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USING MULTIVARIATE STATISTICAL METHODS FOR THE ASSESSMENT OF THE SURFACE WATER QUALITY FOR A RIVER: A CASE STUDY

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ABSTRACT

Multivariate statistical methods, such as principal component analysis (PCA) and cluster analysis (CA) were utilized to the surface water quality data of the Shatt Al Arab River (Iraq), over 4-year period on a monthly basis, with tracking at five different monitoring sites across the river for seven water quality parameters. The study area included the Shatt Al-Arab River, which is one of the most essential rivers that formed because of the confluence related to the Euphrates along with Tigris at the city of Al-Qurnah in Basrah province, southern Iraq. Water samples were analyzed for dissolved oxygen (DO), phosphate (PO_4), calcium (Ca), magnesium (Mg), nitrate (NO_3), chloride (Cl), and sulphate (SO_4) were analyzed making use of standard methods. This research assessed and clarified the complex data sets of water quality and apportioned of pollution sources to obtain better information concerning water quality and to demonstrate the data structure as well as to analyze temporary and spatial variations regarding the water quality. The results of this research were exposed to principal component and factor analysis with three latent factors which were extracted with 98.9 % of the total variance explained. Based on gaining information, it will be possible to design a future, ideal sampling approach, which might minimize the number of monitoring sites and additionally associated cost.

Key words: Water Quality, Principle Component Analysis, Cluster Analysis.

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1. INTRODUCTION

The most important factor that maintaining health and the state of disease, for human and animals, is the surface water quality. Surface water quality in a location is mostly determined by natural processes (soil erosion and weathering) and also by anthropogenic inputs (discharge of municipal and industrial wastewater). The anthropogenic discharges appoint a constant polluting source, while surface runoff, largely influenced by climate within the basin, is regarded a seasonal phenomenon [1-2]. Atmospheric pollution, land use, use of agricultural chemicals, effluent discharges, eroded soils and other human activities are the major factor determining the quality of both surface and ground water [3].

Environmental pollution, mostly of water sources, comes to be public interest. Large researches being done on anthropogenic contamination of the ecosystems [4-5]. Nonetheless, because of spatial and temporary variations in water quality, is required to provide a representative and reliable estimation of the surface water quality, by a monitoring program [6]. The monitoring program is necessary for the evaluation of surface water quality. Nonetheless, monitoring programs for water quality generate complicated and large data sets that are usually complicated to interpret by traditional statistical analyses.

Shatt Al-Arab River is one of the most crucial irrigation and drinking water resources in the south of Iraq and it is the main water source for Basrah city, south of Iraq. There is a large quantity of uncontrolled wastewater discharges into the Shatt Al Arab River without monitoring. Discharge of uncontrolled wastewater causing instant and long-term water quality influences on the users [7]. Presently, disposal of domestic, industrial, and agricultural effluents into the natural water bodies, such as Shatt Al-Arab River, results increased salinity and serious surface and ground water pollution. Shatt Al-Arab River's water is used for domestic, industrial, and irrigation uses, and it is the main source of water for a great number of citizens in Basrah. In Basrah city, drinking water comes from treated surface water of the Shatt Al-Arab River.

In the last decade, the application of various multivariate statistical techniques, such as cluster analysis (CA), principal component analysis (PCA), and factor analysis (FA), has been used extensively for data reduction, interpretation, and classification [8-10]. Multivariate statistical techniques are helpful in the explanation of complex data matrices for better comprehending of water quality and ecological status of any study area under investigation. Multivariate statistical techniques enhance drawing meaningful information from matrices of complex data such matrices created by long-term water quality monitoring programs. These techniques permit the detection for the possible sources that affect water systems and provide a tool that is important for dependable management of water resources, including quick solution for pollution problems [11-12].

In the current study, seven water quality parameters in the collected water samples for a period of four years (2011–2014) from the surface water of the Shatt Al Arab River, analyzed on a monthly basis. The large data set obtained in the present study was exposed to the PCA and CA multivariate techniques in order to evaluate the information about the similarities and/or dissimilarities existing among the sampling that is different, and to determine the impact of the pollution sources on the parameters of the water quality and to find out water quality variables concerning spatial dissimilarity. The raw data must be standardized before using it in the CA, because the variables of water quality have various units of measurement [13]. The Standardization process often tends to reduce the impact of the difference on the variance of the variables and removes the effect of different units of measurements as well as it makes the data dimensionless. The objective of applied extensively multivariate statistical techniques for water quality data of the Shatt Al-Arab River in the present work is to interpret the data structure and to assess temporal variations in the quality of raw water before it pass to the water treatment plants.

