Application of Sequential Analysis and Geographic Information Systems for Hydrochemical Evolution Survey, Shagari Environ, Southwestern Nigeria

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Abstract

Integrated multivariate statistical, spatial, and graphical methods were applied to some hydrochemical data in Shagari area, Akure, southwestern Nigeria with a view to elucidating groundwater hydrochemical evolution. Water samples from 23 dug wells were clustered into distinct groups by hierarchical cluster analysis to depict different hydrochemical facies. Factor analysis reduced bulk hydrochemical data to principal components explaining possible dominant processes controlling water chemistry. Three factors which together explain 83.48 % of the total variance in the dataset were retained and interpreted. Factor 1 explains 35.82 % of the total variance and indicates atmospheric controls and silicate mineral weathering processes. Factor 2 explains 35.41 % of the total variance and reflects atmospheric controls, acid rain and speciation reactions producing inorganic carbon ions in solution. Factor 3 explains 12.24 % of the total variance, indicating silicate mineral weathering processes resulting in elevated pH. Generally, water types tend towards sodium chloride bicarbonate.

Key-words: Geographic information systems; groundwater quality; hydrchemical evolution; sequential analysis.

1.0 Introduction

Shallow weathered Basement rock aquifers are the major sources of water for domestic purposes in the sudy area. Groundwater quality in many parts of the region is often questionable due to anthropogenic impacts from sewage, fertlizers and refuse dumps. Mineral enrichment from host rocks also alter groundwater chemistry appreciably in some parts, thereby making its usability objectionable. Consequently, groundwater characterization is inevitable in most parts of the region. Several wokers (like Elueze et al., 2001 and Ehinola, 2002) had used the traditional graphical approach to characterize groundwater geochemistry in parts of southwestern Nigeria. The absence or inadequacy of input data is a major limitation in groundwater models application in developing countries like Nigeria.

However, evolving emperical assessment methodologies (EAM) are common in recent years in groudwater hydrochemical studies. Multivariate statistical methods have been employed to extract critical information from hydrochemical datasets with respect to groundwater quality assessment in several places (Olobaniyi and Owoyemi, 2006; Shiab and Hashim, 2006; Petalas et al., 2006; Papatheodorou et al., 2007; Belkhiri et al., 2010).

Locsey and Cox (2003) differentiated groundwaters sourced from diferent lithological formations by multivariate analysis of physico-chemical data for easy identification of the likely host rocks of groundwaters from unidentified lithological units, and better understanding of groundwater resource. Yidana (2011) applied multivariate statistics and GIS in a sequential manner to understand hydrochemical processes in a tropical setting on a regional scale. An integrated approach that uses hydrochemical data to improve characterization of watershed hydrology by standard multivariate statistical techniques, spatial analysis and inverse geochemical modeling had also been reported (Thyne et al., 2004). The current study explores an integration of the strengths of multivariate statistical, spatial, and graphical methods in a sequential manner for a robust interpretation of hydrochemical dataset. This is with a view to elucidating possible underlying hydrochemical processes responsible for variability of groundwater composition, and hydrochemical evolution of water in Shagari area, Akure, southwestern Nigeria. Multivariate factor analysis (FA) by principal component extraction method with varimax rotation is used to characterize groundwater hydrochemical facies in the area.

Factor analysis is often used in hydrochemical studies to interprete the structure within the variance-covariance matrix obtained from a collection of multivariate hydrogeochemical observations by extracting the eigenvalues and eigenvectors from the matrix of correlations or covariances of measured standardized variables (Davis, 1973). Bulk hydrochemical data reduction gives factor score groups that correspond to distinguishable underlying controlling environmental factors. Determination of the number of components to retain and interprete is often based on some criteria, viz: components with eigenvalue > 1, components accounting for at least 70% total variability, and components within the sharp descent before eigenvalues level off on the scree plot.

1.1 Description of the study area

The study area lies within latitudes 7^{o} 16^{l} N and 7^{o} 18^{l} N of the equator and longitudes 5^{o} 10^{l} E and 5^{o} 13^{l} E of the Greenwich meridian. It is accessible by footpaths and secondary roads. The topography is generally characterized by hills of varying heights ranging from about 300m to 400m (Fig. 1). The climate is of the West African monsoonal type, characterized by distinct wet and dry seasons typical of West African tropical regions. Average temperatures reach a peak of about 32^{o} C around February and a threshold of about 21^{o} C around August. Relative humidity ranges from about 70% around January to about 90% in July. Typically, the vegetation of the study area is the tropical rain forest with thick undergrowth but had in many parts been modified by human activities such as urbanisation, construction, land cultivation and deforestation.

