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The use of multivariate statistical techniques in the assessment of river water quality

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ABSTRACT

This study assessed the temporal and spatial water quality variability to reveal the characteristics of the Shatt Al-Arab River, Basrah, Iraq. A total of 14 water quality parameters (water temperature (T), pH, electrical conductivity (EC), Alkanets (Alk), total dissolved solids (TDS), turbidity (Tur), total hardness (TH), calcium (Ca), magnesium (Mg), chloride (Cl), sulphate (SO4), total suspended solids (TSS), sodium (Na), and potassium (k)) were analyzed Use of multivariate statistical methods in a total of three stations for the period 2016-2017. In this study was use a statistical approach to determine the water quality using the Pearson Correlation Index (PCI), Principal component analysis (PCA), and Factor Analysis (FA) were used to analyze the data. Main water pollutant sources were wastewater from agricultural drainage and industrial wastewater. Significant relationships recorded between the investigated parameters based on the results of PCI, at the 0.01 and 0.05 significance levels. Per the FA results, 77.1 % of the total variance explained by two factors.

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1. Introduction

In recent decades, human agricultural and industrial activities have greatly affected the quality of water. To identify and control the water pollution, it is necessary to manage water resources through a water body monitoring program and to analyze the quality of water parameters. Because Shatt Al-Arab River is the main source of water in Basrah, prevention and control of river pollution and reliable water quality information are essential for efficient water resources management. Due to the recent industrial and residential developments in the region, the water quality for Shatt Al-Arab River has become a common research topic. Shatt Al-Arab River flows from north to south through major districts, including Qurna, Shatt Al Arab, and Fao. The Shatt Al Arab River's main economic origin is agriculture, irrigation and plant growth. The river covers a wide area and it is also a major source of drinkable water. The quality of water in the river therefore has a significant impact on life and natural climate. Water quality is directly linked to its various uses, including households, hydropower, agricultural production, fisheries, recreation, industries, ecological systems, navigation and hydropower [1]. The temporal and spatial variability characteristics of river water

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quality can provide complex data to manage the water environment effectively and have become a significant way to manage the water environment [2-4].

The water quality of the river could be evaluated by evaluating some physical, chemical and biological criteria, which vary depending on location, time, weather and pollution sources [5-6]. Anthropogenic actions, including processes of urbanization, agricultural and industrial activities, can lead to water quality deterioration and environmental conditions in the study area [7-8].

Assessment of the quality of river water is needed, in particular, where water from the river is a source of drinking water and is threatened by pollution associated with various human activities along the river [9-10].

Cluster Analysis (CA) is a multivariate technological category whose primary purpose is to arrange objects in a pre-determined criteria for selection resulting in high internal (in cluster) homogeneity and external heterogeneity (between clusters). Hierarchic agglomeration is the most common technique, which offers logical similarity-relationships between a sample and the entire data set and is usually shown by a dendrogram [11]. The Euclidean distance gives the similarity between two samples and a distance can be represented by the difference between analytical values from the samples [12]. In this study, hierarchical agglomerative CA was performed on the normalized data set by means of the Ward's method, using squared Euclidean distances as a measure of similarity. The Ward's method uses an analysis of variance approach to evaluate the distances between clusters in an attempt to minimize the sum of squares (SS) of any two clusters that can be formed at each step. The spatial variability of water quality in the whole river basin was determined from CA, using the linkage distance, reported as Dlink/Dmax, which represents the quotient between the linkage distances for a particular case divided by the maximal linkage distance. The quotient is then multiplied by 100 as a way to standardize the linkage distance represented on the y-axis [13-14,2]. The findings of the key component study show that water quality differences were primarily related to three factors: non-point source pollution, point source contamination and other natural water processes. Generally speaking, the quality of water is significantly detrimental to customers ' safety and urban waste water treatment system effluent is the major source of pollution. Sensitive regulation of the anthropogenic activity in the surrounding area was proposed [15]. Their research supports river water quality management by showing the usefulness of multivariate statistical methods for the study and evaluation of complex data sets, defining contamination mechanism and underlying water quality changes.

