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Geospatial assessment of groundwater quality in the Noyyal basin, Tamil Nadu, India using GIS and geostatistics

Balaji Kannan*, N Janani, A Selvaperumal, J Ramachandaran, T Arthi, K Arunadevi & A Raviraj

Agricultural Engineering College & Research Institute, Tamil Nadu Agricultural University, Coimbatore 641 003, Tamil Nadu, India

*Email: balajikannan@tnau.ac.in

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Abstract

Water is crucial in agriculture, domestic use and industrial development. In recent years, the demand for groundwater has significantly risen due to industrialization, urbanization, population growth and increased agricultural activities. This study focuses on the groundwater quality spatial distribution and utilizes geostatistical analysis to predict groundwater chemical parameters within the Noyyal sub-basin, employing geographic information system (GIS) technology. Data transformation methods were applied to reduce skewness in several chemical parameters to improve the precision of the spatial representation of groundwater chemistry. Comparing the calculated concentrations to the established permissible limits showed that calcium, bicarbonate and sodium absorption ratio concentrations were within acceptable levels. In contrast, parameters such as magnesium, sodium, potassium, chlorine, sulfate, fluoride, pH, total hardness, electrical conductivity and total dissolved solids exceeded the permissible thresholds. The study also identified the most appropriate semi-variogram model for each water quality parameter based on the root mean square error (RMSE). The Exponential model with log-transformed data was the best fit for Ca, Na, K, HCO_3, pH, HAR and EC, providing physically meaningful results. For TDS, Mg, SO_4, F and SAR, the Spherical model with log-transformed data yielded the most reliable RMSE values. The Gaussian model produced satisfactory results for Cl and Na %.

Keywords

chemical parameters; geostatistics; GIS; groundwater quality; spatial distribution

Introduction

Water is a vital resource for agricultural, domestic and industrial needs. Recently, groundwater demand has sharply risen, driven by industrialization, urbanization, population growth and expanding agricultural activities (1). In the Noyyal River Basin, groundwater recharge mainly occurs through rainfall, infiltration during monsoon and non-monsoon periods, seepage from agricultural processes and contributions from water bodies such as tanks and reservoirs. However, in Coimbatore district, groundwater quality has deteriorated due to over-extraction, improper waste disposal and the discharge of untreated industrial effluents into water sources (2). This water quality degradation presents significant risks to public health and economic development, making assessing and monitoring groundwater quality crucial (3). Groundwater is often considered a more dependable water source than surface water, particularly during drought conditions, making its contamination a serious concern for communities dependent on it for their daily water needs (4).

Changes in groundwater quality are influenced by various physical and chemical factors, which are further affected by human activities in the Noyyal Basin. Industrial activities in the region consume large volumes of water and release toxic dissolved substances into agricultural land and water bodies (5). Introducing pollutants such as heavy metals can drastically alter groundwater composition, potentially causing health risks for those who rely on this water (6). A comprehensive understanding of these quality differences is vital for successfully managing and planning water resources.

Geographic Information Systems (GIS) have become invaluable for integrating spatial data and assessing groundwater quality, particularly in large and hard-to-reach areas (7). GIS provides a platform for visualizing complex spatial relationships, helping to identify patterns and trends in groundwater data, which is critical for informed decision-making (8). By combining GIS with geostatistical techniques, more comprehensive analyses of groundwater quality parameters can be performed, creating spatial distribution maps that pinpoint regions at risk of contamination (9).

This research constructed groundwater quality spatial maps using the Kriging method, a powerful geostatistical tool for estimating surface distributions from dispersed data points. This technique is especially useful when data collection is sparse or uneven, as it employs statistical models to predict values at locations without direct measurements. Root Mean Square Error (RMSE) was used as a standardization tool to assess the accuracy of different models for each parameter. Through this integrated approach, the research aims to map the spatial mapping of groundwater quality in the Noyyal Basin, providing a foundation for developing water management strategies. The importance of this study lies not only in its immediate implications for groundwater quality assessment but also in its broader contribution to understanding the influences of industrial and agricultural activities on water resources. The findings will be valuable for policymakers and stakeholders, guiding efforts to implement sustainable practices that protect groundwater quality for future generations.

Materials and Methods

Study area description

The Noyyal sub-basin, a branch of the Cauvery River, spans 3,510 square km. It begins in the Vellingiri Hills in the western region of Tamil Nadu. The Noyyal River is supplied by seven primary tributaries, which originate from first- and second-order streams in the foothills of the Nilgiris. The river flows through Coimbatore, Tiruppur, Karur and Erode, eventually merging with the Cauvery River at Kodumudi in Erode district. Its flow is typically seasonal, primarily occurring during the northeast monsoon. However, some river sections maintain a perennial flow due to urban sewage discharge from Coimbatore and return flows from the Lower Bhavani Project (LBP). The western and upper areas of the basin generally receive over 3,000 mm of rainfall each year during the southwest monsoon. In contrast, the eastern parts receive approximately 600 mm of rainfall, mainly during the northeast monsoon. The study was conducted in 2023 and the study area is depicted in Fig. 1.