1.2 Geological and hydrogeological setting

The study area is underlain by the Precambrian Basement Complex of southwestern Nigeria. The assemblages within the Basement Complex had been grouped into four, viz: minor intrusives, Older granites, schist belts and migmatite-gneiss-quartzite complex (Adekoya et al., 2003). The lithologic units encountered in the study area include granite gneiss, porphyritic gneiss, pelitic schist, charnockite, and migmatite gneiss complex (Fig. 2). They vary in texture, and range from fine to medium to coarse porphyritic grains. Structural features occurring on the lithologic units include veins, veinlets, foliations, intrusions and rock-to-rock contacts. Other structures include joints, faults and folds. Generally, the fissure zones trend north-south while the foliation trends are NNW-SSE and NNE-SSW (Olorunfemi et al., 1999). Availability of groundwater in the area often depends on the thickness of the weathered overburden and the frequency of fractures within the crystalline rocks. Depth to static water level in the area range between 1.47m and 8.74m. Groundwater recharge is primarily through infiltration by direct precipitation which reaches mean annual value of about 1350mm. The wet season spans between April to September while the dry season period is between October and March. Secondary recharge occurs by influent from rivers and their tributaries. Discharge of groundwater occurs through seepages, springs, well water abstraction, and flow into rivers and streams. The area is drained by streams and rivers displaying dendritic pattern and maintaining a meandering pattern of flow in south-eastern and southwestern directions.

2.0 Methodology

2.1 Sample collection and laboratory analysis

A total of twenty-three (23) groundwater samples were collected from hand dug wells in Shagari area for chemical analysis. Samples were taken from wells with a rubber container to avoid metallic contamination, and storage was by the use of plastic containers.

Total dissolved solids (TDS), pH, Temperature and electrical conductivity (EC) were measured in situ using the HANNA COMBO meter (HI 98129 model). Samples were analysed in the laboratory using JENWAY Flame photometer (PFP 7 model) for major cations (Na^+ and K), while JENWAY Colorimeter (6015 model) was used for analysing SO_4^{2-}, and EDTA Titrimetric method for Ca^{2+}, HCO_3^- and Cl^- as well as total hardness and alkalinity. The concentrations of the major ions and the ionic balance of the chemical analyses were combined in validating the data for further analysis.

2.2 Data preparation

The data obtained from laboratory analysis were standardized to their standard scores (*z*-scores) by setting the mean and standard deviation to zero and one respectively so that each of the variables will have equal weight in the multivariate statistical analyses. This helps in minimizing the effects of different units and variance of variables by rendering the data dimensionless (Liu, et al., 2003; Singh et al., 2004). Data were evaluated to screen for outliers and assess normality and linearity using Mahalanobis distance. A scatterplot matrix reveals fairly normal distributions and linear relationship among variables. The results were subjected to statistical analysis at 5% level of significance (i.e. $\alpha=0.05$).

2.3 Multivariate data analysis

Multivariate sequential analysis which employs standard methods in a way that each step builds on the prior analysis was adopted. The effort is expected to provide increasing confidence and greater insight into the hydrochemical evolution of the study area, culminating in a robust interpretation. Q-mode Hierarchical cluster analysis (HCA) was performed with assumptions of homoscedasticity of variables (Mertler and Vannatta, 2005). Samples were grouped into distinct clusters of hydrogeologic and statistical significance. The Group Average (Unweighted Pair-Group) linkage and Euclidean distance methods were used. R-mode factor analysis (FA) by principal component extraction method with varimax rotation and Kaiser normalization was employed to reduce bulk hydrochemical data into components that explain possible underlying structures existing among the clustered variables.

Three steps were followed in carrying out the FA, viz: computation of correlation matrix by determining the correlation coefficient, estimation of the factor loadings, and factor rotation and interpretation. For the initial factor extraction, Kaiser's (1958) eigenvalue criterion of retaining only those components/factors whose eigenvalues are greater than 1 was adopted. Other criteria used to determine the appropriate number of components to retain include, scree plot, variance and residuals. Kaiser's varimax rotation, an orthogonal rotation procedure which produces a set of component loadings having the maximum variance of the squares of the loadings is used in conducting the principal component analysis to make the factor solutions more interpretable without altering the underlying mathematical structure (Mertler and Vannatta, 2005). The scheme operates by adjusting the factor loadings to either near ±1 or near zero which is a way of maximizing the variance of the loadings on the factors. Tests indicating factorability such as Kaiser-Meyer-Olkin (KMO) and Bartlett's test were conducted and the various indicators were good, and the residuals indicate that the factor solution was a good one too. SPSS® Statistics 17.0 (SPSS Inc., 2008) was used for the multivariate statistical analysis.

3.0 Results and Discussion

Table 1 gives the summary of the result of laboratory analysis which shows that the water in the area is of moderate mineralization on the basis of the moderate TDS values ranging from 50mg/l to 297mg/l.

3.1 Statistical Analysis

The univariate descriptive statistical overview of the hyrochemical data of groundwater sampled in August, 2010 including major cations and anions is presented in Table 2. The distributions of the water quality parameters were assessed by determining minimum, maximum, mean and standard deviation for each of the 11 variables. Na^+ and K^+ are relatively high in abundance compared with Ca^{2+} and Mg^{2+}. This may be responsible for the moderate TDS, very low hardness and alkalinity of the water samples. Ca^{2+} and Mg^{2+} values are low, and range from 0.9 mg/l to 5.7 mg/l and 0.2mg/l to 0.92mg/l, with mean±s.d. of 2.43±1.15mg/l and 0.5±0.2mg/l respectively. Na^+ and K^+ values range from 12.0mg/l to 76.0mg/l and 15.0mg/l to 88.0mg/l, with mean±s.d. of 33.83±15.67mg/l and 31.09±16.07mg/l respectively.

The total dissolved solids (TDS) in the water samples varied over a wide range of 50 to 297 mg/l with an overall mean ±s.d. of 126.26 ±62.16mg/l. The pH values varied between 5.42 and 6.52 with mean±s.d. of 5.99±0.31.