2. MATERIALS AND METHODS

2.1. Study Area

The study area in this research includes the Shatt Al-Arab River (Figure1). The Shatt Al-Arab River is a river consisting of the confluence of the Tigris and Euphrates rivers in the southern part of Iraq. The two rivers meet in Qurna city, the northern entrance to the Basrah city. The Shatt Al-Arab River is about 190 km long and is flow to the Arabian Gulf at the edge of the Faw city, which is the most extreme point in southern Iraq.

All waters of the Shatt Al Arab River till 1975 were a part of Iraq, but under the Algiers agreement, Iraq relinquished the eastern coast bordering Iran. Shatt Al-Arab River is the main source of drinking and irrigation water for many cities in Basrah. It may be assigned to the effluents of different industrial wastes approaching at the river water.

The south part of the river constitutes the border between Iraq and Iran until eventually it discharges into the Arabian Gulf, with a total length of 190 km, the Shatt Al Arab River widens over its course, expanding from a width of 250-300 m near the Euphrates-Tigris confluence to almost 700 m near the city of Basrah and more than 800 m as it approaches the river mouth. There are many tributaries which are feeding the Shatt Al-Arab River with small sources of water. These tributaries are Al-Huyaza, Al-Hammar, Al-Qurna marshes as well as Al-Karoon River which flows with its left part.

2.2. Data Analysis

Water samples from the Shatt Al-Arab River regularly analyzed over a four year period (Jan 2011–Dec. 2014), on a monthly basis, for dissolved oxygen (DO), phosphate(PO4), calcium (Ca), magnesium (Mg), nitrate (NO3), chloride (Cl), and sulphate (SO4). The water samples were stored after collected from the river for tests. All the units of the collected water quality parameters are expressed in mg/l. The analyses of the previously mentioned parameters were executed in the environmental laboratory of south region in Basrah and were implemented by methods outlined in the Standard Methods for the Examination of Water and Wastewater [14].

2.3. Data Treatment by Statistical Methods

All mathematical and descriptive statistics were prepared to make use of statistical packages SPSS 22 and Minitab 16 software that were used for PCA and CA, respectively. Multivariate analysis of the river water quality data set has done through utilizing of principal component and cluster analysis techniques.

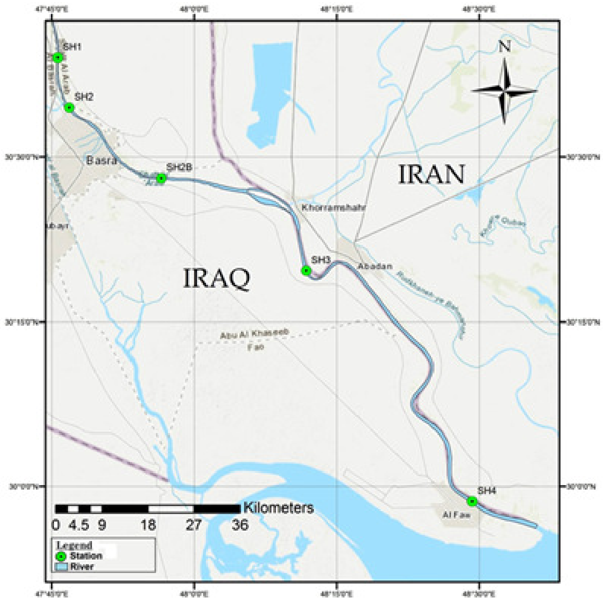

Figure 1 Map of Shatt Al-Arab River and Basrah, south of Iraq

2.4. Multivariate Statistical Methods

Principal components analysis (PCA) is structured to turn the original variables to new, un-correlated variables, known as the principal components (PC), that are linear combinations regarding the variables being original. The new un-correlated variables lie along with the maximum variance directions. PCA provides a means that the objective of indices of this type, hence the variation within the data is accounted for as briefly as possible [15]. To reduce the large data sets of correlated variables into limited composite indices, PCA/FA can be applied for that reason. The main purpose of using of PCA/FA is to define the underlying structure and to offer initial visual information regarding the temporal structure of variation.