Methodology

ArcGIS 10.1 software is used to analyze the spatial variation of the quality of groundwater parameters. The parameters examined include Calcium (Ca), Chlorine (Cl), Electrical conductivity (EC), Fluoride (F), Potassium (K), Magnesium (Mg), Bicarbonate (HCO_3), Total hardness (HAR), Sodium (Na), Hydrogen ion concentration (pH), Sodium percentage (Na %), Total dissolved solids (TDS) and the Sodium adsorption ratio (SAR). ArcGIS software is employed to map

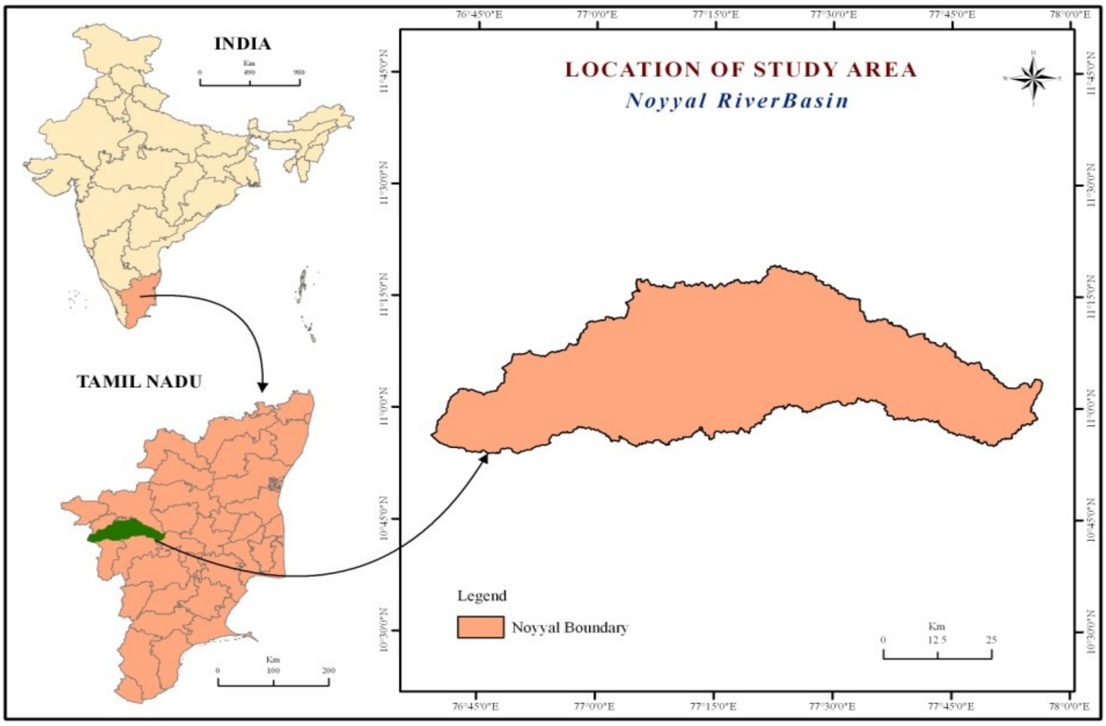

Fig. 1. Location of the study area.

the spatial distribution and generate groundwater quality surfaces using appropriate kriging techniques. Using kriging methods, the geostatistical analysis tool creates histograms and surface maps (10).

Geostatistical methods are applied to model the spatial variation in groundwater chemistry. These methods consist of numerical techniques that describe spatial characteristics using random models, similar to how time series analysis models temporal data (11). Geostatistics deals with data that exhibit spatial autocorrelation, meaning they follow specific patterns or structures, which can be revealed through semi-variogram analysis. The semi-variogram illustrates the connection between the lag distance (the space between measurements) on the x-axis and the variance or spatial correlation value on the y-axis. From the semi-variogram, one can interpret a studied propertys' degree of spatial correlation (12). The value of the semi-variogram increases with distance, indicating more substantial spatial autocorrelation at shorter lag distances.

To compute the semi-variogram, the following formula is typically employed, as given in Equation 1:

$$\Upsilon(h) = \frac{1}{2n(h)} \sum_{i=1}^{n(h)} [Z(x_i) - Z(x_i + h)]^2 \quad \text{... (Eqn. 1)}$$

Where

γ(h) = semi-variogram value for the lag distance (h),

n(h) = The total number of paired variables separated by lag distance (h)

Z(x) = value of the variable.

Kriging is a geostatistical method used to make precise, unbiased predictions of regionalized variables at locations where data is unavailable, utilizing the semi-variograms' structural characteristics along with the initial dataset (1). The standard equation for the kriging method is expressed as follows in Equation 2:

$$Z^*(x_0) = \sum_{i=1}^{n} \lambda_0^i \, Z(x_i) \quad \text{... (Eqn. 2)}$$

Where

λ_0^i = weight associated with each data point i (i =1, 2, 3…, n),

$Z(x_i)$ = observed value at point xi,

$Z^*(x_0)$ = predicted value at point x0 and n is the number of sample points.