3.2 Q-and R-mode Analyses

Q-mode analysis which grroups samples on the basis of similarities in multidimensional space was employed to classify the dataset into clusters and shown as a dendogram (Fig. 3). From the dendogram, 3 preliminary clusters were selected by visual inspection to depict different hydrochemical facies. Generally, the order of enrichment in all the chemical constituents is such that cluster 3 > cluster 2 > cluster 1 (Table 3). The correlation matrix of these groundwater quality parameters was composed for R-mode factor analysis (Table 4) using principal component extraction method with varimax rotation and Kaiser normalization. Three components were retained and interpreted on the basis of Kaiser's criterion of eigenvalues >1.0 (Tables 5 & 6) and indications from the scree plot (Fig. 4). The three components together explain 83.48 % of the total variance in the dataset (Table 7). Factor 1 shows high positive loadings of Total hardness (TH), Ca^{2+}, Mg^{2+}, Cl^- and TDS, and explains 35.82 % of the total variance. It indicates atmospheric controls and silicate mineral weathering processes. Factor 2 with high loadings of Na^+, K^+, HCO_3^- and Alkalinity, and average loadings of Total hardness, Ca^{2+} and Mg^{2+} concentrations explains 35.41 % of the total variance. It reflects atmospheric controls and speciation reactions producing inorganic carbon ions in solution. Factor 3 associated with high pH explains 12.24 % of the total variance. It reflects silicate mineral weathering processes associated with increased pH. There is a very high degree of consistency between the results of factor analysis by principal component extraction and those of HCA. The plot of the first two factor scores produced three distict clusters which correspond well with the clusters produced by HCA (Fig. 5).

3.3 Hydrochemistry

Plots of hydrochemical data on Piper (1944) trilinear diagram (Fig. 6) show the distribution of chemical constitiuents (cations and anions) in groundwater within the the area. This was accomplished by using the GW_Chart package (USGS, 2000). From the plot, three different water types were identified in the study area, viz: $Na^+ - K^+ – Cl^- - SO_4^{2-} - HCO_3^-$, $Na^+ - K^+ - HCO_3^- - Cl^- - SO_4^{2-}$, and $Na^+ - Ca^{2+} - Cl^- - SO_4^{2-} - HCO_3^-$ water types. The water types tend towards sodium chloride bicarbonate which is consistent with expected water-rock interactions in such basement complex terrain (Bala and Onugba, 2001; Ehinola, 2002). These water types would probably have resulted from precipitation of meteoric water through the different lithologic units (granite gneiss, porphyritic gneiss, pelitic schist, charnockite, and migmatite gneiss) in the area. The Na^+ and K^+ may have resulted from silicate mineral weathering while Cl^- may have originated from evapotranspiration process, and HCO_3^- may be inorganic carbon ions produced when infiltrating water reacted with soil CO_2. The order of dominance of cations and anions is $Na^+ > K^+ > Ca^{2+} > Mg^{2+}$ and $HCO_3^- > Cl^- > SO_4^{2-}$ respectively. The spatial distribution of statistical water groups in the study area is as presented in Figure 7. It is observed that water samples in the same statistical group are in close proximity spatially.

Generally, there is a high degree of spatial, statistical and hydrochemical coherence (Figs. 3, 5 & 7). The low TDS group 1 water samples occur at relatively highest elevations, while Group 2 water samples which are characterized by intermediate TDS values occur at lower elevations than group 1. Group 3 water samples which are associated with the highest TDS values occur along topographic lows and flowpaths where more water-rock and soil-rock interactions that would increase TDS is expected. This agrees with the findings of Thyne et al. (2004).

4.0 Conclusions

This study has employed an integrated approach to groundwater hydrochemical system characterisation using standard multivariate statistical techniques, spatial analysis, geographic information systems (GIS) and traditional graphical methods in a sequential manner in Shagari area, southwestern Nigeria. The study showed that atmospheric, geologic and hydrogeologic controls are possibly behind the geochemical processes responsible for variation in water quality in area. Three different water types were identified in the study area, viz: $Na^+ - K^+ – Cl^- - SO_4^{2-} - HCO_3^-$ water type, $Na^+ - K^+ - HCO_3^- - Cl^- - SO_4^{2-}$ water type, and $Na^+ - Ca^{2+} - Cl^- - SO_4^{2-} - HCO_3^-$ water type. The water types tend towards sodium chloride bicarbonate which is consistent with expected water-rock interactions in such basement complex terrain.

Generally, there is a high degree of spatial, statistical and hydrochemical coherence. The study had demonstrated the integration of the strengths of multivariate statistical, spatial, and conventional graphical methods in a sequential manner for a robust interpretation of hydrochemical dataset.

