GEOSTATISTICS AND MULTIVARIATE ANALYSIS OF HYDROGEOCHEMICAL PARAMETERS OF ELEYELE LAKE, IBADAN, SOUTH WEST NIGERIA

Iheme, K. O, Olelewe, M. C, Omotoso, O. A, Okolo, C. J, Atanu O.
Department of Geology And Mineral Sciences University of Ilorin,
Ilorin, Kwara State, Nigeria
Corresponding Author: Iheme.ko@Unilorin.edu.ng

Abstract
Evaluation of Eleyele Lake and Wetland, Ibadan South Western Nigeria was carried out to acertain the contamination state of the water bodies. 29 water samples were collected from the lake and its effluents streams, and were geochemically analzyed using Inductively Coupled Plasma-Mass Spectrometery (ICP-MP) while the pH, total dissolved solids (TDS), and electrical conductivity (EC) were measured insitu during the sampling operations. Values of pH, TDS, EC, and metals with significant concentrations in the samples were selected as variables used for geostatistical analysis, and multivariate analysis; principal component analysis (PCA) and hierarchical cluster analysis (HCA). Comparison of geostatistical analysis result with Nigerian Standard for Drinking Water Quality, shows that EC, TDS, iron (Fe), and aluminum (Al) concentration were above the recomended limits in many locations. PCA results show that the first 2 principal components accounts for 79.7% of the variability or information in the samples. PC scores clearly revealed two clusters which was indicative of where the water sample was collected; Lake or Tributary/effluent streams. Hierarchical clustering identified three clusters of samples but subsequent piper digram of the clusters revealed that clusters 2 and 3 were more alike and less contaminated by sodium (Na) compared to water samples in cluster 1.

Keywords: Geostatistics, Principal component analysis (PCA), Hierarchichal cluster analysis (HCA).

1.0 Introduction

Large population centers are often accompanied by large scale industrial development, this can lead to multiple contamination and pollution of surface water bodies from different points and non point sources such as agricultural discharges, unsafe sewage disposal, mining, direct dumping of domestic waste into surface water bodies *etc*. Some contaminated and polluted water bodies can be identified by their foul smell, unpleasant colour, and presence of large amounts of decaying organic matter. However most contamination and pollution of surface water bodies are not easily identified without conducting proper sampling investigation and chemical analyses. Consequently when contamination and pollution is suspected, a method has to be found to evaluate if the contaminant species exceeds sanitary levels, the volume/area of contamination, cleanup methods, and how to mitigate against future occurrence. This research evaluates eleyele lake and wetlands using geochemical, geostatistical and multivarent models. Sampling programs with the aim of geochemically investigating the contamination state of water bodies was designed to measure several variables from samples, and these samples were collected between sampling stations of wide spatial intervals/extents due to costs and time constraints. Geostatistical interpolation (kriging) was used to make an unbiased estimate of each individual environmental variables/parameters at unmeasured locations, from measured values. Unbiased estimation of environmental variables at unmeasured locations was possible because the spatial correlation information captured by variograms is incoporated during

geostatistcal spatial interpolation (kriging). Many of the variables in a collated data set generated from surface water contamination studies are highly correlated and thus provides redundant/repeated information. Principal component analysis (PCA) which is a multivariate analytical technique was used to summarize the collected dataset into a few variables called principal components which retains most of the variability or information contained in the original dataset. Hierarchical cluster analysis (HCA) was used to classifiy the samples into groups or clusters based on a measure of the distance between samples; this distance is often the euclidean distance measured by comparing the variable values of each sample with those of other samples in the data set, and those with small distance distances are group together using a number of algorithms. Geostatistics, PCA, and HCA have been used as tools to investigate and characterize the contamination state of water bodies by several researchers like [3],[2],[4],[1],[[8],[16],[11],[12] and it has been proven to be an effective method.

1.1 Location and Land Use

Eleyele Lake and Wetland which is located in North-Western part of Ibadan, South-Western Nigeria within latitudes 07º36'00''N and 07º39'00''N and longitudes 03º51'00''E and 03º53'00''E, covers an area of about 12km^2. The study site is surrounded by Eleyele community and is bounded in the South by Apete and Awotan communities by the North, and Ijokodo to the East (Figure 1a). The water from Eleyele Lake is dammed and serves as a very important source of domestic water supply, transportation, farming, fishing, and recreation to these communities [13]. The site is enclosed by Alapata Road, New Eleyele Road, and Sango Eleyele Road. Unsurpervised classification of Sentinel2A image of Eleyele area with confirmation from Google Earth image classifies the landcover/land use of the area into four categories (Figure 1b); lake water body (Eleyele Lake, 0.75sq.km), wetlands (5.55 sq.km), Urban (11.25 sq.km), and grassland/cropland (6.21 sq.km).

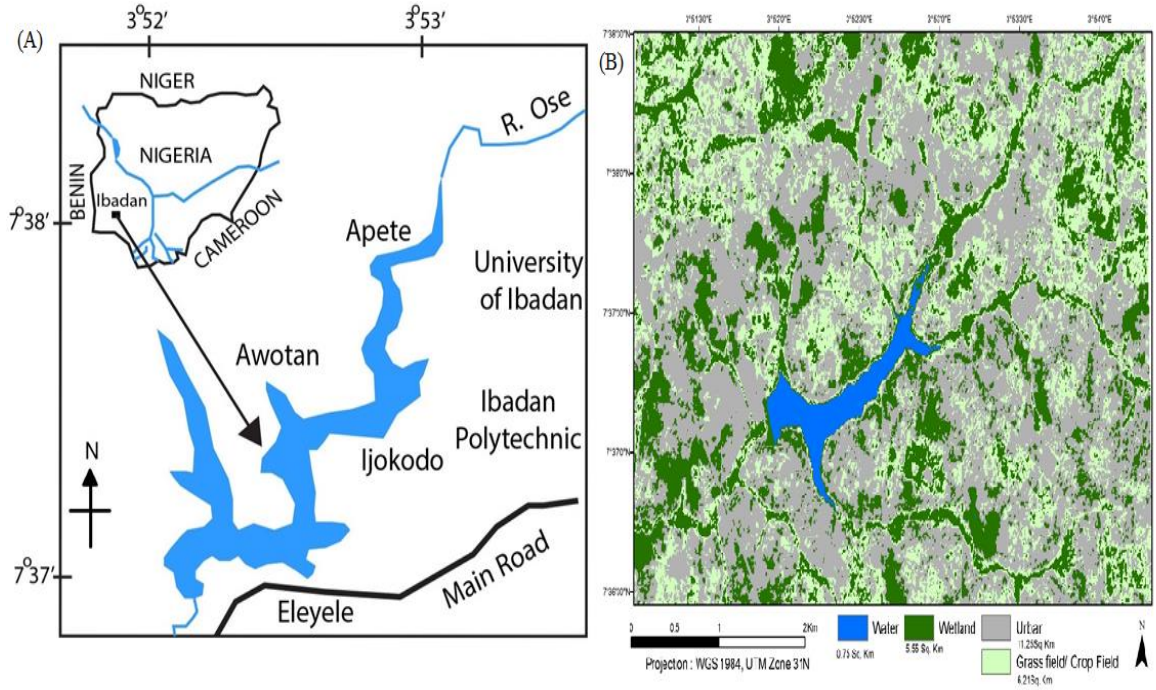

Figure 1: A; Location map (modified after [15]), and B; land use map of the Eleyele and environs