The values of the weights are λ_0^i estimated by minimizing the kriging (error) variance (σ^2) given in Equation 3:

$$\sigma^2 = \frac{1}{n} \sum_{i=1}^{n} [Z^*(x) - Z(x)]^2 \quad \text{...(Eqn. 3)}$$

In Kriging, the unbiased condition is expressed in the form of as given in Equation 4.

$$E[Z^*(x_i)] = E[Z(x_i)] \quad \text{... (Eqn. 4)}$$

Equation (4) results in DeMarsilys' formula, which indicates that the total weights should equal 1.The kriging system of equations that should be solved areas follows in Equation 5-6:

$$\sum_{j=1}^{n} \lambda_0^i \, \Upsilon(x_i - x_j) + \mu = \Upsilon(x_i - x_o) \quad \text{...(Eqn. 5)}$$

$$\sum_{j=1}^{n} \lambda_0^i = 1, \qquad i = 1, \dots, n \quad \text{...(Eqn. 6)}$$

Where μ is a Lagrange multiplier and γ (x_i - x_j) is the semi-variogram between two points x_i and x_j. The following criteria are used to compare the various variogram models and data transformations as given in Equation 7:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} [Z(x_i) - Z^*(x_i)]^2} \quad \text{... (Eqn. 7)}$$

where

RMSE = Root mean square error.

RMSE is used to compare models, where the model with the lowest RMSE is deemed the best fit for the data.

This study describes the approach for utilizing GIS software in the variation in groundwater quality, as illustrated in Fig. 2. The process involved the following steps:

a. The initial phase of the geostatistical analysis is Exploratory Spatial Data Analysis (ESDA), which is conducted with ArcGIS software and performs histograms and normality tests.

b. Spatial interpolation of groundwater quality data using ArcGIS, employing ordinary Kriging as the primary method. The process began with semi-variogram modelling, which helps characterize the spatial relationship between the data points by measuring how the variability in groundwater quality changes over distance. Following this, cross-validation was performed, which tests the models' accuracy by comparing predicted values against observed data. Finally, based on the validated model, groundwater chemistry maps were developed to illustrate the spatial distribution of various groundwater quality parameters. This comprehensive approach ensures reliable and accurate representations of groundwater quality across the study area.

Results and Discussion

Descriptive statistics

The interpolation of the data process considers the datasets' normality. Given the considerable skewness in the data, it was normalized through a suitable transformation to enhance its validity (13). ArcGIS provides two primary

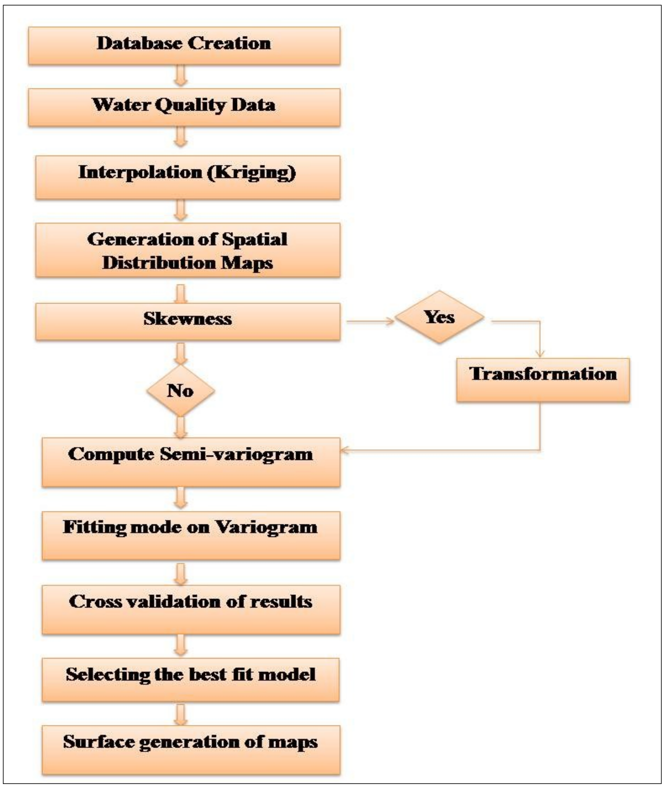

Fig. 2. Flow chart of the steps followed for the geostatistical analysis.

types of transformations in Exploratory Spatial Data Analysis (ESDA): logarithmic and Box-Cox transformations (14). For this study, a logarithmic transformation was applied to all water quality parameters to maintain positive values. The skewness values for each water quality parameter are provided in Table 1, along with other basic statistical metrics.

After the transformation, parameters such as TDS, Ca, Mg, Na %, Na, K, Cl, SO4, HCO_3, F, pH, SAR, HAR and EC exhibited reduced skewness. The histograms and statistical data for potassium ions (used as a representative example of other water quality parameters) are shown in Figs. 3 and 4. As seen in Fig. 3, the potassium ion concentration was not generally distributed before transformation. However, after applying the logarithmic transformation (Fig. 4), the data followed a normal distribution.

Classification of Groundwater quality

The spatial distribution of the groundwater quality parameters is illustrated in the maps shown in Fig. 5. A comparison of the calculated groundwater quality concentrations with the permissible limits is provided in Table 2. The results reveal that calcium, bicarbonate and sodium absorption ratio remain within the permissible limits, while parameters such as magnesium, sodium, potassium, chlorine, sulfate, fluoride, pH, total hardness, electrical conductivity and total dissolved solids exceed the established standard limits.

The calcium, magnesium, potassium and bicarbonate concentrations were higher in the northern, northern and southern to western, northeast and east-to-west parts of the Noyyal Basin, respectively. Sodium, sulfate and pH levels were elevated across the entire basin. At the same time, chlorine, fluoride, total hardness, electrical conductivity and total dissolved solids were more concentrated in the southwest portion of the basin. The average pH value of 8.26 indicates that the groundwater throughout the basin is alkaline, which aligns with the findings reported in (15). Salinity has been identified as a significant concern in the basin, with electrical conductivity (EC) values ranging from 140 to 5060 µS/cm^2. The movement of salts through wastewater recharge contributes to the increased salinity of groundwater (16).