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Table 1: Water Analysis Result

Location	Longitude (E 005^O)	Latitude (N 07^O)	TDS (mg/L)	pH	TH (mg/L)	K (mg/L)	Na (mg/L)	Ca (mg/L)	Mg (mg/L)	Cl (mg/L)	HCO_3 (mg/L)	SO_4 (mg/L)	Alkalinity
1	11.871	16.898	129.00	5.93	4.40	38.00	52.00	2.30	0.62	1.30	2.70	0.05	2.50
2	11.483	17.150	157.00	5.99	3.70	30.00	42.00	2.50	0.50	2.40	2.20	0.10	1.80
3	11.413	17.252	148.00	5.87	3.10	22.00	34.00	2.10	0.40	2.60	1.60	0.06	1.50
4	11.437	16.978	146.00	6.10	4.70	20.00	31.00	2.70	0.64	2.00	2.10	0.05	1.50
5	11.288	17.034	73.00	5.98	2.90	32.00	18.00	1.00	0.50	1.00	1.40	0.02	1.00
6	11.257	16.953	120.00	6.01	3.90	34.00	40.00	1.90	0.60	1.60	2.00	0.03	1.70
7	11.307	16.768	86.00	5.93	3.60	15.00	24.00	2.10	0.50	1.40	4.10	0.04	1.20
8	11.357	16.470	64.00	5.99	2.20	18.00	26.00	1.80	0.24	1.00	1.30	0.08	1.22
9	10.820	16.918	60.00	5.88	1.40	22.00	19.00	1.00	0.20	1.20	0.90	0.01	1.00
10	10.971	16.730	57.00	5.94	2.10	24.00	32.00	1.60	0.26	0.70	1.30	0.04	1.30
11	10.966	16.595	64.00	6.09	2.12	20.00	28.00	1.62	0.23	0.80	1.10	0.20	1.32
12	10.949	16.486	91.00	6.15	3.10	38.00	51.00	1.81	0.42	1.00	2.20	0.02	2.20
13	11.051	16.346	135.00	5.83	3.60	15.00	21.00	1.83	0.52	2.00	1.10	0.03	1.20
14	11.727	16.215	234.00	6.49	5.80	24.00	32.00	4.20	0.70	3.60	1.70	0.10	1.40
15	12.034	16.611	261.00	6.61	7.70	88.00	76.00	5.71	0.92	3.30	5.20	0.12	4.30
16	11.792	16.631	137.00	6.09	5.10	32.00	42.00	3.20	0.70	1.70	1.40	0.03	1.70
17	10.820	17.050	105.00	6.21	4.90	40.00	53.00	2.60	0.71	1.20	2.50	0.04	2.20
18	10.728	17.292	102.00	6.58	4.20	31.00	50.00	3.60	0.50	0.80	2.20	0.01	2.40
19	11.077	17.143	147.00	5.98	4.80	48.00	12.00	3.90	0.54	2.20	1.90	0.15	0.50
20	11.199	17.303	103.00	5.70	3.10	16.00	13.00	2.00	0.22	1.50	1.20	0.05	0.70
21	10.884	16.388	170.00	6.30	3.70	26.00	32.00	2.20	0.52	2.80	1.60	0.09	1.40
22	11.824	16.198	262.00	6.55	6.10	30.00	37.00	3.50	0.83	3.90	1.70	0.11	1.50
23	11.976	16.392	83.00	5.64	1.60	54.00	14.00	0.90	0.23	1.50	0.60	0.06	0.70

Table 2: Descriptive statistics of water quality data from Shagari

Variable	Min	Max	Mean	Std. Deviation
TH	1.40	7.70	3.82	1.52
Ca^{2+}	0.90	5.70	2.43	1.15
Mg^{2+}	0.20	0.92	0.50	0.20
Cl^-	0.70	3.90	1.80	0.92
Na^+	12.00	76.00	33.83	15.67
K^+	15.00	88.00	31.09	16.07
HCO_3^-	0.60	5.20	1.91	1.02
Alkalinity	0.50	4.30	1.57	0.79
pH	5.42	6.52	5.99	0.31
TDS	50.00	297.00	126.26	62.16
SO_4^{2-}	0.01	0.20	0.06	0.05

Table 3: Mean water chemistry of the HCA water clusters

Cluster	TH	Ca^{2+}	Mg^{2+}	Cl^-	Na^+	K^+	HCO_2^-	Alk.	pH	TDS	SO_4^{2-}
Cluster 1	2.86	1.87	0.36	1.64	24.17	27.25	1.35	1.13	5.94	105.08	0.07
Cluster 2	4.24	2.53	0.59	1.38	42.88	30.75	2.40	1.93	6.16	114.50	0.03
Cluster 3	6.53	4.47	0.82	3.60	48.33	47.33	2.87	2.40	6.55	252.33	0.11

Table 4: Correlation matrix of water quality parameters from Shagari

	TH	**Ca^{2+}**	**Mg^{2+}**	**Cl^-**	**Na^+**	**K^+**	**HCO_3^-**	**Alk.**	**pH**	**TDS**	**SO_4^{2-}**
TH	1.000										
Ca^{2+}	0.913	1.000									
Mg^{2+}	0.947	0.765	1.000								
Cl^-	0.684	0.633	0.628	1.000							
Na^+	0.608	0.567	0.623	0.181	1.000						
K^+	0.499	0.534	0.455	0.253	0.548	1.000					
HCO_3^-	0.644	0.618	0.611	0.245	0.672	0.530	1.000				
Alk.	0.619	0.600	0.606	0.196	0.962	0.630	0.750	1.000			
pH	0.517	0.455	0.537	0.258	0.527	0.012	0.338	0.468	1.000		
TDS	0.783	0.680	0.769	0.925	0.329	0.270	0.311	0.306	0.434	1.000	
SO_4^{2-}	0.235	0.373	0.102	0.409	-0.018	0.216	0.083	0.005	-0.102	0.346	1.000