1.2 Geology of The Study Area

Geology of Ibadan and environs, including Eleyele Lake and environs, falls within the Precambrian rocks of southwestern Nigeria (Figure 2a) which is part of the Nigerian Basement Complex. The major rock types within the southwestern Nigerian Basement complex includes schist-quartzites, granite-gneiss, banded gneiss, augen-gneiss, and migmatites [5],[13], while minor rock types such as pegmatite, aplites, quartz veins, and dolerite dykes intrudes the main rocks in sevaral places. Gneisses are migmatized in some places, and characterized by predominantly medium-sized grains while schist-quartzites occur as elongated ridges striking NW-SE [13]. The major rock exposures within Ibadan area includes Pegmatite/quartz vein, biotite granite gneiss, hornblende-biotite-granite, migimatite biotite-hornblend gneiss, quartz, gneiss schist complex rocks. (Figure 2b). The drainage system is controlled by the bedrock geology with a characteristic dendritic pattern of the streams and rivulets being structurally controlled [19].

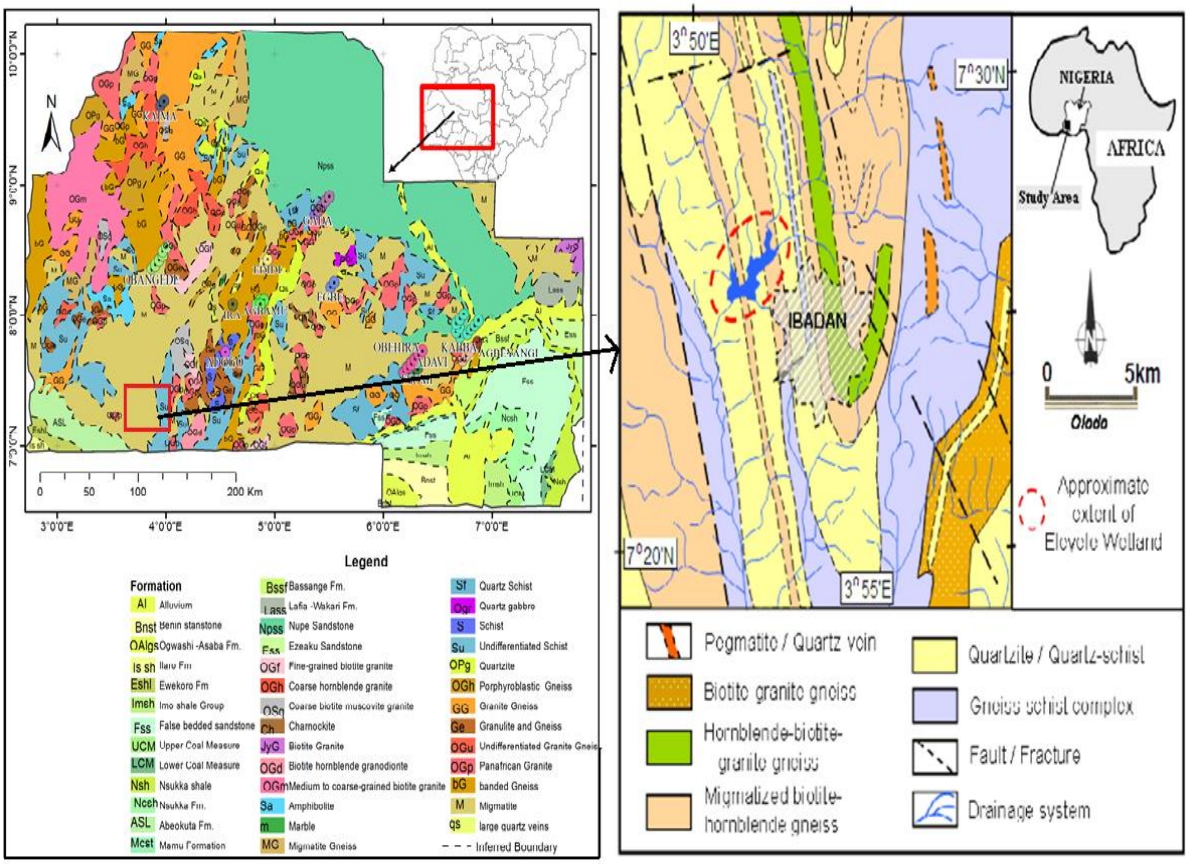

Figure 2: Geology map of southwest Nigerian Precambrain Basement Complex [10], and lithological map of map of Ibadan[19]

2.0 Methology

For the Purpose of this research, twenty nine (29) water samples were collected from Eleyele Lake and wetland (Figure 3a). Twenty (20) of the samples were collected from the main lake, and the rest (9) were colleted at the different points where effluent streams enters the lake. Various hand held meters were used to measure the insitu temperature, pH, total dissolved solids (TDS), and electrical conductivity. Two types of water samples were collected at each

site in polythene bottles of different sizes; unfiltered un-acidified (UFUA) water filling 1000mls size and ensuring no air bubble is trapped in them, and 125mls size unfiltered and acified with drops of 1 molar $HNO_{3(aq)}$ to make water sample pH equal 2, and this is to prevent the precipitation of cations on the walls of the plastic container, and preserve various reactions taking place within the flowing water. On site observation of water colour, and turbidity was done. The unfiltered un-acidified Water samples were tested for pH, total alkalinity, electrical conductivity (EC), total disolved solids (TDS), carbonates(CO_3^-), bicarbonate(HCO_3^-), nitrate (NO_3^-), and sulphate (SO_4^{2-}) at a laboratory close to the field base camp. Chemical analyses was done using inductively coupled plasma–mass spectrometry (ICP–MS) to analyzed for 60 suites of elements present in water samples at Veritas laboratories, Ontario Canada. The data set generated from physical and chemical analysis of the samples were analyzed using exploratory/descriptive statistics to help understand the distribution of various parameter, and it involves sumarizing the information in a data set and presenting it in a tabular format with categories such as sample count, minimum and maximum values, mean, and count of samples that exceeds Nigeria Standard for Drinking Water Quaility threshold for a given parameter in water. Geostatistical modeling involved log transformation of the data set to get them to follow a normal distribtuion requirement, structural analysis (variography) involved the computation of omnidirectional semivariogram to produce the variogram cloud, and the experimental variogram is gotten by binning the variogram cloud and computing the average within each bin, the theoretical variogram models is fitted to the experimental variogram and parameters that capture spatial correlation or depedence (range, sill, and nugget) are measured. Ordinary kriging involved the spatial estimation/interpolation approach adopted, and the grid used has a dimention of 25x25meters (Figure 3b), and all sample locations were used for interpolation. Two maps were produced for geostatistical estimation effort; these are the estimation (parameter), and estimation variance maps. The estimation variance is a measure of estimation error. The estimation variance is used to compute the lower and upper confidence limit map and is based on probability theory that has a two tailed distribution, and the probability of containing the true value, Z is 1-α [18], and α is level of signifcance. The formular proposed by [18] for the computation of the lower and upper confidence limit is given in Equation (1).