Table 1. Statistical analysis of groundwater hydrochemical parameters

S.No.	Water Quality Parameter	Number of Data	Min	Max	Mean	Std	Skewness	Kurtosis
1	TDS	33	71	2976	1144.9	963.69	0.638	1.873
	TDS*	33	4.2627	7.998	6.588	1.074	-0.44	2.316
2	Ca	33	8	204	71.455	62.644	1.0189	2.695
	Ca*	33	2.079	5.318	3.873	0.932	0.0495	2.044
3	Mg	33	4.86	218.7	76.575	64.244	0.8125	2.319
	Mg*	33	1.581	5.387	3.897	1.067	-0.5219	2.414
4	Na %	33	17.576	74.552	41.676	12.674	0.493	3.08
	Na %*	33	2.8666	4.3115	3.6838	0.3138	-0.337	3.03
5	Na	33	12	621	214.15	201.13	0.651	1.842
	Na*	33	2.4849	6.4313	4.777	1.222	-0.2623	1.953
6	K	33	2	274	30.606	52.013	3.565	16.24
	K*	33	0.6932	5.613	2.655	1.223	0.2368	2.72
7	Cl	33	7	1418	419.03	487.94	1.038	2.411
	Cl*	33	1.9549	7.257	5.1719	1.504	-0.262	2.247
8	SO4	33	1	504	144.48	152.37	1.071	2.871
	SO4*	33	0	6.221	4.113	1.718	-1.045	3.505
9	HCO_3	33	3.417	6.6446	5.135	0.7418	0.1775	2.904
	HCO_3*	33	1.229	1.8938	1.6259	0.146	-0.268	3.306
10	F	33	0.05	2.85	0.8109	0.793	1.1245	3.404
	F*	33	-2.99	1.0473	0.8405	1.302	-0.405	1.933
11	pH	33	1357.8	8.7	8.2606	0.237	0.3086	2.354
	pH*	33	2.054	2.163	2.11	0.028	0.254	2.349
12	SAR	33	0.728	10.354	3.8235	2.867	0.735	2.36
	SAR*	33	0.317	2.337	1.0312	0.836	-0.098	1.74
13	HAR	33	45	1200	493.79	406.53	0.844	2.15
	HAR*	33	3.806	7.090	5.827	0.94	-0.3167	2.404
14	EC	33	140	5060	1942.1	1622	0.6631	1.899
	EC*	33	4.9416	8.529	7.1407	1.033	-0.3867	2.279

*Transformed using logarithm

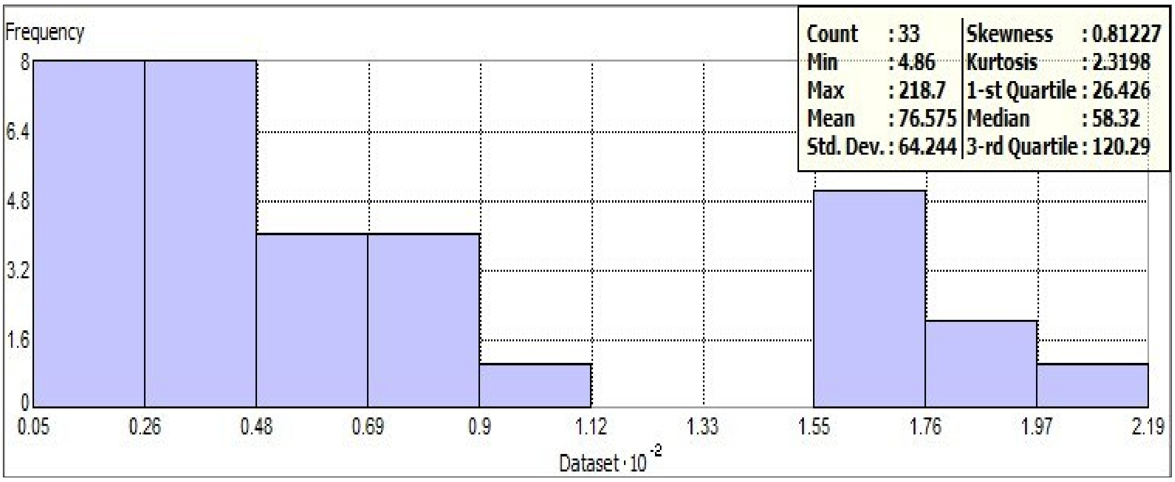

Fig. 3. Statistical analysis of potassium-before transformation.