Table 5: Eigenvalues of Factors extracted through PCA, Differences between Factors and proportion of variance explained by factors

Factors	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**
Eigenvalues	6.080	1.889	1.213	0.613	0.417	0.313	0.221	0.178	0.043	0.022	0.010
Difference	4.191	0.676	0.600	0.196	0.104	0.092	0.043	0.135	0.021	0.012	
Proportion	0.553	0.172	0.110	0.056	0.038	0.028	0.020	0.016	0.004	0.002	0.001
Cummulative	0.553	0.725	0.835	0.891	0.929	0.957	0.977	0.993	0.997	0.999	100.000
Eigenvalues of the Correlation Matrix; Total = 11; Average = 1											

Table 6: Variance explained for factors retained before and after varimax rotation

Factor	**Extraction Sums of Squared Loadings**			**Rotation Sums of Squared Loadings**		
	Total	**% of Variance**	**Cumulative %**	**Total**	**% of Variance**	**Cumulative %**
1	6.080	55.273	55.273	3.941	35.824	35.824
2	1.889	17.173	72.446	3.895	35.407	71.231
3	1.213	11.029	83.475	1.347	12.244	83.475

Table 7: Varimax rotated factor loadings and communalities

Variable	**Factor 1**	**Factor 2**	**Factor 3**	**Communalities**
TH	**0.785**	0.554	0.067	0.928
Ca^{2+}	**0.710**	0.567	-0.091	0.833
Mg^{2+}	**0.739**	0.529	0.193	0.864
Cl^-	**0.918**	0.038	-0.183	0.877
Na^+	0.194	**0.874**	0.269	0.874
K^+	0.125	**0.778**	-0.402	0.783
HCO_3^-	0.235	**0.812**	0.045	0.716
Alk.	0.170	**0.928**	0.181	0.924
pH	0.473	0.275	**0.687**	0.771
TDS	**0.951**	0.134	-0.014	0.922
SO_4^{2-}	0.409	0.018	-0.723	0.690
% Variance	**35.824**	**35.407**	**12.244**	**83.475**

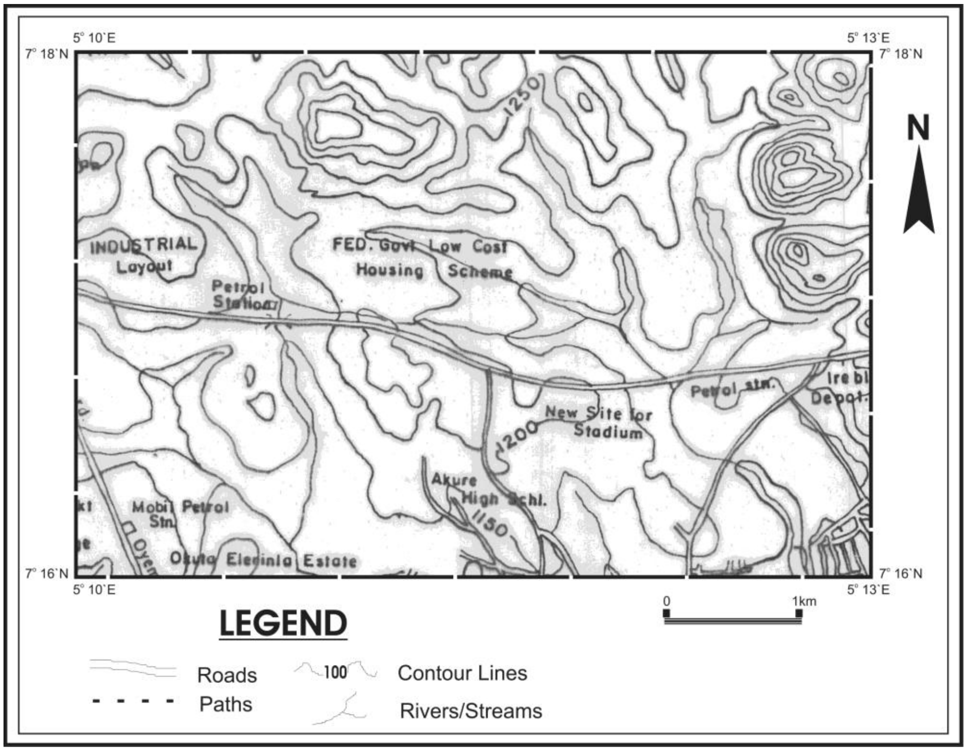

Figure 1: Topographical map of study area (Fed. Survey Nig., 1964)