Factor analysis goes one-step further and attempts to figure out the underlying structure or construct. It tries to show exactly variables being certain correlated. PCA is usually used as a primary-step to ascertain how many factors to be used in the factor analysis. PCA is a mathematical technique used for data-reduction and it generally does not assume any specific distribution of the data. All used variables should be as near to a normal distribution as possible prior to carrying out PCA/FA [16]. Thus, all the variables were tested for normality and those that disregarded this assumption were changed just before the consecutive analyses. Standardization of the data must be used to prevent possible consequences because of a different order of the magnitude of the variance for the variables [1,17]. The eigenvalues criterion and the scree-plot were used to determine the number of factors that extracted.

The CA technique is a category this is certainly unsupervised that requires measuring either the similarity or the distances between the objects come to be clustered. CA had been utilized to identify the natural groupings of data with regards to the variability that is temporal. The observations had been grouped into clusters to ensure that each cluster was as homogeneous as possible pertaining to the clustering variables and the groups were as various as possible.

Hierarchical agglomerative clustering (HAC) is one of common method, which supplies instinctual similarity relationships between any sample and total data set, additionally is usually explained as tree diagram, generally known as the dendrogram [18]. The dendrogram introducing a picture of the groups and their distance and offers a visual overview of the clustering process. The Euclidean distance, commonly provides the similarity between two samples and a distance, and can be exemplified by the difference between analytical values from the samples [19].

In this study, PCA was utilized to summarize the statistical correlation between the components in the collected water samples from the Shatt Al Arab River. The clusters were created by the use of hierarchical agglomerative CA which doesn't include being familiar with the number of clusters in advance. Cluster analysis was used to discover the spatial similarity for sites group within the monitoring network. To measure the similarity between each data point, Squared Euclidean Distance (SED) was applied. The Ward's linkage method was applied to measure the distances between clusters. The concentration order between all the studied parameters was greatly differ; hence, the statistical results must certainly be strongly biased by any parameter with higher concentrations.

3. RESULTS AND DISCUSSION

The range of values, means and standard deviations of the obtained results are presented in table 1. The concentration of dissolved oxygen in water is impacted by the water temperature and the chemical or biological processes that occur in the aquatic system. The monitoring of oxygen concentration is an essential matter in the aquatic system [20]. The low level of DO concentration may be due to the untreated sewage or due to the organic pollutants that attach the intake of dissolved oxygen in the water during warm conditions. The results also show that there is a high level of major cations concentrations (Ca and Mg) and also high concentrations of major anions (Cl and SO4) in river water samples that was collected. Based on Versari et al. [21], when the chloride concentrations in water are higher than 200 mg/l, it may cause unpleasant taste of water and the water regarded to be a risk for human wellness. Phosphate and nitrate concentrations (Table 1) varied significantly because of river water contamination causing from domestic sewage and agricultural sources that arrived from the upstream agricultural areas in which the common use of phosphate and nitrogen fertilizers. The higher concentrations of phosphate are due to anthropogenic activities, as for example, organic pollutants releases, fertilizer usage, and release of wastewater from domestic sources [22].

Low DO concentrations, 2.19 mg/l, was noticed on the monitoring site 3 (SH3), while the high level of DO concentrations was observed in the monitoring site 1 (SH1) during the study period. Mean of DO concentrations in the collected water samples from all sites (SH1, SH2, SH2B, SH3, and SH4) was found to be 7, 6.8, 7, 6.5, and 6.8, respectively. Mean of phosphate concentrations during the study period showed no significant variations, presenting averages ranged between 0.27 mg/l and 0.32 mg/l for all of the monitoring sites.