$$\left(\hat{z} - t_{\frac{\alpha}{2},n-1} . s_{\hat{z}}\right) \leq \hat{z} \leq \left(\hat{z} + t_{\frac{\alpha}{2},n-1} . s_{\hat{z}}\right) \quad (1)$$

Where $\hat{z}$ is the estimated value, $t_{\alpha\frac{1}{2},n-1}$ is the Student's t with n-1 degrees of freedom at α/2 significance level. $s_{\hat{z}}$ is the sample standard deviation and n is the sample size. Back transformation of all the parameter interpolation maps was done, and binary estimate map was also generated by comparing the upper confidence limits estimate of each parameter with the Nigerian Standard for Drinking Water Quality , NSDWQ [9] threshold values in which areas below these threshold are delineated in green and those above in red.Ba, Na, Fe, Al, Mg, Pb, pH, EC, and TDS were the variables selected for exploratory/descriptive statistic, and geostatistical modeling and estimation. Multivatriate analyses of Eleyele Lake data set was done using principal component analysis(PCA), and hierarchical cluster analysis (HCA). Ca, Cl, K, Mg, Mn, Na, P, Si, Fe, S, HCO3, NO3, SO4, CO3, PH, EC, and TDS were the variables selected for use in these analysis. All variables in the data set were log transformed and scaled to set the standard deviations to 1. This is to remove outliers and achieve multivariate normality. After running the principal component analysis algorithm, scree plot (Bar plot of the percentage of variability or information explained by each principal component) was used to select the optimal number of principal components (PCs) to use for subsequent

interpretation. Pricipal component score (PC-scores) which is used to show how each observation plots on the principal component space/dimensions, and were ellipses were drawn on the PC scores plot based on were the samples were collected effluent/feeding streams, or main lake. To generate the dendrogram that shows the result of HCA, the Ward method was used to join clusters, because it is considered to be efficient, and uses the analysis of variance (ANOVA) approach to evaluate the distances between clusters, and also the Hopkins statistic was computed to evaluate if the dataset is ameanable to cluster analysis and was in the affirmative. Elbow plot was use to determine the optimum number of clusters, and three clusters was found to be optimum for this dataset. Qgis was used to to digitize the outline of the lake into a shapefile, which was imported into R statistical software for geostatistical modeling and estimation with the help of sp, lattice, rgdal, and gstat extension packages. Multivariate analysis was done with the help of FactoMineR and factoextra R packages based on the procedures outlined by [7][8].

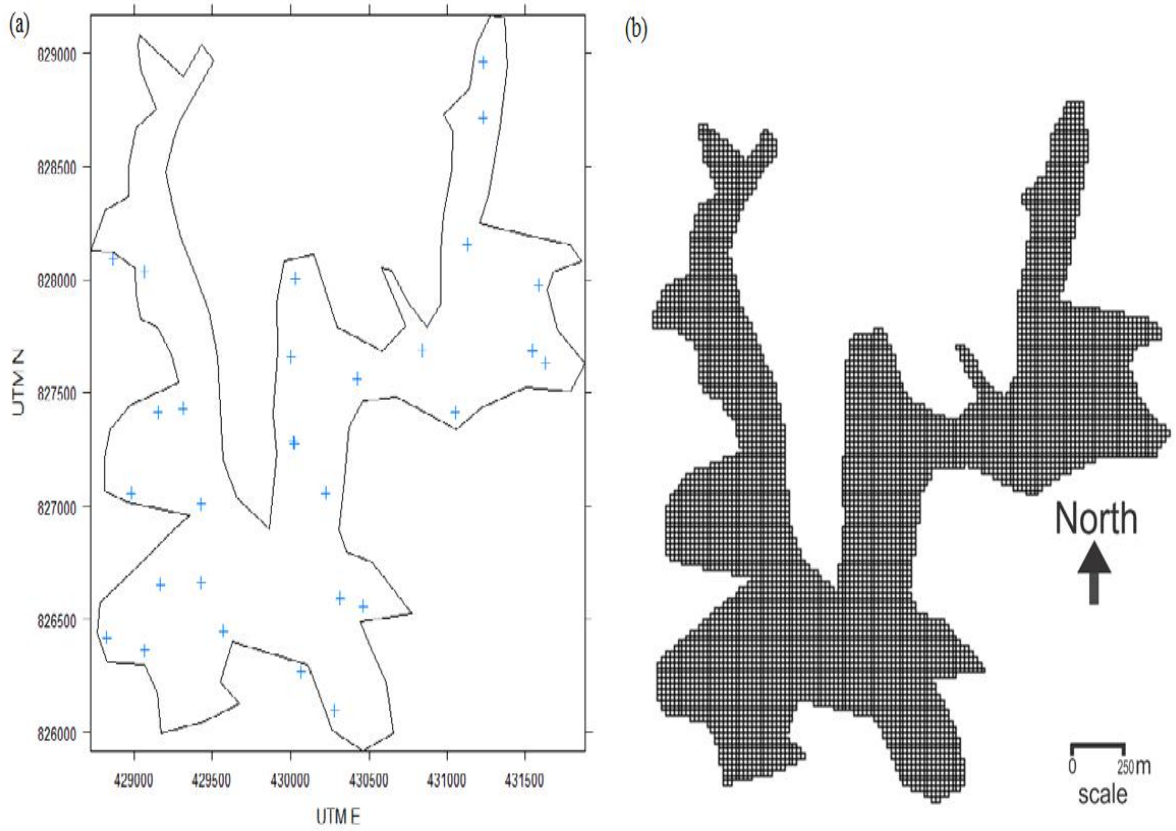

Figure 3: Sampling location of Eleyele Lake (a), and Grid mesh (b) used for geostatistical interpolation of Eleyele Lake physichochemical parameters (Cell dimension is 25m).

3.0 Result and Discussions

3.1 Exploratory/Descriptive Statistics

Table 1 presents the summary statistics of some physicochemical parameters of the water samples, and count of samples with parameter values exceeding the threshold stated in Nigeria Standards for Drinking Water Quality, NSDWQ [9]. The average pH of the water samples is alkaline with a value of 7.34 and ranges between 6.87 and 7.71. Electric Conductivity (EC),

varies widely with a minimum of 290µS/cm and maximum of 1090µS/cm (mean= 456.6 µS/cm); higher values of EC corresponse to higher dissolved species/ions. Total dissolved solids varies between 193 to 726mg/L; and has an average value of 303.98mg/L, Ba, Na, Fe, Al, Mg, and Pb have ranges beween 0.07- 0.29mg/L, 20.46-117.52mg/L, BD-14.57mg/L, BD-1.53mg/L, 7.13-18.41mg/L, and 0.00-0.02mg/L respectively. From column 7 of table one in which count of samples exceeding NSDWQ threshold for each parameter is presented, it can be seen that 17 out of 29 samples have Fe concentrations more than NSDWQ. Other parameters that could also be a source of concern include Al (NSDWQ exceedance count =7), TDS (NSDWQ exceedance count = 4), EC (NSDWQ exceedance count = 2), and Pb (NSDWQ exceedance count = 3).