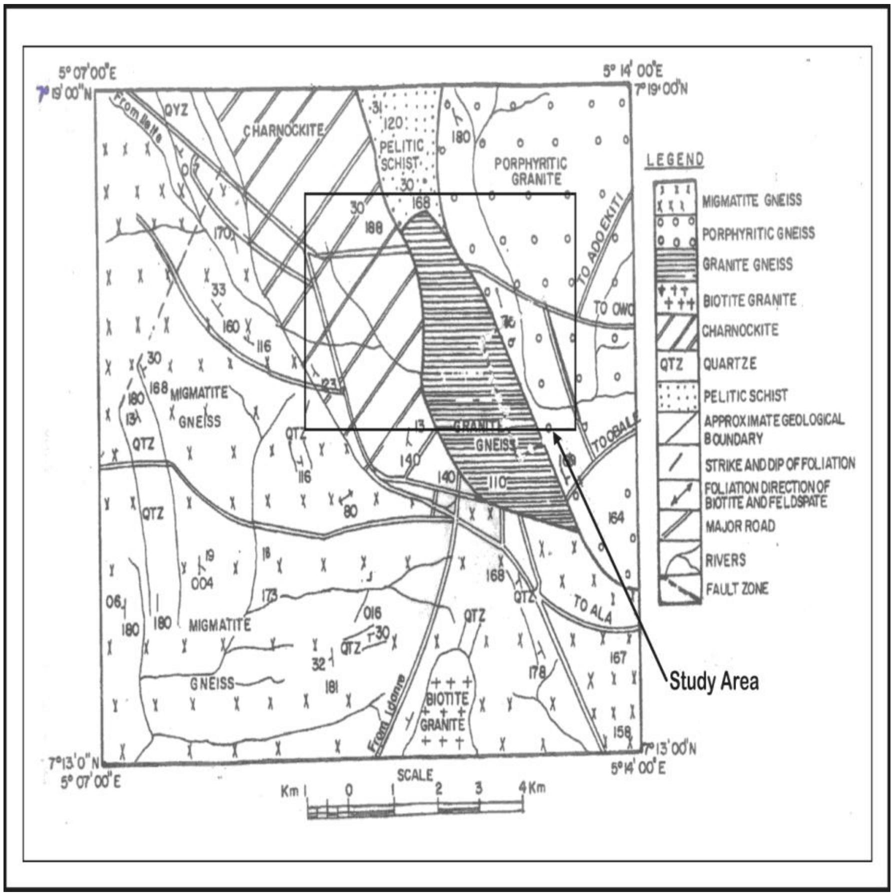

Figure 2: Geological map of study area

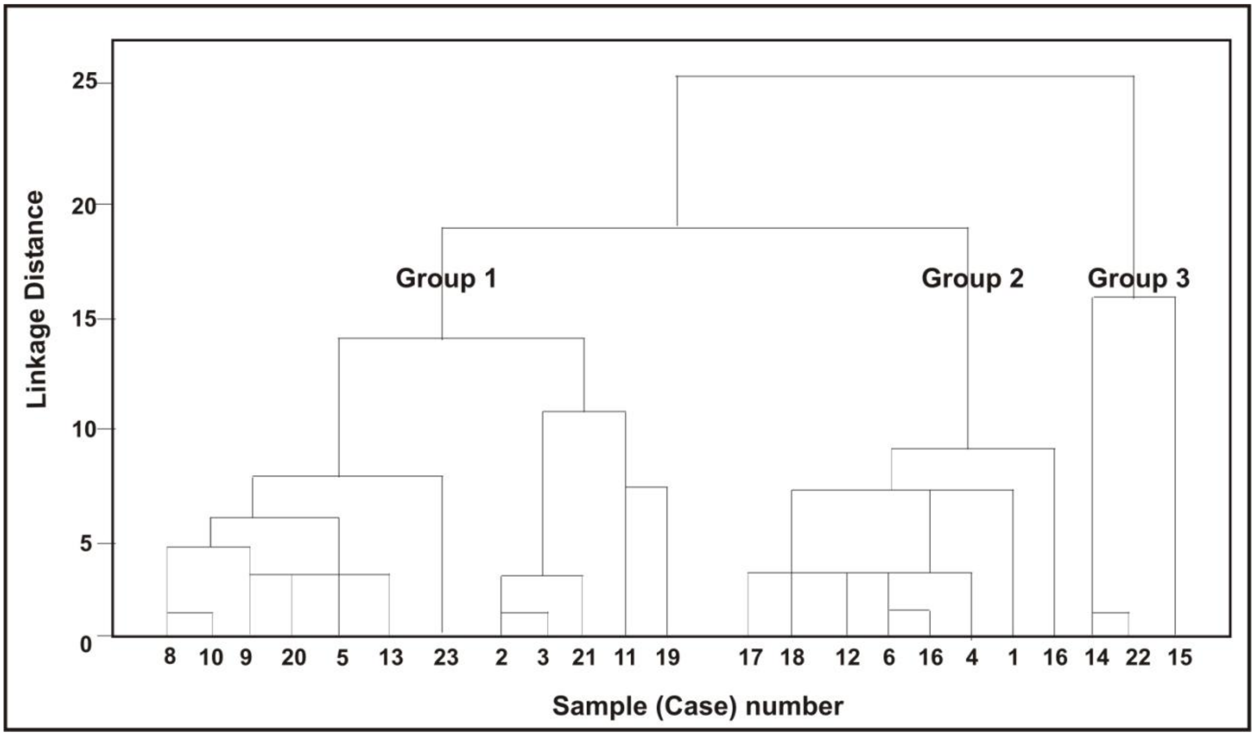

Figure 3: Dendogram of hydrochemical data depicting associations between groundwater samples from Shagari.