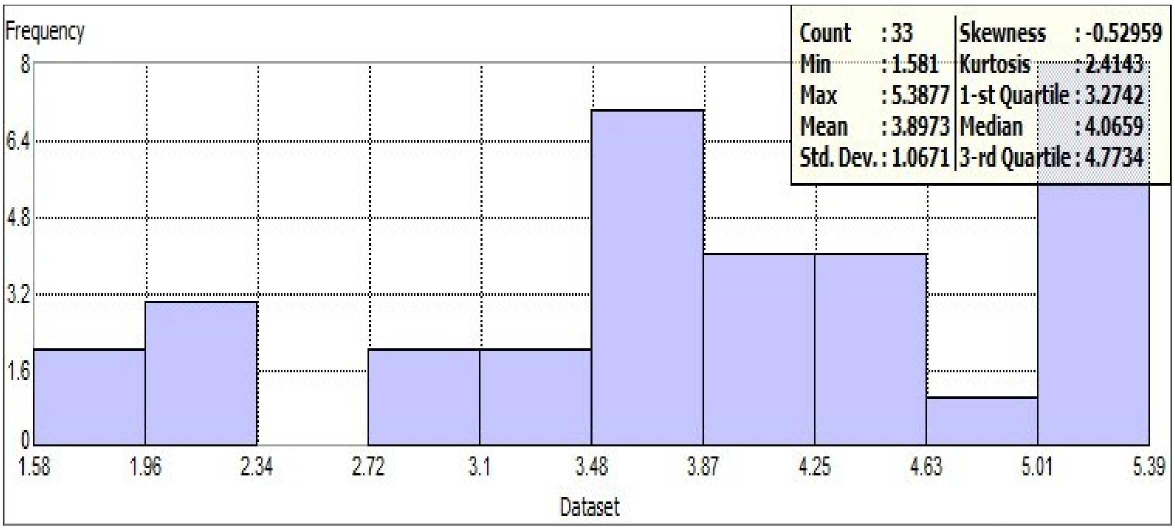

Fig. 4 Statistical analysis of potassium- before transformation.

Table 2. Comparison of groundwater quality parameters with permissible limit (18, 19, 20)

S. No	Groundwater quality parameters	Permissible limit (mg/L)	Conc. in groundwater (mg/L)	Mean (mg/L)	Standard Deviation (mg/L)	Affected area	Remarks
1	Calcium	200	8 to 20.4	71.45	62.64	Northern part of Noyyal basin.	Within permissible limit
2	Magnesium	100	4.86 to 218.7	76.57	64.24	Northern and Southern to the Western part of the basin	Exceeds permissible limit
3	Sodium	20	12 to 621	214.1	201.13	Throughout the basin	Exceeds permissible limit
4	Potassium	14	2 to 274	30.60	52.01	North-east part of Noyyal basin	Exceeds permissible limit
5	Chlorine	1000	7 to 1418	419.0	487.94	southwest side of the basin	Exceeds permissible limit
6	Sulphate	400	1 to 504	144.4	152.37	Throughout the basin	Exceeds permissible limit
7	Bicarbonate	600	3.417 to 6.6	5.13	0.74	East to west side of the basin	Within permissible limit
8	Fluorine	1.5	0.05 to 2.8	0.81	0.79	Southwest part of the basin	Exceeds permissible limit
9	pH	6.5 to 8.5	7.8 to 8.7	8.26	0.2370	Throughout the basin	Exceeds permissible limit
10	Sodium absorption ratio	26 to less than 10	0.728 to 10.35	3.82	2.86	Throughout the basin	Within permissible limit
11	Total hardness	600	45 to 1200	76.57	64.24	Southwest part of the basin	Exceeds permissible limit
12	Electrical conductivity	2000 µS/cm^2	140 to 5060 µS/cm^2	1942	1622	Southwest part of the basin	Exceeds permissible limit
13	Total dissolved solids	600	71 to 2976	1144	963.69	Southwest part of the basin	Exceeds permissible limit