Table 1: Summary statistics, and countof samples with parameter values greater than threshold valuestated in Nigeria Standards for Drinking Water Quality (NSDWQ, 2015)

Parameter	Sample count	Minimum	Maximum	Mean	NSDWQ	NSDWQ Exceeded Count
Ph	29	6.87	7.71	7.34	6.5 - 8.5	0
EC (µS/cm)	29	290.00	1090.00	456.55	1000.00	2
TDS (mg/L)	29	193.00	726.00	303.93	500.00	4
Ba (mg/L)	29	0.07	0.29	0.12	0.70	0
Na (mg/L)	29	20.46	117.52	39.93	200.00	0
Fe (mg/L)	29	BD	14.57	1.84	0.30	17
Al (mg/L)	29	BD	1.53	0.12	0.20	7
Mg (mg/L)	29	7.13	18.41	8.89	20.00	0
Pb (mg/L)	29	BD	0.02	0.003	0.01	3

BD = below detection

3.2 Variography or Structural Analysis

The semivariogram modeled of various considered parameters from the study area is presented in Figure 4, and the various parameters estimated from a semivariogram is presented in Table 2. The semivariogram is used for kriging interpolation because it contains information about spatial autocorrelation between observation locations, and between observation locations and estimation locations.

Table 2 shows that the gaussian model was fitted to all except Fe semivariogram, to which was fitted in an exponential model. Al has the highest distance of spatial autocorrelation (range = 525.63m), while Pb has the least (range=276.42).

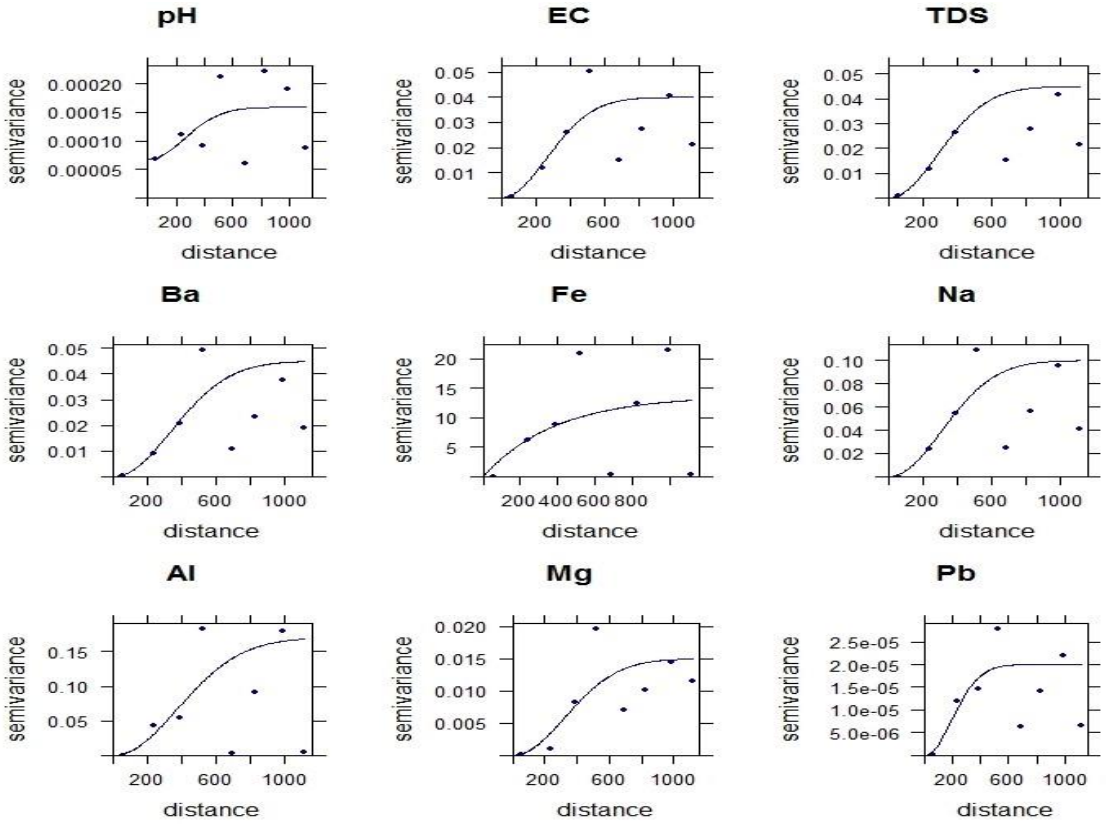

Figure 4 : Fitted ominidirectional semivariogram for various parameters of Eleyele Water Samples

Table 2: Measured semivariogram parameters for selected physico-chemical parameters of Eleyele water samples

Parameter	Transformation	Theoretical Model	Nugget	Sill	Range (m)
pH	Log10	Gaussian	6.7×10^{-5}	9.1×10^{-5}	361.11
EC	Log10	Gaussian	0.0	0.04	377.63
TDS	Log10	Gaussian	0.0	0.045	408.28
Ba	Log10	Gaussian	0.0	0.045	475.55
Na	Non	Exponential	0.0	13.74	390.22
Fe	Log10	Gaussian	0.0	0.1	438.39
Al	Log10	Gaussian	0.0	0.17	525.63
Mg	Non	Gaussian	0.0	0.015	458.59
Pb	Non	Gaussian	0.0	2.0 x 10-5	276.42

3.3 Spatial Interpolation – Ordinary Kriging

The resulting estimation maps shown in Figure 5a and Figure 5b are the possible condition of the Eleyele Lake based on the samples collected for this research. The first, second and third columns in Figure 5a and Figure 5b displays the lower confidence limit, the estimation map, and upper confidence limit map of the modeled paramters respectively. The last column are

binary maps showing areas where the upper confidence limit value of the estimation map has exceeded Nigerian Standard for Drinking Water Quality (NSDWQ) values in red and below in green. These binary maps of the water quality indicators/paramters show that EC, Fe,Na, Al, and Pb concentration are above the NSDWQ threshold values in many locations.