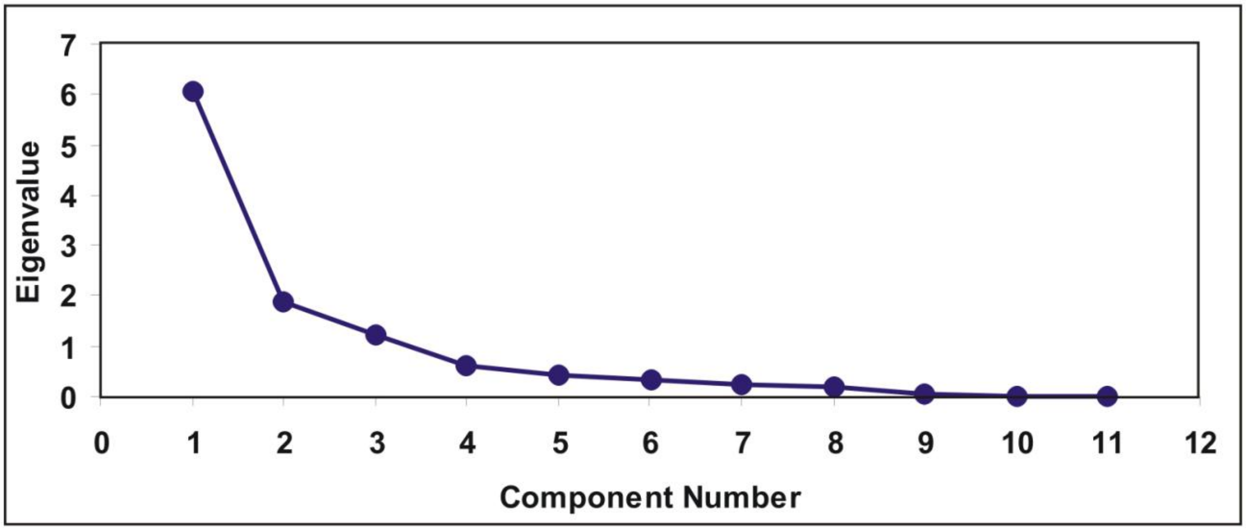

Figure 4: Scree plot for selecting number of factors to retain and interpret.

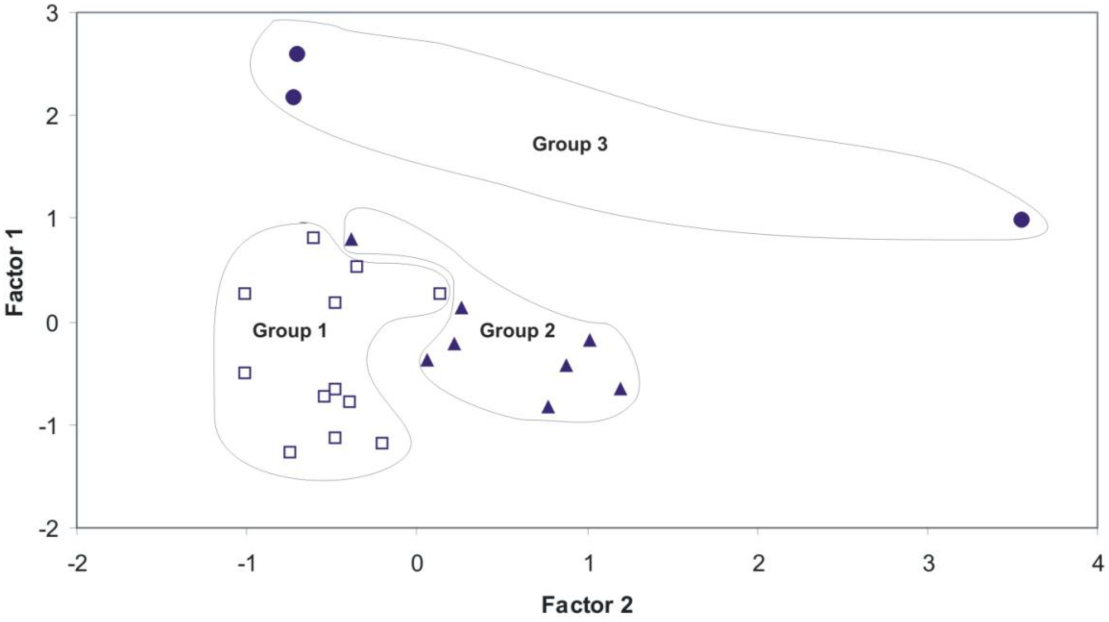

Figure 5: Distribution of HCA-derived classification of samples using factor analysis results