The application of descriptive statistical analysis is to interpret surface water quality and to detect the long-term correlation between variables as well as to show the inefficient delimitation of the source of the variation [16]. Techniques such as Multivariate statistical have therefore recently been widely used as standard methods for analyzing water quality data in order to obtain meaningful information [14,17-18]. Principal component analysis (PCA) and factor analysis (FA), and cluster analysis (CA) are the most popular multivariate statistical methods that are widely used throughout the world. PCA and CA, are used to classify and evaluate surface water quality as they can verify temporal and spatial differences due to natural and anthropogenic factors associated with seasonality [3,19-20]. These techniques or methods also enable the classification of necessary factors / sources responsible for water quality variations and influence and quality of water systems [21].

Multi-statistic approaches, which can easily help to analyze the complex data matrices in order to have better understand of the ecosystems being studied, are commonly used in large numbers of countries in studies of water quality in general. Factor analysis is one of the most popular multivariate statistical methods that are widely used throughout the world.

In the paper of [22], the permeability index (PI), sodium adsorption ratio (SAR), percentage of sodium (Na%), and residual sodium carbonate (RSC), which are known as effective groundwater quality management strategies. Their work aimed at analyzing the physicochemical parameters of groundwater content at Basrah site using the data obtained and the criteria for water quality, by assessing their adequacy for irrigation purposes. The work is used as a supplementary tool for identifying areas of water quality degeneration and discovering possible sources of pollution at the site of test, the principal component analysis and the cluster analysis.

The results of [23] worked which is revealed parameter variation over time due to, at most, the increasing pollution levels at the monitoring stations along the Shatt Al Arab River during the 2011-2014 period. Throughout current research, a comparative evaluation of large and complex datasets has

been used and extended throughout order to obtain more valuable information on surface water quality, sample design and measurement procedures, effective pollution control and successful surface water management.

This research aims to examine temporal and space water quality variations by evaluating primary sources of pollution in Basrah, Iraq, on the Shatt Al-Arab River. In 2016-2017, water samples from various assigned sampling stations along the river were investigated into the hadrochemical system of the Shatt Al-Arab Riverbank. The water quality metrics for the river included physical and chemical parameters which are evaluated using correlation analyzes by Pearson, key analysis of components and analysis of the element. The average water quality tests have shown that consistency is above acceptable standards. Review of their current study has shown that water quality is mainly controlled by household waste, industrial waste and agricultural waste. Out of 14 factors, there are only three important factors. We constitute 84,926 percent of the total variance, with the first factor describing 60,935 percent of the total difference. The second factor was 15,528 percent of the total variation. When describing the Third Element, the gap is 8,464%. The study of key components led to the categorization of contributing variables or improvements in water quality at the source. Such findings should be considered for the future planning of drinking water consumption [15].

These approaches can be used as tool for designing suitable objectives to manage water resources accurately and rapidly resolve pollution problems [14,17]. This research used the Data sets gained from the River and were subject to various multivariate statistical methods for analysis the temporal and spatial varieties in water quality. For the data analyzed from the River water measurements, the Pearson Correlation Index (PCI), PCA, FA, and CA were applied to assess the water quality.

The findings from this study provide a scientific basis for management of the ecological system, environmental protection and regulation of water pollution in the River basin.

2. Materials and Methods

2.1. Characterization of the study area

Al-Arab River (30º24'26"N The Shatt 48º09'06"E) is comprised of the confluence of the Euphrates and the Tigris in al-Qurnah town, located in the southern Iraq (Fig. 1). The selected section of the study area for the Shatt Al-Arab River is located in the middle of the Shatt Al-Arab basin, and the quality of water in the river in that section influenced by upstream water quality and influences the water quality in the downstream. The Shatt Al-Arab river of about 200 km in length, with an annual average calculated temperature of 24.3 °C and an average annual precipitation of 152 mm of falls annually (Fig. 2). The rainy season stretches from October to May [24].



Figure 1. Location of water stations (water sampling points) for study area (Shatt Al-Arab River) basin, in Basrah Province, Iraq.