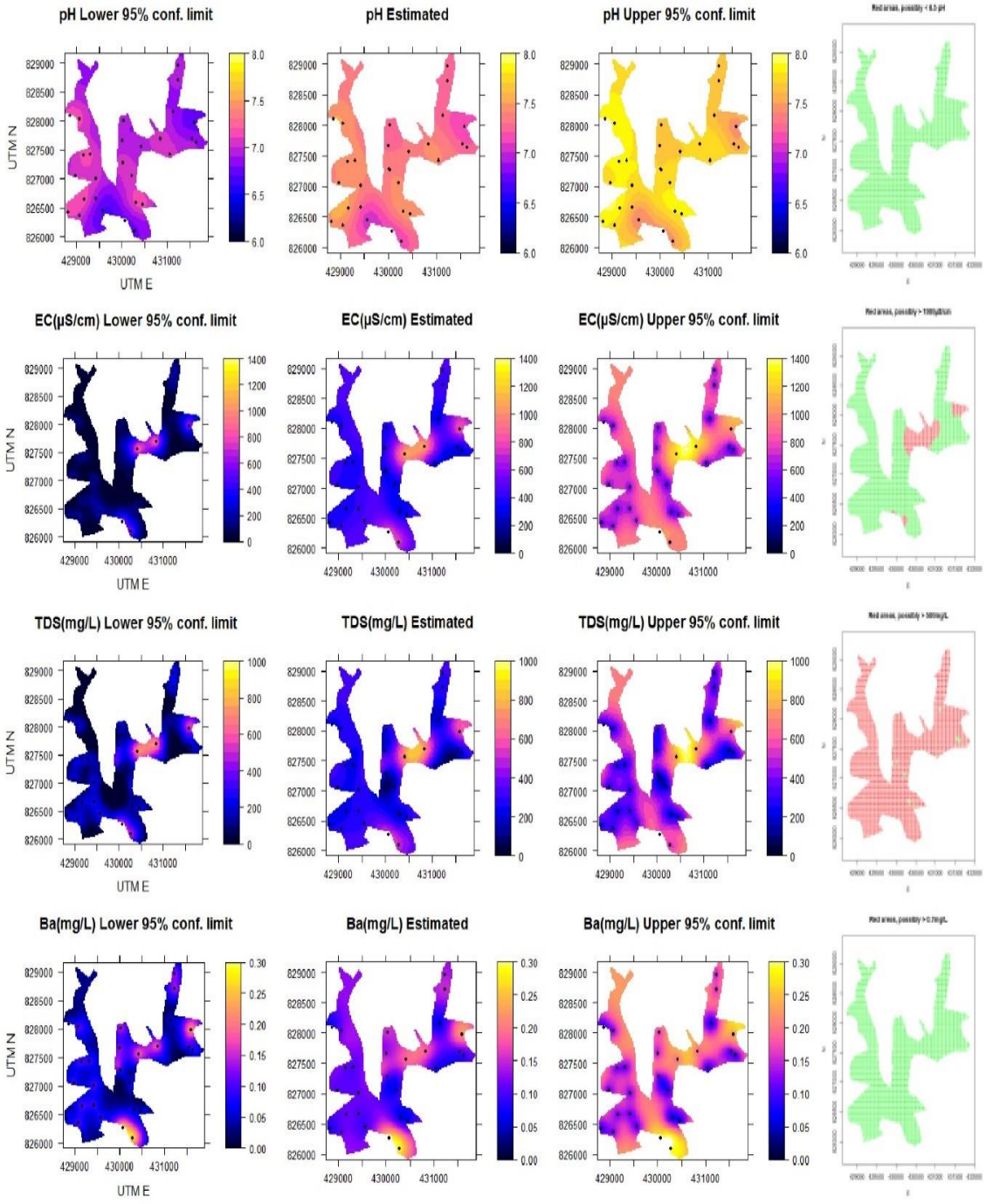

Figure 5a : Ordinary Kirging estimation map of water quality parameters in the second column, the lower and upper confidence limit of estimation map are displayed in the first and third columns respectively. The last column is a binary map showing possible cotaminated areas i.e. where Nigerian Standard for drinking water quality has been exceed in red.

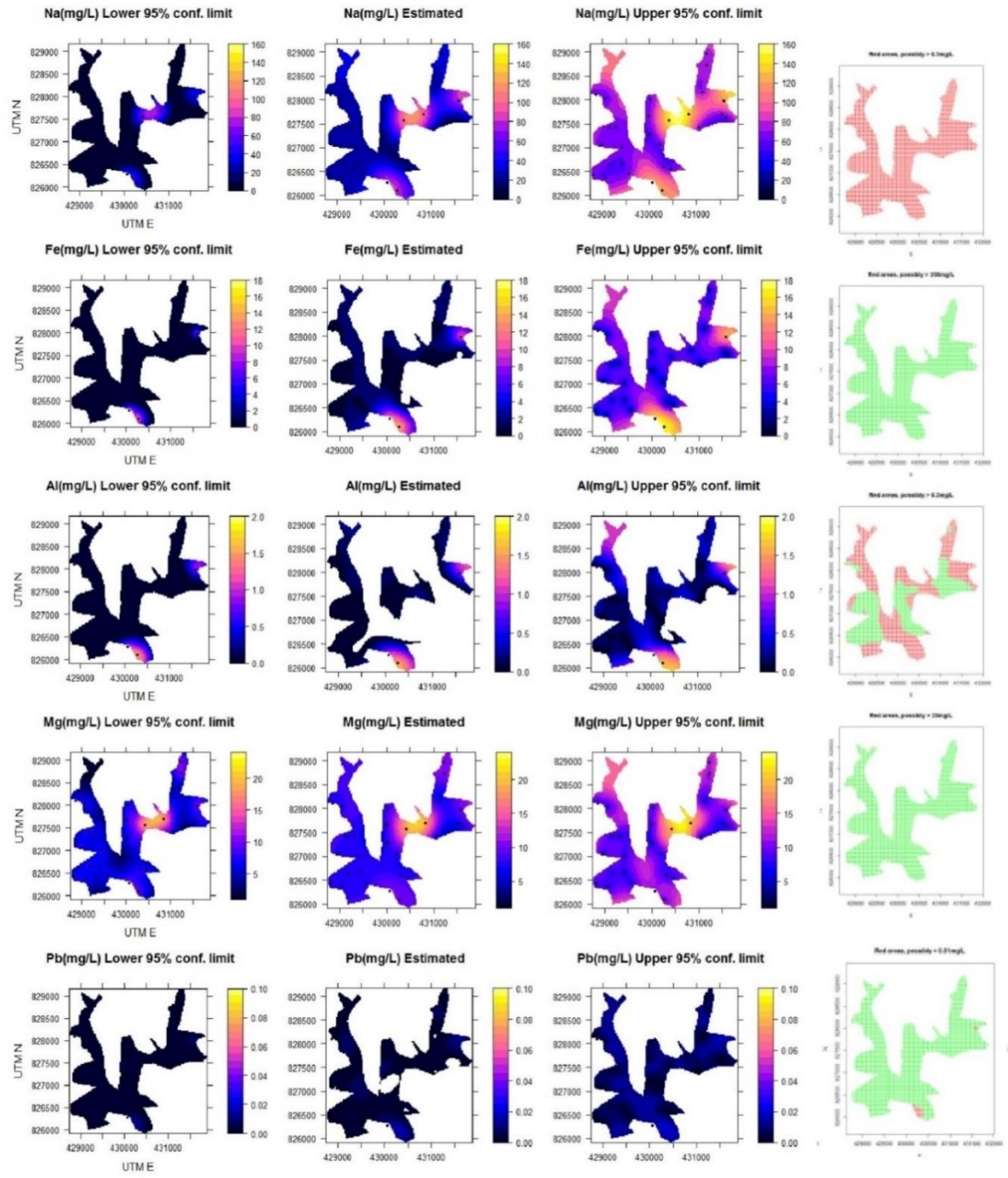

Figure 5b : Ordinary Kirging estimation map of water quality parameters in the second column, the lower and upper confidence limit of estimation map are displayed in the first and third columns respectively. The last column is a binary map showing possible cotaminated areas i.e. where Nigerian Standard for drinking water quality has been exceed in red.

3.4 Multivariate Analysis

Principal component analysis (PCA), and hierarchical cluster analysis (HCA) are the mulivariate analytical techniques used to characterize Eleyele water samples. Ca, Cl, K, Mg, Mn, Na, P, Si, Fe, S, HCO3, NO3, SO4, CO3, PH, EC, and TDS were the variables used for both PCA and HCA.