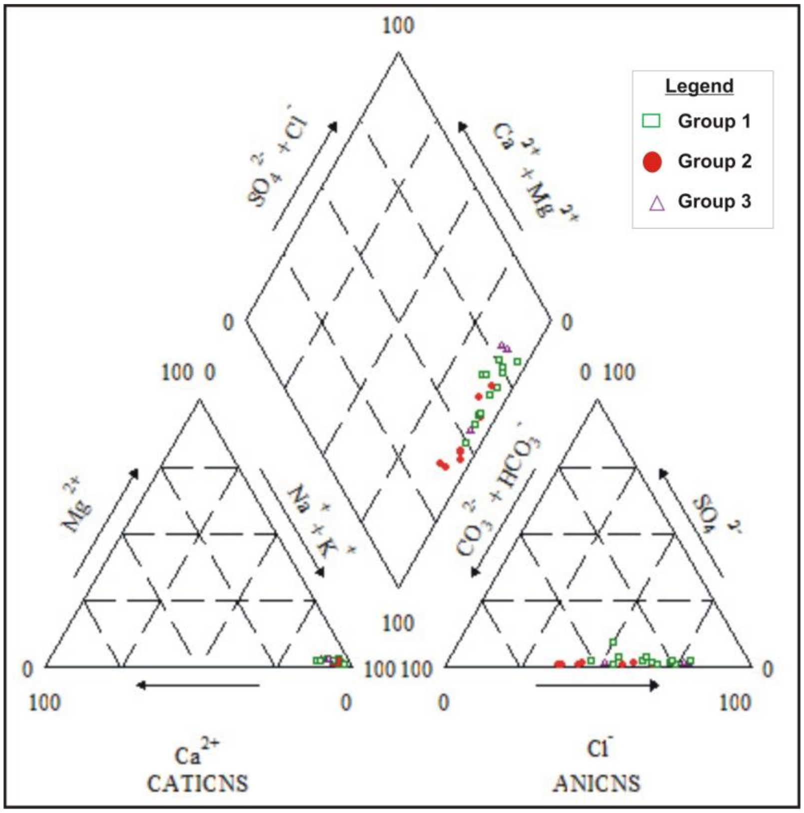

Figure 6: Piper trilinear diagram depicting variation in groundwater chemistry of Shagari area

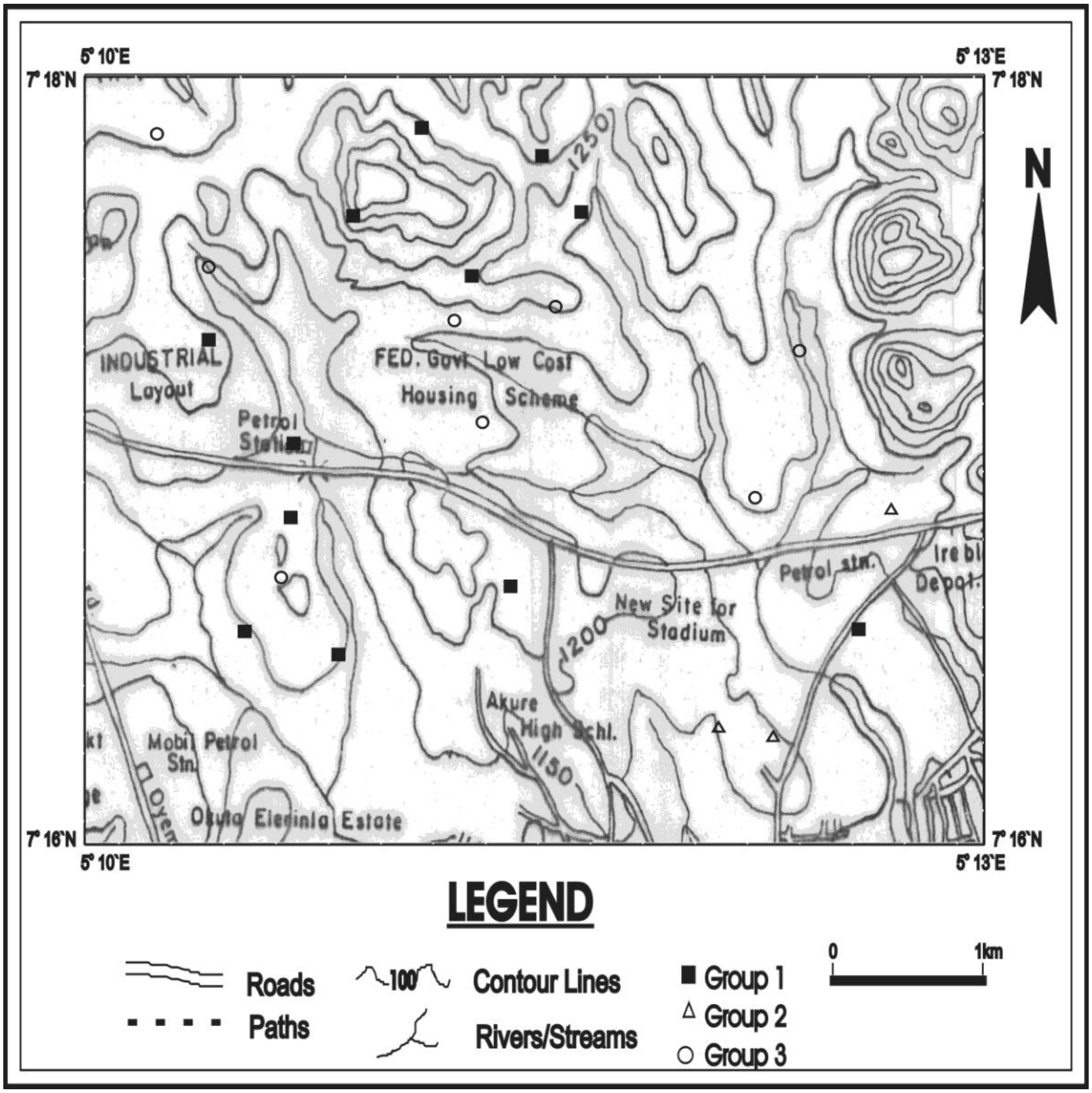

Figure 7: Spatial distribution of HCA-derived water groups for Shagari area.