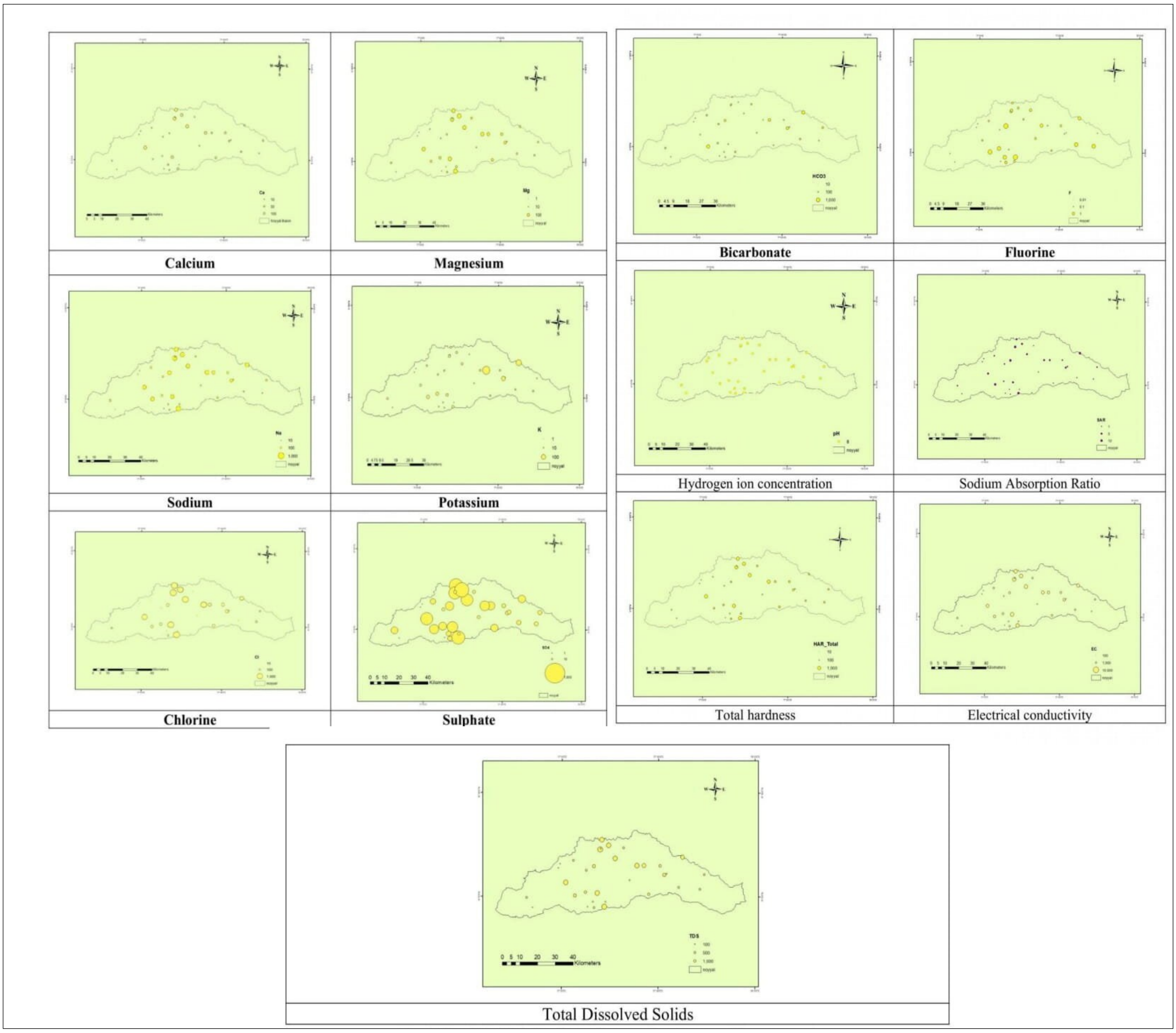

Fig. 5. Spatial distribution of groundwater quality parameters.

Geostatistical analysis

Semi-variograms were computed after normalizing the data in the Universal Transverse Mercator (UTM) coordinate system using ArcGIS Geostatistical Analyst, with ordinary Kriging applied for this procedure. The semi-variogram model was created by adjusting parameters to fit the experimental semi-variogram derived from the data. The angle direction and angle tolerance were kept constant to ensure consistency across different semi-variogram models. The most suitable semi-variogram model was selected based on the Root Mean Square Error (RMSE) criterion. The experimental semi-variogram, represented by scatter points and the omnidirectional semi-variogram model, depicted by the blue line, are shown in Fig. 6. The characteristics of the selected semi-variogram models for map generation are detailed in Table 3.

Table 3. Suitable semi-variogram model characteristics for map generation

Hydrochemical parameters	Number of Data	Transformation	Model	Nugget	Partial sill	Range	Sill	Nugget/ sill	Nugget/ sill
TDS	33	Logarithmic	Spherical	0.95	0.41	0.8563	1.36	0.69	Moderate
Ca	33	Logarithmic	Exponential	0.83	0.071	0.554	0.9	0.92	Weak
Mg	33	Logarithmic	Spherical	0.69	0.462	0.095	1.15	0.59	Moderate
Na %	33	Logarithmic	Gaussian	0.03	0.071	0.144	0.11	0.35	Moderate
Na	33	Logarithmic	Exponential	1.20	0.488	0.8487	1.68	0.71	Moderate
K	33	Logarithmic	Exponential	1.24	0.455	0.977	1.69	0.73	Moderate
Cl	33	Logarithmic	Gaussian	1.91	0.575	0.478	2.49	0.76	Weak
SO_4	33	Logarithmic	Spherical	2.46	0.884	0.7699	3.34	0.73	Moderate
HCO_3	33	Logarithmic	Exponential	0.47	0.136	0.977	0.60	0.77	Weak
F	33	Logarithmic	Spherical	0.81	0.742	0.0942	1.55	0.52	Moderate
pH	33	Logarithmic	Exponential	0.00	4.345	0.1357	4.34	0.00	Strong
SAR	33	Logarithmic	Spherical	0.51	0.147	0.099	0.66	0.78	Weak
HAR	33	Logarithmic	Exponential	0.66	0.345	0.7482	1.0	0.66	Moderate
EC	33	Logarithmic	Exponential	0.83	0.395	0.8715	1.22	0.67	Moderate