Figure 2. Monthly distribution of temperature (minimum, maximum, and average) and rainfall in Basrah Province, Iraq [24].

2.2. Water quality evaluation

The monitoring of water quality in the Shatt Al-Arab River basin was carried out twice a month. Field measurements and water sampling were conducted at three sites, namely, Al-Jabila water station (WS1), Al-Biradieih 2 water station (WS2), and Al-Libaniu water station (WS3), to cover areas with different characteristics of land use. Water stations on the river basin are given in Figure 1. Set of water samples were started sampling in January 2016 and ended in May 2017 and two water samples collected as monthly intervals. Water samples were collected by Basra Water Directorate (BWD).

Fourteen parameters were selected depended on their sampling continuity at all the testing sites listed. These water parameters included water tem-



perature (T), pH, electrical conductivity (EC), Alkanets (Alk), total dissolved solids (TDS), turbidity (Tur), total hardness (TH), calcium (Ca), magnesium (Mg), chloride (Cl), sulphate (SO4), total suspended solids (TSS), sodium (Na), and potassium (k). All of

these measured parameters, except for Tur (NTU), pH, EC (μ S/cm), and TEMP (C), are expressed in mg/L. Measurements of Temp, EC, pH, Turb and TDS had been carried by using of multiparameter probes onsite.

Water samples were collected in plastic bottles for physico-chemical research, and after frozen in ice at 4 ° C and moved for analysis in the Laboratory of Basra Water Directorate (LBWD). Parameters for the quality of the water were analyzed as per the methodologies recommended by the Standard Methods for Examination of Water and Wastewater [25].

2.3. Statistical analysis

The results were subjected to use of Pearson Correlation Index (PCI) to assess the relations among the physico-chemical parameters by using the statistical package software called SPSS 22. The results were also subjected to Factor Analysis (FA) to assess the useful varifactors in the Shatt Al-Arab River according to correlated variables by using the same statistical package software SPSS 22.

The application of principal component analysis (PCA) on the results is supposed to eliminate the data overlapping between variables consequently, suggests the scope for their contribution to the phenomenon's variability in an individual manner. PCA gives information about the most important parameters which characterize the data set that helps data reducing with minimal loss of original information [14].

The application of Cluster Analysis (CA) for the water quality data set was conducted in different field of water quality [20,26-28]. CA is an investigative analysis which classifies objects in order to be identical to each other in the cluster on the basis of a predetermined classification criterion. The resulting object's clusters should be within-cluster is highly internal homogeneous and it should be between-cluster is highly external heterogeneous [28]. In this research, the Ward's method with squared Euclide-an distances, was performed, as CA on the standard-ized data sets, to measure of similarity [26]. The computations of mathematical and statistical methods in this study has been done with SPSS 22 software.

3. River water for agricultural uses

The irrigation water with a high Electrical conductivity (EC) value has a negative effect on yield potential; it is an important measure of the salinity risk for plants. Excess salinity results in a reduction in plant osmotic activity; it thus interferes with nutrient and water absorption from the soil [29]. Electrical conductivity for total dissolved ions is called an arbitrary indicator and both (EC and TDS) are reliable [30]. Any changes in electrical conductivity values therefore allow TDS values to change. The TDS is between (260-839) mg/l in the field of study. Sodium as expressed in a sodium adsorption ratio (SAR) is the most critical chemical parameter for determining the suitability of water for irrigation. Excess sodium ration causes undesirable effects of surface modifications and reduces the soil permeability of irrigational water [31]. Calcium and magnesium ions ration however are very important as they propensity to overcome sodium effect. A major factor in irrigating water quality is the sodium hazard. It is commonly used to test the recognition of irrigation water quality. High levels of sodium in soil water lead to undesirable effects, as soil (Na) responds to decrease its permeability [32]. This will have a negative impact on plant growth [33]. The influence on irrigation water of the magnesium hazards (MH) ratio is known to be an undesirable (harmful) effect on development when the magnesium values are greater or similar to (50). More magnesium in water than calcium concentration contributes to soil structure degradation and soil productivity decrease [34]. Residual sodium carbonate (RSC) is an important parameter for water irrigation assessment [35]. It will be used to determine the dangerous effect on water quality for agricultural purposes of carbonate and bicarbonate. The acceptability of water for irrigation can also be affected by high amounts of carbonates or bicarbons in the water relative to calcium and magnesium. Furthermore, when the carbonate content is high, calcium and magnesium can combine to produce a number of solids which are extracted from water [36].