Table 1 Range, mean and SD of water quality parameter at the monitoring station during the study period

Parameters	Station					
		SH1	**SH2**	**SH2B**	**SH3**	**SH4**
DO (mg/l)	Range	4.54-11.2	4.01-9.5	3.73-10.8	2.19-9.1	3.3-9.8
	Mean	7.0	6.8	7.0	6.5	6.8
	S.D.	1.8	1.8	1.8	2.1	1.8
PO_4 (mg/l)	Range	0.21-0.6	0.18-0.5	0.17-0.4	0.17-0.4	0.16-0.4
	Mean	0.31	0.32	0.30	0.27	0.27
	S.D.	0.1	0.1	0.1	0.1	0.1
Ca (mg/l)	Range	87-203	99-192	120-216	153-400	128-680
	Mean	130.9	149.1	175.4	210.2	403.7
	S.D.	34.1	32.2	27.3	68.4	176.7

Mg (mg/l)	Range	46-113	36-235	76-202	48-720	175-1464
	Mean	68.6	105.8	123.6	225.9	778.8
	S.D.	18.3	48.6	38.6	221.3	467.4
NO_3 (mg/l)	Range	6.14-15.8	7.74-15.9	7.01-14.2	7.52-13.3	6.51-13.1
	Mean	8.8	11.8	10.2	10.3	9.6
	S.D.	2.7	2.5	1.9	1.8	1.9
Cl (mg/l)	Range	220-718	260-1445	513-2505	408-8123	730-19110
	Mean	372.1	658.1	1019.5	2625.3	9584.2
	S.D.	124.1	359.5	613.5	2443.3	6070.9
SO_4 (mg/l)	Range	140-406	160-600	250-700	250-1000	300-7000
	Mean	271.3	312.5	391.9	422.5	1409.4
	S.D.	71.5	117.3	112.2	216.6	1588.7

The range of Ca and Mg ions in surface water samples from the monitoring sites was found in the range of 87–680 mg/l and 36 –1464 mg/l, respectively. The nitrate values were found in the range of 6.14 –15.9 mg/l, in the river water samples. The level of Cl and SO4 were found in the range of 220–19110 and 140–7000 mg/l, respectively, corresponding to a higher level than WHO recommended values for drinking and irrigation water (Table 2). The measurement of the major ions, Ca, Mg PO4, NO3, Cl, and SO4 in the study area (Shatt Al Arab River) were higher than their concentrations in various surface water bodies around the world [23].

The extracted factors in the current study were three and explained 98.9 % of the total variance contained in the data-set (Table 3). Where the first factor explains the largest proportion (67.9 %) of the total variance and it has positive loadings for calcium, magnesium, chloride, and sulphate, while it has negative loading for dissolved oxygen, phosphate, and nitrate. This factor is considered to be "major cations and anions" factor and depends mainly on Ca, Mg, Cl and SO4, and that is caused by a number of processes such as for example the exchange between the cations [24].

The second factor explained 20.1 % of the total variance and had high positive loadings for dissolved oxygen, phosphate, calcium, magnesium, chloride, and sulphate, while it had a negative loading for nitrate. Factors that loaded with a a variable this is certainly single be difficult to be interpreted. Furthermore, the third factor explained 10.9 % of the total variance and has negative loadings for all the studied water parameters.

Table 2 Water Quality Parameters and Comparative Standards

Parameters	Water uses	
	Drinking	**Irrigation [c]**
DO (mg/l)	> 5b	NS
PO_4 (mg/l)	NS	NS
Ca^{+2} (mg/l)	< 150 [b]	NS
Mg^{+2} (mg/l)	< 100 [b]	NS
NO_3 (mg/l)	< 10 [a]	5-30
Cl^- (mg/l)	< 350 [b]	< 145
SO_4^{-2} (mg/l)	< 500 [a]	NS

[a]: World Health Organization (WHO) guideline recommended for drinking water;

[b]: Iraqi guideline recommended for drinking water ;

[c]: Food and Agriculture Organization standard for irrigation purpose;

NS: Not specified.

The basic statistics of the river water quality are depending on seven water samples are summarized in Table 1, which shows the range, mean and the standard deviation of the results for each of the seven studied parameters. The monitoring sites were regarded as dependent variables, whereas all the measured water quality parameters established the independent variables. Hence, in summary, three factors were extracted and about 99 % of total variance was explained. The result of the PCA base on the correlation matrix of water parameters is expressed (Table 3).

Cluster analysis was employed on the surface water quality data, to identify the spatial similarity and dissimilarity for grouping of monitoring sites (five sites) spread over the course of the Shatt Al Arab River. The dendrogram offered a visual summary regarding the clustering process. It is showing an image associated with groups and their proximity, along with an amazing decrease in dimensionality of the first data. The resulted of the dendogram (Fig. 2), sorted all the five monitoring sites into two statistically significant clusters, as sites 1 (SH1) and 3 (SH2B) that have low distance as compared to the other sites (SH2, SH3, and SH4). The result of CA that depending on the PCA scores is demonstrated in Fig. 2.