3.4.1 Principal Component Analysis (PCA)

The screen plot (Figure 6) of the principal components (PC) show that the first 2 principal components accounts for 79.7% of the variability while 88.1% is accounted for by the first 3 principal components. This would suggest further interpretation of result of PCA should focus primarily on principal components 1 and 2. Table 3 shows the principal component loadings of the first two PCs. Varimax rotation was applied to the PC loadings so as to filter and to highlight the correlation of the PCs with a few variables and it can be seen that Ca, Cl, K, Mg, Na, P, Si, HCO3, NO3, SO4, CO3, EC, and TDS are highly correlated with PC1, while Mn, Fe, Ph and S are highly correlated with PC2. Figure 7 is the variable factor map which is a visualization of the PC loadings. The length and direction of each variable vector is its magnitude of correlation with the PCs. Variables plots on opposite are negetively correlated with one another; hence it can be seen from figure 7 that as pH decreases the concentration of other variables increases. Ca, Cl, K, Mg, Na, P, Si, HCO3, NO3, SO4, CO3, EC, and TDS have strong effect on PC1, while Mn, Fe, and S dorminate PC2. The plot of sample PC-scores (figure 8) clearly reveals two clusters; PCA was able to group samples based on the environment of sample collection ; main lake (points with blue ellipse) and effulent streams (points with pink ellipse). The clusters may also mean that water in the main lake are of higher quality than the water in effulent streams.

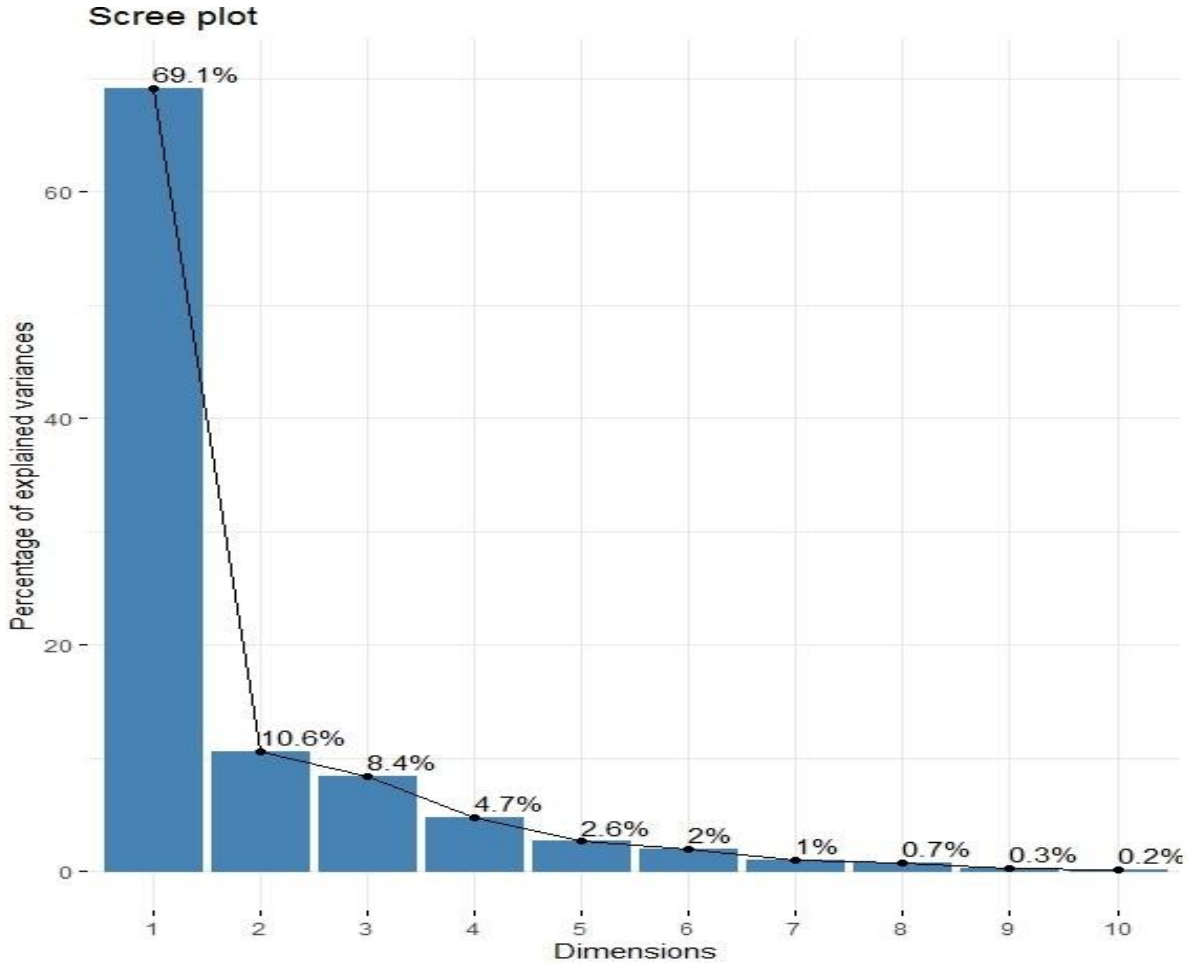

Figure 6:Scree plot of principal components. The height of the bar is proportion to the level of expalined variability by each PC

Table 3: PCA Loadings of the first two principal components. PCA loadings greater than 0.6 are bolded to show strong effect/correlation of the variable on the Principal components

Variables	PC1	PC2
Ca	0.90	0.35
Cl	0.96	0.21
K	0.94	0.30
Mg	0.85	0.18
Mn	0.13	0.89
Na	0.92	0.34
P	0.74	0.59
Si	0.86	0.10
Fe	0.32	0.91
S	0.12	0.62
HCO3	0.73	0.51
NO3	0.79	0.22
SO4	0.88	0.11
CO3	0.81	0.26
PH	-0.20	-0.53
EC	0.85	0.46
TDS	0.85	0.47

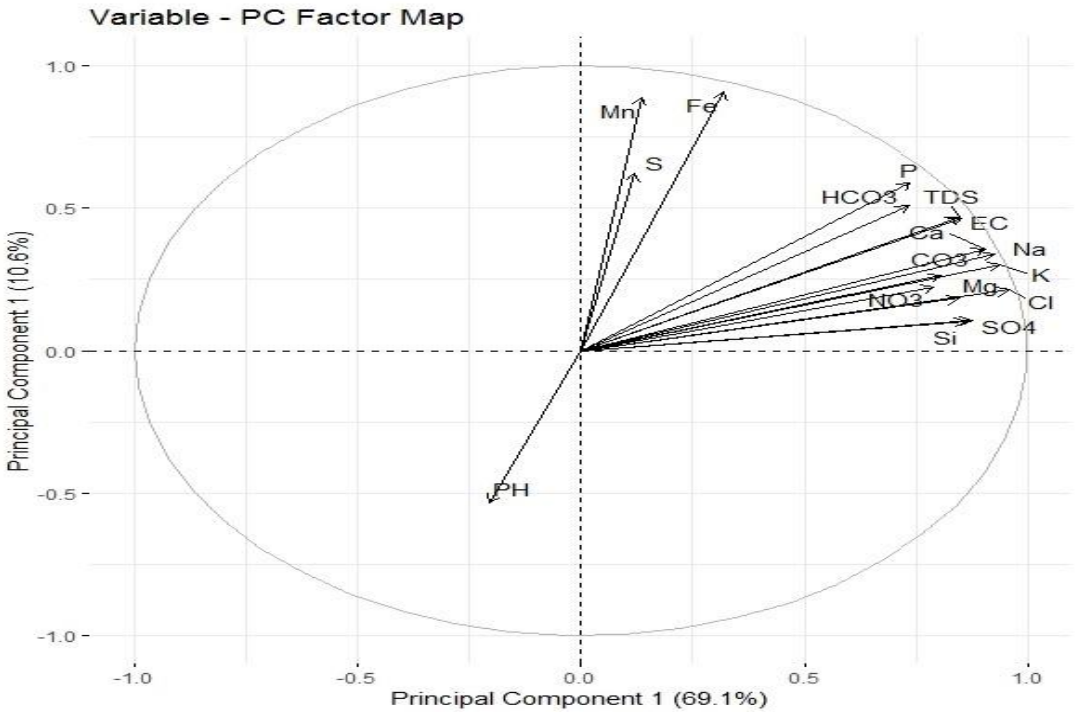

Figure 7: Variable – Factor Map of Eleyele Lake and Wetland hydrogeochemical and physicochemical parameters.