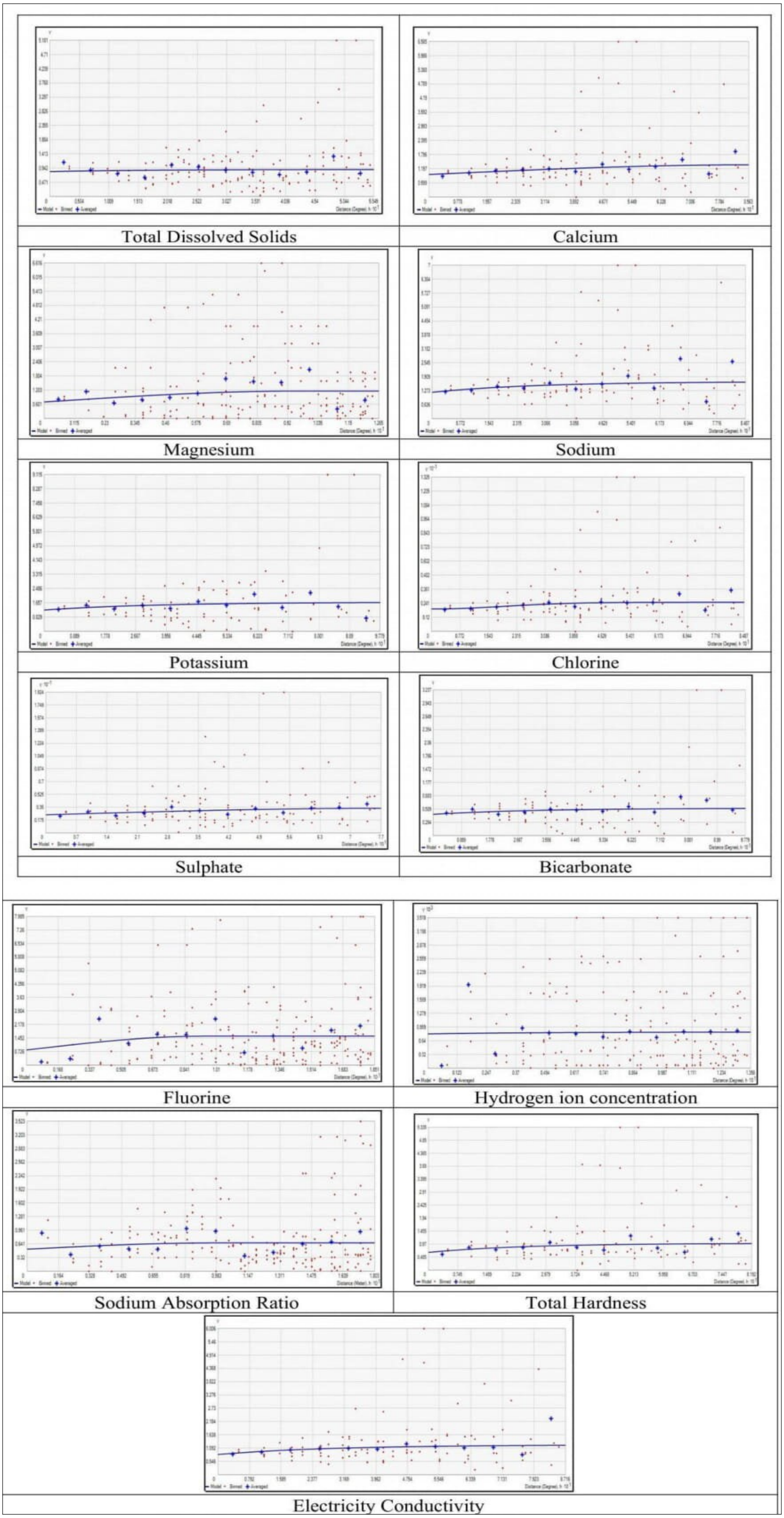

Fig. 6. Semi-variogram of groundwater quality parameters.

The results indicate that the optimal semi-variogram model, determined by the RMSE criterion, differs for each water quality parameter. For parameters like Ca, Na, K, HCO_3, pH, HAR and EC, the Exponential model applied to log -transformed data produced physically reasonable concentration maps. For parameters such as TDS, Mg, SO_4, F and SAR, the Spherical model with log-transformed data was found to be most appropriate. The Gaussian model with the ordinary data yielded satisfactory Cl and Na % results.

The "range" refers to the distance at which the semi-variogram model begins to level off and this distance varies across different hydrochemical parameters. The sill is the value at which the model flattens, while the "nugget" represents the value where the model intersects the y-axis. The difference between the sill and the nugget is called the partial sill. The proportion of the nugget to the sill reflects the spatial dependency of the quality of groundwater parameters. Three categories are used to classify this spatial dependence: strong (if the ratio is less than 25 %), moderate (if the ratio ranges between 25 % and 75 %) and weak (if the ratio exceeds 75 %) (17). pH is classified as having strong spatial dependence, while parameters such as calcium, chlorine, bicarbonate and sodium absorption ratio fall under weak spatial dependence. The remaining parameters are classified as moderate. Once the semi-variogram model was established, the cross-validation tool was used to assess the accuracy of groundwater chemistry predictions at unsampled locations. Cross-validation statistics were then analyzed to determine whether the model and its parameters were reasonable and reliable.

Prediction map of spatial distribution of parameters of groundwater

Using the best model selected through cross-validation, the prediction maps for the spatial distribution of chemical parameters of groundwater are presented in Fig. 7. These maps effectively illustrate the groundwater quality across the Noyyal basin. Ordinary Kriging was practical in determining the regions' groundwater quality parameters and spatial distribution. The predicted maps indicate that, in most areas, hydrogen ion concentration (pH) values exceed 8, suggesting a significant alkalinization of the basin. This trend is expected to worsen over time.

In summary, the relative importance of cations, on average, follows the order: Na > Ca > Mg > K, while for anions, it is Cl > SO_4 > HCO_3 > CO_3. However, this ranking may vary depending on the specific location of the sample, as it is influenced by factors such as climate, the underlying parent material and human activities.