As mentioned above, cluster analysis resulted in two major clusters. Cluster 1 involved the site1 (SH1) and the site 3 (SH2B), approximately corresponding to the low polluted sites. The dendogram (Fig.2) explains the abnormality of the monitoring sites 1 and 3, which create one class as cluster 1. Whereas, cluster 2, (sites 2, 4 and 5) correspond to relatively high pollution regions, which receive and collect the polluted effluents from non-point sources, in other words, from domestic, industrial, and agricultural activities. Cluster 2 involved the remaining Sites (2, 3, and 5), somewhere around corresponding to the other polluted sites.

It is clear that the CA approach is practical by provided a trusted classification of the river waters in the Shatt Al Arab River and will make available to tolerably provide for spatial assessment in an ideal way. Hence, the cost in the monitoring sites as well as the number of the monitoring sites along the river will be decreased with no loses for any significance of the results.

Table 3 Eigenvector and eigenvalues of factor matrix of water quality parameter in the river

Parameter	**PC1**	**PC2**	**PC3**
DO	-0.143	0.731	-0.414
PO_4	-0.393	0.173	-0.488
Ca	0.454	0.022	-0.153
Mg	0.451	0.047	-0.182
NO_3	-0.112	-0.646	-0.671
Cl	0.454	0.040	-0.141
SO_4	0.443	0.114	-0.251
Eigenvalue	4.7530	1.4051	0.7644
% of variance	67.9	20.1	10.9
Cumulative %	67.9	88.0	98.9

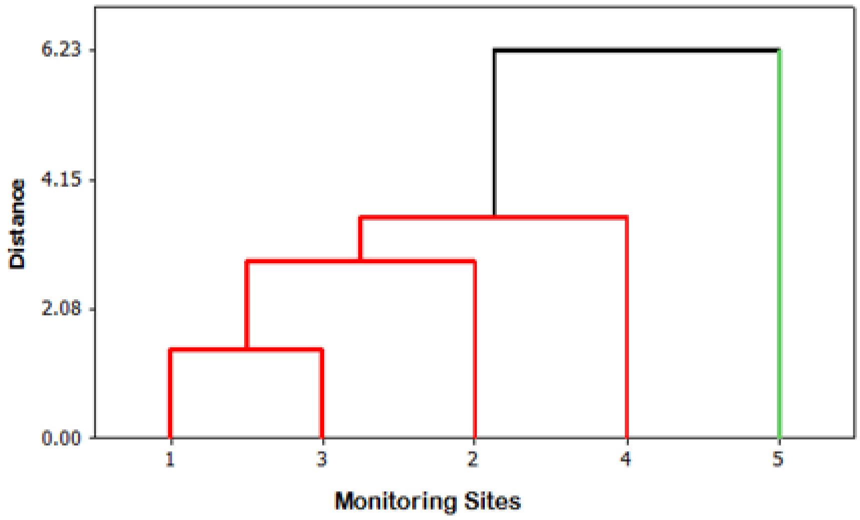

Figure 1 Dendogram for CA based on PCA score. The distance represented by Euclidean and the cluster's combination is supported by Ward method

4. CONCLUSION

In this study, principal component analysis and cluster analysis, which are different of multivariate statistical techniques, are used to evaluate variations in the surface water quality depending on seven original variables that responsible for major variations in the Shatt Al Arab River during 2011-2014. Three potential factors were extracted with 98.9% of the total variance clarified. PCA/CA offered satisfactory indications for detecting variable behavior in the river water data set. The primary cause of degradation of the Shatt Al Arab River is the discharge of municipal sewage, industrial and agricultural wastes of water from the upstream of the Shatt Al Arab River. Cluster analysis reported two major clusters. Cluster analysis grouped the five monitoring sites into two clusters of pollution characteristics. This study shows the effectiveness of utilizing the multivariate statistical techniques for the examination and interpretation of complex data sets, recognition of pollution sources and considering variations in the water quality for effective river water management. Therefore the current study recommends fastening the control on the discharged waste of non-point sources into the Shatt Al Arab River for the protection of the river and its waterways from pollution and to compliance with the general effluent concentration discharge standards. These results should be considered in future planning in using the river's water for drinking purposes.

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