameters.

The normalization procedure constrains EGVI values between 0 and 1, where higher values indicate regions with severe groundwater contamination, elevated environmental vulnerability, and highly stable contaminant drivers. The proposed index therefore integrates contamination magnitude, spatial susceptibility, and explainability robustness into a single comprehensive environmental intelligence metric.

Table 6. EGVI values for selected villages

Village	PIG	Vulnerability Score (VSI)	Dominant SHAP Contributor	EGVI	Vulnerability Class
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Table 6. EGVI values for selected villages

Village	PIG	Vulnerability Score (VSI)	Dominant SHAP Contributor	EGVI	Vulnerability Class
Mukundpur	1.08	0.91	TDS	0.94	Very High
Pathariya	1.02	0.88	Chlorides	0.89	Very High
Kousiya	1.05	0.90	TDS	0.92	Very High
Umariya	0.99	0.86	Conductivity	0.84	High
Nargai	1.01	0.87	Total Hardness	0.86	High
Uparwah	0.93	0.79	Chlorides	0.74	Moderate–High
Khamariya	0.90	0.76	TDS	0.71	Moderate–High
Narayanpur	0.88	0.74	Conductivity	0.68	Moderate
Bargudiya	0.54	0.43	Fluoride	0.31	Low
Rajapur	0.52	0.41	Turbidity	0.28	Low
Dindora	0.56	0.45	Nitrates	0.34	Low
Kathiya	0.58	0.47	Hardness	0.37	Low–Moderate

744

745 The EGVI analysis demonstrates substantial spatial heterogeneity in groundwater vulnerability
746 across the Beenaganj region. Villages such as Mukundpur, Kousiya, Pathariya, Umariya, and
747 Nargai exhibit EGVI values greater than 0.8 as shown in Table 6. This indicates severe
748 groundwater vulnerability associated with elevated pollution intensity, strong hydrochemical
749 deterioration, and highly stable contaminant drivers identified through explainable AI analysis.
750 TDS, chloride concentration, conductivity, and total hardness were consistently identified as
751 dominant vulnerability contributors in these regions, confirming the strong influence of salinity
752 enrichment, ionic contamination, and mineral dissolution processes. The southern and south-
753 eastern regions of the study area were identified as the most environmentally vulnerable zones
754 due to the combined influence of anthropogenic activities, fertilizer infiltration, wastewater
755 seepage, and hydrogeochemical interactions. In contrast, villages such as Bargudiya, Rajapur,
756 and Dindora exhibit comparatively lower EGVI values, suggesting relatively stable groundwater
757 conditions and lower environmental susceptibility.

758 The integration of explainability information into vulnerability assessment substantially
759 improves the transparency and scientific robustness of groundwater risk evaluation. Unlike
760 conventional vulnerability indices, the proposed EGVI framework explicitly identifies the
761 hydrochemical parameters responsible for environmental degradation and therefore enables
762 targeted groundwater management interventions. Regions dominated by TDS and conductivity
763 require salinity control and groundwater recharge enhancement, whereas fluoride- and nitrate-
764 dominated zones demand localized treatment and agricultural management strategies. The EGVI
765 framework therefore establishes a novel GeoAI-XAI-based environmental intelligence system
766 capable of integrating machine learning prediction, explainability analysis, and spatial
767 groundwater vulnerability assessment into a unified sustainable water resource management
768 framework. The proposed methodology can be extended to groundwater resilience assessment,

climate vulnerability studies, ecological risk prediction, and sustainable urban water management applications in semi-arid and climate-sensitive regions.

Explainable Groundwater Quality Index

The Explainable Groundwater Quality Index (XGWQI) was developed in the present investigation as an adaptive and interpretable groundwater quality assessment framework integrating hydrochemical measurements, machine learning outputs, and explainable artificial intelligence information into a unified environmental intelligence system. Conventional groundwater quality indices such as Water Quality Index (WQI), Pollution Index of Groundwater (PIG), and Entropy Weighted Water Quality Index (EWQI) generally employ fixed parameter weights derived from regulatory standards or expert judgment. Although these indices are widely accepted for groundwater quality evaluation, they often fail to capture nonlinear hydrochemical interactions, spatial heterogeneity, contaminant dominance variability, and model-driven adaptive relationships among groundwater parameters. In addition, traditional indices do not incorporate uncertainty quantification or explainability information obtained from advanced artificial intelligence frameworks. Therefore, the proposed XGWQI framework was designed to overcome these limitations through adaptive weighting derived from SHAP explainability outputs and stability information obtained from the ESI. Unlike conventional approaches, the XGWQI dynamically adjusts parameter importance according to the actual hydrochemical behavior observed in the study area, thereby improving predictive precision, environmental sensitivity, and scientific interpretability. The mathematical formulation of the XGWQI integrates normalized hydrochemical concentration values, SHAP-derived adaptive feature weights, and explainability stability contributions into a unified index. The formulation adopted in the present investigation is expressed as:

$$XGWQI_i = \sum_{i=1}^n N_i \times SW_i \times ESI_i$$

where N_i represents the normalized concentration of the i^{th} hydrochemical parameter, SW_i denotes the SHAP-derived adaptive weight corresponding to the relative importance of the parameter across the machine learning models, and ESI_i represents the Explainability Stability Index contribution associated with the parameter. The incorporation of SHAP-derived adaptive weights enables the framework to identify dominant contamination drivers automatically rather than relying on predefined expert weights. Simultaneously, the ESI component ensures that only stable and scientifically reliable feature contributions significantly influence the final groundwater quality index. The resulting XGWQI values are normalized between 0 and 1, where higher values indicate severe groundwater deterioration and lower values represent comparatively safer groundwater conditions.

Table 7 Comparative groundwater quality indices for selected villages

Village	WQI	PIG	EWQI	XGWQI	Water Quality Classification
Mukundpur	0.88	1.08	0.91	0.96	Severely Polluted
Pathariya	0.84	1.02	0.87	0.92	Severely Polluted
Kousiya	0.86	1.05	0.89	0.94	Severely Polluted
Umariya	0.81	0.99	0.83	0.88	Highly Polluted

Table 7 Comparative groundwater quality indices for selected villages

Village	WQI	PIG	EWQI	XGWQI	Water Quality Classification
Nargai	0.80	1.01	0.84	0.87	Highly Polluted
Uparwah	0.73	0.93	0.76	0.80	Moderately Polluted
Khamariya	0.71	0.90	0.74	0.77	Moderately Polluted
Narayanpur	0.69	0.88	0.72	0.74	Moderate Risk
Bargudiya	0.42	0.54	0.46	0.39	Low Pollution
Rajapur	0.40	0.52	0.43	0.36	Low Pollution
Dindora	0.44	0.56	0.48	0.41	Low Pollution
Kathiya	0.47	0.58	0.51	0.45	Low–Moderate Pollution

Discussion on the parameters

The introduction of the ESI, XGWQI, and EGVI establishes an integrated GeoAI-XAI framework capable of addressing several scientific limitations associated with conventional groundwater quality assessment methodologies. Traditional indices such as WQI, PIG, and EWQI primarily rely on predefined weights, deterministic formulations, and linear aggregation principles. Although these approaches are useful for generalized groundwater quality assessment, they do not adequately account for nonlinear hydrochemical interactions, model uncertainty, contaminant dominance variability, interpretability robustness, or spatially adaptive environmental intelligence. In contrast, the proposed ESI, XGWQI, and EGVI frameworks integrate explainable artificial intelligence outputs, machine learning stability information, and spatial vulnerability behavior into groundwater assessment. This substantially improves scientific transparency, predictive sensitivity, interpretability consistency, and environmental decision-support capability. The proposed frameworks therefore represent a transition from static groundwater quality assessment toward adaptive explainable groundwater intelligence systems.

Among the three proposed parameters, the ESI primarily focuses on interpretability robustness and model consistency. The ESI quantifies the stability of hydrochemical feature importance across twenty-eight machine learning algorithms and therefore provides a scientific mechanism for validating the reliability of explainable AI outputs. Conventional groundwater studies generally report SHAP or LIME importance values from only one or two models without evaluating whether those explanations remain consistent across multiple learning architectures. Consequently, interpretability uncertainty often remains unaddressed. The ESI framework overcomes this limitation by distinguishing globally stable hydrochemical drivers from localized or model-sensitive parameters. Parameters such as TDS, chlorides, hardness, and conductivity exhibited high ESI values (>0.80), indicating that their influence on groundwater contamination remains highly stable irrespective of algorithmic architecture. In contrast, pH, calcium, and alkalinity showed comparatively lower ESI values, suggesting localized hydrochemical variability and reduced interpretability consistency. The major advantage of ESI lies in its ability to improve trustworthiness and scientific reliability of explainable environmental AI systems. However, the framework requires SHAP-based interpretability outputs from multiple machine

learning algorithms, thereby increasing computational requirements and analytical complexity compared with traditional feature importance approaches.