4. Results and discussion

Table 1 provides an exploratory analysis for the data collected to assess the water quality at the three monitoring stations in the Shatt Al-Arab River.

It was noticed that there is small variation in water temperature values an increase from upstream to downstream along the Shatt Al-Arab basin. Such variance might also be due to the sampling times.

The mean value of pH for the point WS1 (7.46) met the Iraqi standard [37-38] (pH $6.5 \sim 8.5$). None-theless, the mean values of pH in the waters at points WS2 (7.54) and point WS3 (7.54) as shown in table 1. For the mean pH value for all the water, it had been varied from 7.19 to 7.87 for the study area (Table 1). Based upon this, the detected mean values

are perfectly with the limitations set by WHO [39-40] as well as our Iraqi standards [37-38].

From the three monitored points, WS2 (11.2 NTU) had the smallest mean value of turbidity (Table 1). It was detected that there is an increase in level of turbidity as it moves downstream in the river, that can be related to increased riverbank erosion, with sediments contributing to the flow.

For electrical conductivity (EC), Table 1 signifies that the mean values of this parameter are above the standard limitation values for WHO [39-40] (1500 μ S/cm). The mean values of EC for the examined stations reveal higher levels at points WS2 (6110 μ S/cm) and WS3 (6330 μ S/cm), for which a higher variability was noticed during the year, this might be associated with the monthly differences in the distributions of rainfall took place throughout the study time and discharge of domestic effluents without proper treatment in river waters. For the waters of Shatt Al-Arab River, it was noticed that the average value of total dissolved solids (TDS) for all the stations (2483.7 mg L-1) was above the WHO standards [39-40] (500 ppm) as Iraqi standard [37-38] (1000 ppm) as shown in (Table 1). A similar behavior is recognized for electrical conductivity (EC), which has direct correlation with TDS, showing more increased salt content. In the basin of the Shatt Al-Arab River waters. The average value of turbidity (Turb) was 13.39 NTU, did not meets the WHO [39-40] and Iraqi standards [37-38] that to be 5 NTU, the notable increase in all levels at points WS1, and WS3 (Table 1). However, all values were above the standard limits.

 Table 1. Statistical descriptors of monitored parameters in Shatt Al-Arab River.

	ters	S III SHALL AF	-ALAD KIVE		
Variables	Statistical Parameters	WS1	WS2	WS3	all water sta- tions
	Min.	19.5	18	18	18.50
Temp.	Max.	29.2	31.2	31	30.47
	Mean	25.05	24.56	25.24	24.95
	Min.	7.22	7.15	7.2	7.19
pH	Max.	7.82	8	7.8	7.87
	Mean	7.46	7.54	7.54	7.52
	Min.	1628	1336	1556	1506.7
TDS	Max.	3802	3838	3950	3863.3
	Mean	2502.0	2454.2	2494.9	2483.7