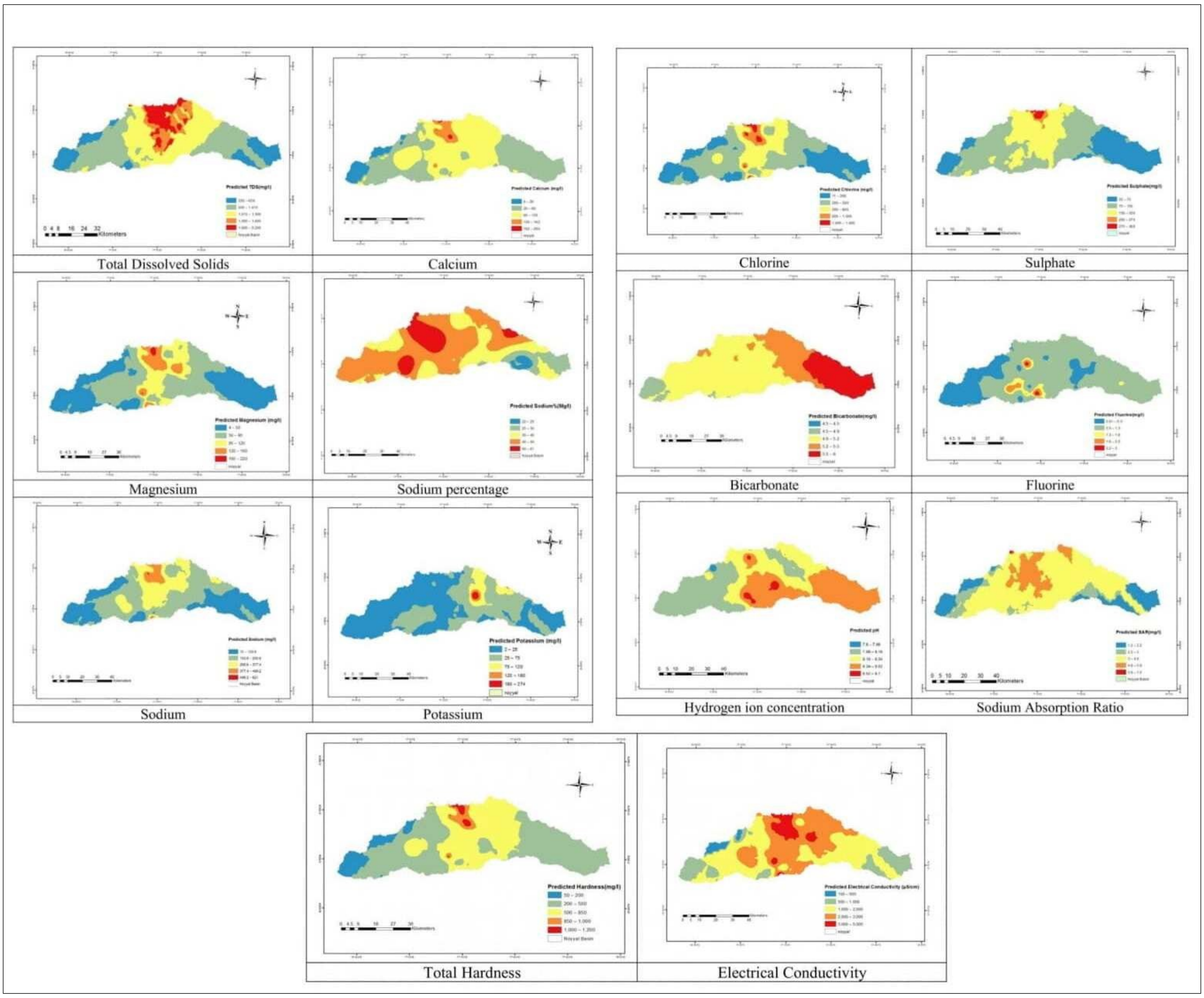

Fig. 7. Spatial distribution of groundwater chemical parameter.

Conclusion

A comparison of the calculated concentrations with the permissible limits revealed that calcium, bicarbonate and sodium absorption ratios fall within acceptable levels, while the remaining parameters exceed the allowable thresholds. The analysis also shows that the optimal semi-variogram model, based on RMSE, varies for each groundwater quality parameter. The predicted maps suggest that the alkalinization of the entire basin is likely to worsen and the extent of the affected areas will increase. In conclusion, the research highlights the importance of geospatial methods as essential tools for policymakers and planners, aiding in developing strategies for efficient groundwater resource management.

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Authors' contributions

BK highlights the alarming trend of groundwater quality deterioration, noting that key parameters such as magnesium, sodium and total dissolved solids exceed permissible limits. NJ focuses on the innovative use of geostatistical analysis and GIS to map and predict groundwater chemistry, ensuring that our findings are based on robust data transformations. AS discusses the significance of semi-variogram models, which reveal the variability in water quality across the basin, providing insights into specific contaminants. JR underscores the implications of high pH values, warning of the severe risks of alkalinization to the ecosystem and agriculture. TA addresses the need for sustainable groundwater management strategies to mitigate these challenges. KA assisted in the data collection interpretation of results and provided revisions to the manuscript. AR conducted detailed statistical analyses on the groundwater quality data, identifying trends and anomalies that informed the overall findings.

Compliance with ethical standards

Conflict of interest: Authors do not have any conflict of interest to declare.

Ethical issues: None

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