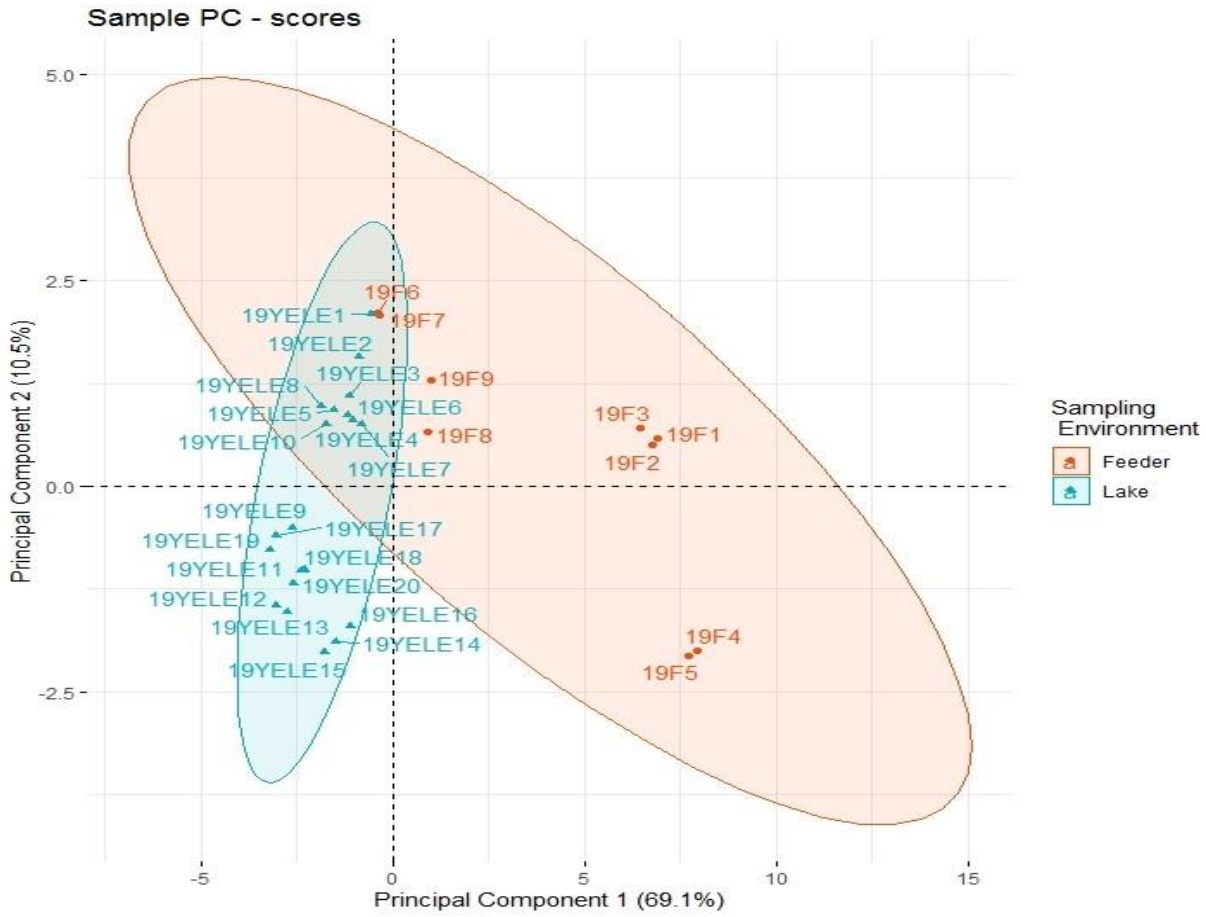

Figure 8: Eleyele Lake and wetland sample – PC scores. This shows separation of samples from the two sampling domain beautifully, with a perfect separation.

3.4.2 Hierarchical Cluster Analysis (HCA).

Hopkins statistics for Eleyele hydrogeochemical dataset is 0.176 meaning the dataset is ameanable to clustering (0.176<<0.5). Elbow plot (Figure 9) of Eleyele dataset reveals 3 optimum cluster groups. Figure 10 is the dendrogram plot of Eleyele hydrogeochemical dataset from hierarchical clustering. From left to right of figure 9, samples 19F1, 19F2, 19F3. 19F4 and 19F5 belong to the cluster 1 tree. 19F6, 19F3, 19F8, 19YELE1, 19YELE2, 19YELE3, 19YELE4, 19YELE5,19YELE6, 19YELE7, 19YELE8, and 19YELE10 belong to cluster 2 tree. 19YELE9, 19YELE19, 19YELE11, 19YELE12, 19YELE13, 19YELE17, 19YELE18, 19YELE20, 19YELE14, 19YELE15, and 19YELE16 belong to the cluster 3 tree. Since the clustering is based on water quality indicators/parameters, it is probable that water quality might be increasing from left to right of the dendrogram. Piper diagram [17] of the samples colour coded based on their cluster group(figure 11) shows that cluster 2 and cluster 3 samples are significantly alike and are of Ca^{2+}-HCO_3^-hydrochemical water type. Clusters 1 sample plots on the mixed Ca^{2+}-Na^+-HCO_3^- hydrochemical type field. Enrichment of Na in the cluster 1 samples may be as a result of household discharges of soapy/ detergent water into effulent streams.