	Min.	2680	2220	2545	2481.7
EC	Max.	6014	6110	6330	6151.3
	Mean	4008.8	3957.2	4013.5	3993.2
	Min.	6.9	2	4	4.30
Turb	Max.	24.3	23.3	42	29.87
	Mean	13.01	11.20	15.95	13.39
	Min.	680	552	584	605.33
TH	Max.	1252	1212	1126	1196.7
	Mean	871.5	828.4	821.7	840.5
	Min.	62	20	38	40.0
TSS	Max.	148	138	136	140.7
	Mean	101.9	90.9	103.53	98.8
	Min.	142	112	115	123.00
Ca	Max.	256	244	230	243.33
	Mean	178.1	170.1	168.9	172.35
	Min.	79	66	72	72.33
Mg	Max.	149	147	135	143.67
	Mean	103.88	98.59	97.47	99.98
	Min.	278	258	286	274.00
Na	Max.	938	922	1024	961.33
	Mean	552.79	555.71	578.53	562.34
	Min.	7.5	7.3	7	7.27
k	Max.	31.3	23.4	29.4	28.03
	Mean	12.83	11.93	12.48	12.41
	Min.	440	395	450	428.33
Cl	Max.	1405	1390	1550	1448.33
	Mean	836.74	842.8	878.6	852.72
	Min.	494	398	417	436.33
	Max.	1041	1037	980	1019.33
SO4	1010071				
SO4	Mean	699.53	663.3	654.3	672.38
SO4		699.53 120	663.3 126	654.3 128	672.38 124.67
SO4	Mean				

The concentrations of TDS and Turbidity, greatly increase in the downstream direction (Table 1). The reported of mean values for TDS concentrations which include those acquired in other studies of the Shatt Al-Arab River basins in the study area, as reported by [23,41]. The mean values of the Alkalinity (Alk) (154.04 ppm) were actually above the WHO limits (up to 10 ppm) as shown in Table 1. As for TH, a higher mean level were noticed in the waters at station WS1 (1252 ppm) and WS2 (1212 ppm), with the water of other station in addition displaying very high TH concentration values. That it is nearly all expected due to releases of untreated effluents from domestic sewage near station WS1 in the measurement time-period.

As for magnesium (Mg) concentration in water, the average value for all the three stations was 99.98 ppm (Table 1), satisfying the Iraqi standard for water (100 ppm) (Table 1). Unfortunately, the highest concentration for Mg (103.88 ppm) discovered at station WS1. A similar behaviour is regarded for calcium (Ca), which has direct relationship with Mg, showing more increased of its level.

As for the measured anionic concentrations (Cl and SO4) in water, the average values for all the three stations was 852.72 ppm and 672.38 ppm, respectively (Table 12), not satisfying the Iraqi and WHO standards for drinking water. The mean values of the potassium (k) (12.41 ppm) were actually above the WHO limits [39-40] (up to 10 ppm) as noticed (Table 1). As for sodium (Na), a higher mean concentration was found in the third water station (1024 ppm) with the water of other stations additionally revealing very high Na level values.

Box plots (**Fig. 3**) show spatial changes in water quality parameters during the study period (Jan 2016- May 2017) for the three water stations.

The relationships involving the physical and chemical parameters levels in the study area of Shatt Al-Arab River Basin were established by using observed data (n = 14) and all recognized relationships are provided in Table 2.

In the current study, if the Pearson Correlation coefficients values is near to 1 or exactly 1, there is a good positive relationship between the two studied variables, while when its value near 0 means there is no relationship between them.

















Figure 3. Box plots for the spatial variations in water qualityparameters during the study period (Jan 2016- May 2017) for thethreewaterstations.

	k	Na	TSS	TDS	SO4	Cl	Mg	Ca	TH	Alk	EC	pН	Turb	Temp
k	1.000													
Na	.701	1.000												
TSS	236	121	1.000											
TDS	.732	.983	137	1.000										
SO4	.703	.849	166	.924	1.000									
Cl	.692	.998	109	.980	.837	1.000								
Mg	.695	.835	095	.915	.983	.829	1.000							
Ca	.723	.846	131	.924	.984	.842	.976	1.000						
TH	.715	.845	115	.925	.989	.840	.994	.994	1.000					
Alk	219	146	.419	185	263	154	196	261	230	1.000				
EC	.732	.983	146	.998	.924	.980	.912	.921	.922	196	1.000			
pН	411	397	.198	443	465	391	440	474	459	.206	444	1.000		
Turb	163	009	.710	037	112	.004	061	062	064	.413	051	.033	1.000	
Temp	469	368	.450	394	412	358	386	405	399	.326	393	.198	.328	1.000

Table 2. Pearson Correlation Index coefficients

Based on the results of table (2), Na showed excellent positive correlation with each of (TDS, Cl, and EC) and a very good positive correlation with (SO4, Mg, Ca, and TH). it is shown from the same table, that k is correlated with each of (TDS, Na, SO4, Cl, Mg, Ca, TH, and EC) in approximately a good positive correlations.