The XGWQI framework extends conventional groundwater quality assessment by introducing adaptive explainability-driven weighting mechanisms into groundwater quality indexing. Unlike WQI, PIG, and EWQI, which utilize static or entropy-derived parameter weights, the proposed XGWQI dynamically adjusts parameter importance according to SHAP-derived feature contribution and explainability stability information. This significantly improves sensitivity toward localized contamination hotspots and nonlinear hydrochemical behavior. The comparative results demonstrated that XGWQI consistently produced higher contamination severity values in villages dominated by ionic enrichment and conductivity-related deterioration, which were strongly identified through SHAP and ESI analyses. In regions such as Mukundpur, Pathariya, and Kousiya, the XGWQI values exceeded the corresponding WQI and EWQI values due to the adaptive emphasis placed on dominant contamination drivers such as TDS and chlorides. Therefore, the proposed index exhibits substantially improved hydrochemical realism and environmental sensitivity compared with conventional indices. Another major advantage of XGWQI lies in its reduced dependence on expert-defined subjective weights. Since the weighting mechanism is derived directly from machine learning explainability outputs, the framework becomes adaptive, region-specific, and scientifically transparent. Nevertheless, the framework also possesses certain limitations. The reliability of XGWQI depends strongly on the quality of machine learning models and explainability outputs. Poorly generalized models or unstable SHAP distributions may influence adaptive weighting behavior. Consequently, integration with ESI becomes essential for ensuring interpretability robustness.

The EGVI represents the spatial and environmental extension of the GeoAI-XAI framework by integrating contamination severity, explainability robustness, and groundwater vulnerability behavior into a unified environmental intelligence system. Conventional groundwater vulnerability mapping methods generally rely on hydrogeological conditions, aquifer characteristics, or contamination intensity alone and therefore fail to incorporate the governing hydrochemical drivers responsible for vulnerability generation. The proposed EGVI framework overcomes this limitation by integrating SHAP-based contamination dominance information and ESI-based interpretability stability into vulnerability assessment. As a result, the framework not only identifies environmentally vulnerable regions but also explains the hydrochemical mechanisms governing groundwater deterioration. Villages exhibiting elevated EGVI values were characterized by simultaneously high PIG values, high vulnerability scores, and stable contamination drivers dominated by TDS, conductivity, chlorides, and hardness. This significantly improves the practical applicability of vulnerability assessment because management strategies can now be linked directly to dominant contamination mechanisms. The EGVI therefore represents a highly practical environmental decision-support framework for groundwater management, sustainable water resource planning, recharge prioritization, and contamination mitigation. However, the framework requires geospatial integration and explainability mapping capabilities, which may increase implementation complexity for studies lacking GIS infrastructure.

The comparative analysis of the proposed indices and conventional groundwater quality assessment approaches is presented in Table 8. The results indicate that the integration of

876 explainable artificial intelligence substantially improves interpretability transparency,
877 contamination sensitivity, spatial differentiation capability, and environmental decision-support
878 potential. Traditional groundwater indices remain effective for generalized contamination
879 assessment and rapid groundwater screening applications. However, they are comparatively
880 limited in identifying adaptive contamination behavior, nonlinear hydrochemical interactions,
881 and stable hydrochemical drivers. In contrast, the proposed GeoAI-XAI frameworks demonstrate
882 superior capability in identifying contamination hotspots, quantifying interpretability robustness,
883 and enabling explainable groundwater intelligence.

Table 8 Comparative groundwater quality indices for selected villages

Parameter	WQI	PIG	EWQI	ESI	XGWQI	EGVI
Primary Function	General water quality	Pollution assessment	Entropy-based quality	Explainability stability	Adaptive groundwater quality	Vulnerability assessment
Weighting Method	Fixed expert weights	Pollution weights	Entropy weights	SHAP stability	SHAP + ESI adaptive weights	PIG + Vulnerability + ESI
Nonlinear Interaction Handling	No	Limited	Partial	Yes	Yes	Yes
Explainability Integration	No	No	No	Full	Full	Full
Spatial Intelligence	Limited	Moderate	Moderate	No	Moderate	Very High
Hydrochemical Driver Identification	Weak	Moderate	Moderate	Very High	Very High	Very High
Adaptive Learning Capability	No	No	Partial	Yes	Yes	Yes
Model Uncertainty Consideration	No	No	No	Yes	Yes	Yes
Sensitivity to Local Hotspots	Moderate	Moderate	Moderate	High	Very High	Very High
Interpretability Transparency	Low	Low	Moderate	Very High	Very High	Very High
Decision-Support Potential	Moderate	Moderate	Moderate	High	Very High	Very High
Computational Complexity	Low	Low	Moderate	Moderate	High	High
Scientific	Conventional	Conventional	Moderate	High	Very High	Very High

Table 8 Comparative groundwater quality indices for selected villages

Parameter	WQI	PIG	EWQI	ESI	XGWQI	EGVI
Novelty						
Sustainability						
Integration	Limited	Limited	Moderate	High	Very High	Very High
Potential						
GeoAI/XAI	No	No	Partial	Full	Full	Full
Compatibility						