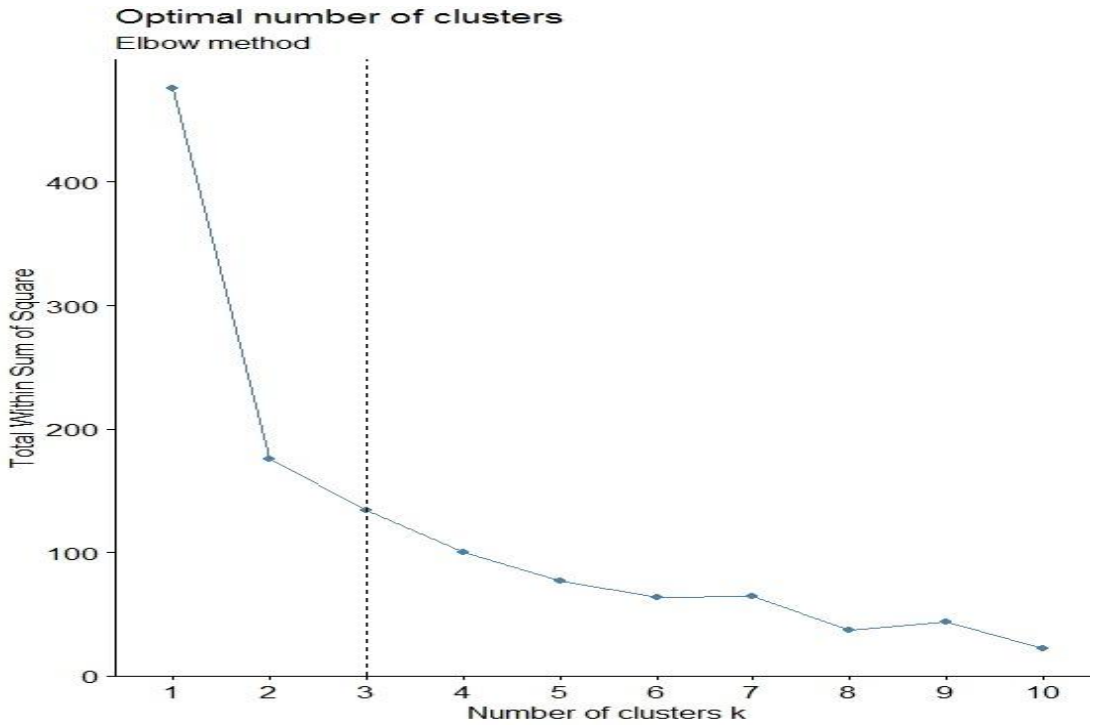

Figure 9: Eleyele Lake and wetland elbow plot. There are 3 optimum cluster represented by vertical dotted line is the line of optimum clusters.

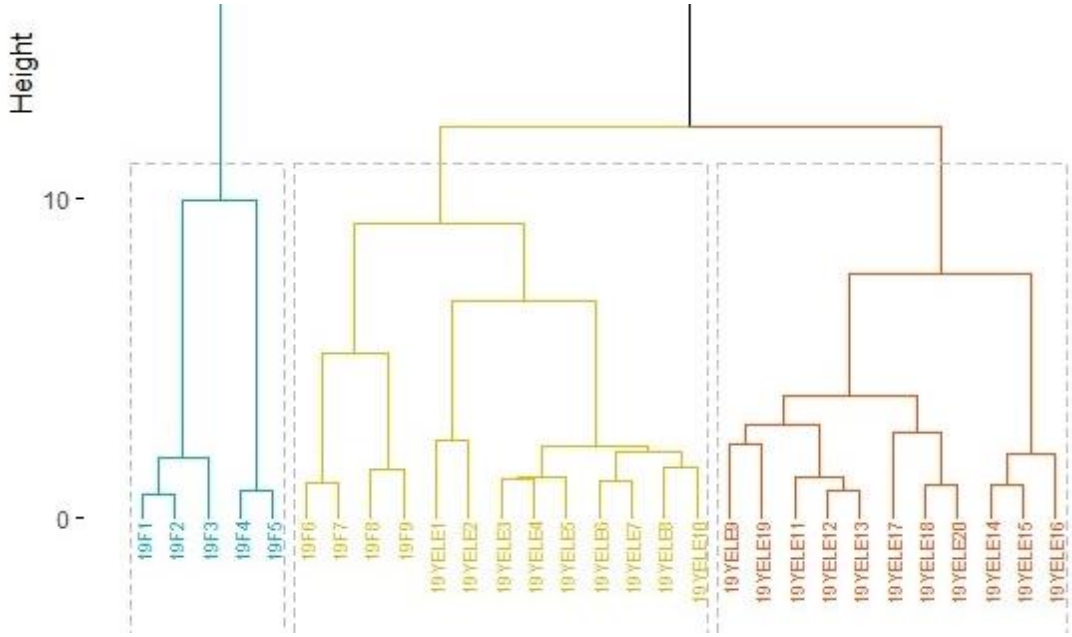

Figure 10: Dendrogram showing result of Hierarchical Clusting Analysis for Eleyele physicochemical dataset. Water quality might be increasing from left to right of the dendrogram.

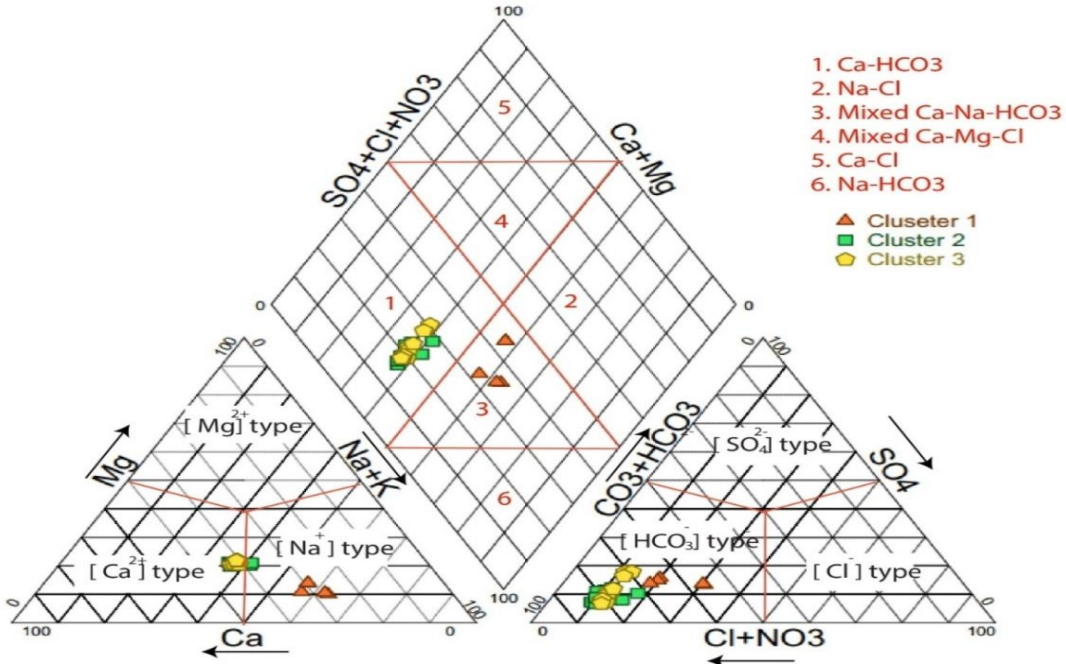

Figure 11: Piper Diagram [17] of Eleyele Lake and Wetland samples

4.0 Summary And Conclusion

Geostatistical analysis result, and the subsequent binary map of exceedence of a parameter threshold show that EC, Fe, Na, Al, and Pb concentration are above the Nigeria standard in many locations. PCA component analysis result shows that 79.7% of the variability in the original data set is contained in the first two principal components, and plot of the principal component loadings on the factor – variable map indicates that pH influences the concentrations of several other parameters. Principal component analysis was also able to identify two clusters which was indicative of where the water sample was collected; Lake or effluent/Tributary stream. Hierarchical clustering identified three clusters of samples but subsequent piper digram of the clusters revealed that clusters 2 and 3 samples were alike and less contaminated by sodium (Na) when compared to cluster 1 water samples.

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