TDS and SO4 showed excellent positive correlation with each of (Cl, Mg, Ca, Th, and EC) as well as their excellent positive correlation between each of them (TDS and SO4).

Correlation analysis showed that EC is highly positively correlated with each of (TDS, TH, Ca, Cl and Mg). this means that increases of EC in water samples is similar trend for other correlated variables.

Commonly the factor loadings is categorized into three classes as "strong" (values greater than 0.75), "moderate" (0.75–0.50) and "weak" (0.50–0.30). Eigenvalues above one were chosen as the criterion for determining the main components needed to demonstrate the origins of data variability. Based on the rotated cumulative percentage variance, two factors explained 77.1% of the total variance (Table 3) and the FA scree plot is given in the Figure 4.

		Table 3.	Factors	of the	e matrix components	
5 7	•	1 1		DC1	DCO	

_	Variables	PC1	PC2	
	k	.792	100	
	Na	.933	.151	
	TSS	223	.851	
	TDS	.977	.125	
	SO4	.964	.041	
	Cl	.928	.160	

Mg	.951	.112
Ca	.964	.075
TH	.963	.093
Alk	282	.620
EC	.977	.113
pН	512	.075
Turb	126	.846
Т	485	.496
Eigenvalues	8.603	2.193
Explained variance	0.614	0.156
Total variance	0.614	0.771

PC principal components 1 and 2

^a Bold values represent strong loadings

PC1, that accounts for 61.4% of the total variance, seems to have strong positive loads on k, Na, TDS,SO4, Cl, Mg, Ca, TH, and EC, and moderate negative loads on pH. This component concentrates almost all of the impacts of agricultural activities, that increase the concentration of EC and TDS that can also be affected by agricultural activities and domestic sewage and fertilizers that are added to crops in the basin. but has increased its value in some waters of the river. Therefore, so much of the spatial variability of water quality in the basin can be correlated with the land use/land cover situation, that is defended by other studies [6,42].

PC2 represented 15.6 % of the total variance. Strong positive TSS, Ca, ph, and Turb. highest TH loads were noted, and moderate positive Temp loads were observed. This component could be correlated to water pollution that indicating that this component is correlated with soil particles and influence on water quality parameters. PC2 also has medium positive loading on Alk.



Figure 4. Scree plot of FA for water quality variables .

Table 4. Factors of the matrix components						
Total Variance Explained						
G	I	nitial Eigenval	ues			
Component	Total	% of Variance	Cumulative %			
1	8.603	61.448	61.448			
2	2.193	15.661	77.109			
Comment	Extraction Sums of Squared Loadings					
Component	Total	% of Variance	Cumulative %			
1	8.603	61.448	61.448			
2	2.193	15.661	77.109			
German	-	Rotation Sums Squared Loadir				
Component	Total	% of Variance	Cumulative %			
1	8.319	59.418	59.418			
2	2.477	17.691	77.109			

Conclusions

In this study, Factor Analysis was used to evaluate the water quality of the Shatt Al-Arab River by using a large number of physical, chemical and biological data. Factor Analysis assisted to recognize the effective factors on the system and 2 effective factors were determined that were explained 77.1 % of the total variance. The first component accentuating the concentration of variables linked to the influence of agricultural land use and domestic wastewater discharged to the river, which results in 61.4% of the total variation of water quality in the study area. PC2 accounted for 15.6 % of the total variance; this component was related to soil particles in surface runoff. Higher magnesium than calcium leads to an increase in magnesium saturation in irrigation water which decreases soil productivity.

In conclusion, multistatistical evaluation is necessary for a sophisticated environmental evaluation especially in water quality assessment studies, because of obtained large numbers of different parameters and difficulty of the interpretations of all parameters.

This study provides an improved understanding of the temporal and spatial variations in the water quality of the Shatt Al-Arab River river.

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