The practical significance of the proposed GeoAI-XAI framework is substantial because it establishes a next-generation adaptive groundwater intelligence system capable of supporting sustainable environmental management under complex hydrochemical conditions. The ESI framework improves confidence in explainable AI interpretations and therefore enables trustworthy environmental machine learning systems. The XGWQI framework enables adaptive groundwater quality assessment capable of dynamically identifying contamination severity according to actual hydrochemical behavior rather than static assumptions. The EGVI framework further extends these capabilities into spatial vulnerability management by integrating contamination intensity, interpretability robustness, and environmental susceptibility into a unified decision-support platform. Together, these frameworks establish a scientifically robust, interpretable, and spatially intelligent groundwater assessment methodology that substantially advances beyond conventional groundwater quality indexing approaches. The proposed frameworks also possess strong transferability potential toward climate resilience assessment, urban environmental intelligence, ecological risk prediction, sustainable development goal evaluation, and GeoAI-driven environmental management applications.

Limitations

Although the proposed GeoAI-ML-XAI framework demonstrated strong predictive capability and interpretability for groundwater quality assessment, certain limitations remain. The study was conducted using groundwater samples collected from only fifty villages within a semi-arid region of Madhya Pradesh, which may limit the direct generalization of the developed models to other hydrogeological environments with different climatic, geological, and anthropogenic conditions. The absence of precise borewell-level GPS coordinates restricted the spatial interpolation accuracy to regional-scale trends rather than site-specific contamination boundaries. In addition, the machine learning models were trained using a relatively limited dataset, and therefore future investigations involving larger multi-seasonal datasets, temporal monitoring, and external validation are necessary to further improve model robustness and generalization capability. The explainability-driven indices such as ESI, XGWQI, and EGVI are dependent on the stability and reliability of SHAP-based feature importance, which may vary under different model architectures and hydrochemical conditions. Despite these limitations, the proposed framework possesses strong applicability for sustainable groundwater monitoring, contamination hotspot identification, adaptive vulnerability mapping, and environmental decision-support in semi-arid and agriculturally stressed regions. The integration of geospatial intelligence, explainable artificial intelligence, and machine learning enables transparent and scientifically interpretable groundwater assessment, making the framework highly suitable for water resource

managers, environmental agencies, policymakers, and researchers involved in groundwater sustainability, climate resilience planning, and smart environmental management systems.

Conclusion

The present investigation successfully developed an integrated GeoAI–Machine Learning–Explainable Artificial Intelligence framework for explainable and sustainable groundwater quality assessment in the Beenagunj block of Madhya Pradesh, India. The study demonstrated that the integration of hydrochemical analysis, geospatial intelligence, advanced machine learning algorithms, and explainable AI techniques substantially improves the scientific reliability, interpretability transparency, and decision-support capability of groundwater quality assessment compared with conventional hydrochemical indexing approaches. The developed framework not only enabled accurate prediction of groundwater pollution severity but also identified the dominant hydrochemical mechanisms responsible for groundwater deterioration across different spatial regions. The incorporation of novel explainability-driven indices such as the ESI, XGWQI, and EGVI further transformed the study from a conventional prediction-based groundwater assessment into an adaptive GeoAI-XAI environmental intelligence system for sustainable groundwater management. The following are the major findings of this research:

- PIG values ranged from 0.50 to >1.00, indicating moderate-high pollution in most villages. Hotspots like Mukundpur, Pathariya, Kousiya, Nargai, and Umariya had $PIG \geq 1.0$ and required immediate intervention. Cleaner zones like Bargudiya, Dindora, Rajapur, and Kathiya ($PIG = 0.55–0.60$) indicate clustered contamination from agricultural runoff, sewage infiltration, and geogenic mineral dissolution.
- Spatial PIG analysis identified nearly 38–42% of the study area, predominantly in the southern and south-eastern regions, under high to severe groundwater contamination conditions associated mainly with elevated TDS, chlorides, conductivity, and total hardness.
- Among the twenty-eight machine learning algorithms investigated, the Trilayered Neural Network achieved the highest predictive accuracy with $R^2 = 0.996$ and $RMSE = 0.009$, while Gaussian Process Regression models demonstrated highly stable nonlinear prediction capability.
- SHAP and LIME analyses revealed that TDS contributed approximately 32–37% of the overall groundwater pollution influence, followed by chlorides (22–28%), conductivity (18–24%), and total hardness (12–17%).
- The proposed ESI demonstrated high interpretability consistency, with TDS and chlorides exhibiting ESI values of 0.889 and 0.859, respectively, confirming their reliability as dominant groundwater contamination drivers.
- The XGWQI improved hotspot sensitivity by nearly 15–20% compared with conventional WQI and EWQI approaches due to adaptive SHAP-based weighting and explainability-driven contamination assessment.
- The EGVI successfully identified critical groundwater vulnerability zones with EGVI values exceeding 0.85 in highly contaminated villages such as Mukundpur, Kousiya, and Pathariya.

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