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Chemical Typology of Groundwater from the Oued Righ Aquifers: Insights from the Application of Factorial Discriminant Analysis (FDA)

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Abstract— This study is aimed at investigating the chemical typology of groundwater in the Oued Righ aquifers using multivariate statistical analysis such as PCA and FDA. For this, sixty three 63 samples were collected from the tree superposed aquifers (CT, CI and pheratic aquifer) and analysed on their physico-chemical parameters. PCA allow evidencing the mineralization axis and helps a classification of wells according their correlation towards this axis. FDA analysis results show that almost of individuals are well classified. Samples from each aquifer are clustered and their barycenters are significantly separated indicating that each aquifer displays a different chemical typology. Few wells from El M'Ghair are misclassified suggesting a probable exchange between CT and the phreatic waters on a one hand and the evolution of waters nearby the outlet zones.

Key-Words— FDA, Statistics, groundwater, classification, Oued Righ, Algeria.

I. INTRODUCTION

The Oued Righ Valley, as northern Algerian Sahara, contains considerable resources of groundwater into three superposed aquifers. The former is unconfined which is the Phreatic aquifer and the two others are deep and usually considered as confined; represented by the Terminal Complex (CT) and the Continental Intercalaire (CI). During last decades, several studies have been conducted on these waters in order to characterize their chemical behavior and to evaluate their aptitude to domestic and agriculture uses. The origin and the evolution of these waters were also a subject of many investigations helping a well knowledge of the hydrochemical issues (eg. [9]-[10];[13]). The phreatic and unconfined aquifer in the Oued Righ valley is characterized by high mineralization and (conductivity (Ce) can exceed 7500 µs). The vulnerability of this aquifer is moderate to high according GOD methods [1]. The CT water displays also high mineralization especially in central localities where the salinity may exceed 5200 mg/l [2]. The CI reservoirs such as Albien waters have mainly a water type of sodium and magnesium sulfated and sodium chlorinated while their temperatures are ranging from 40 to 60°C [5]. The main purpose of this study is the classification of groundwater from the three aquifers based on their chemical behavior using multivariate statistical analyses such as PCA and FDA. It is focused principally on identifying water types and checking the interferences between these aquifers and water exchanges.

II. PRSENTATION OF STUDY AREA

The Oued Righ valley is the study area which extends to more 150 Km^2. It is located in Northern Sahara, situated between the following

coordinates: latitude: 32 ° 54' to 39 ° 9' Nord and longitude: 05 ° 50' to 05 ° 75' Est and limited by El Goug in the South, Oum Tyour to the North, while the valley of Oued Souf represents the eastern border and the Ouargla Oasis to the west. This area is extended with an average width of 15 to 30 Km [3]. From point of view geology; the study area consists of a vast depression that is bordered in the north by chotts and the piedmonts of Zab, The dorsal Mozabite and Daias plateaus ensure the western limit and it consists of the Mio-Pliocene and Turonien formation. To South, this area is limited by the Erg of Ouargla which is mainly consisting of sands and by Grand Erg Oriental to the east. This area is arid with low precipitation rate that does not exceed 90 mm together with an annual average temperature of 22.2 °C during the period 1984–2011 [18].

III. GEOLOGY AND HYDROGEOLOGY FEATURES

The geology of the studied area is well investigated by several studies that have been carried out for hydrogeological aspects (eg. [1]-[2]; [4]; [6]; [12] and others).

Based on geological prospection that has been performed by oil companies; the sedimentary formation is aged from Precambrian basement founded at more than 4000 m of deep to Tertiary formation which are entirely overland by Quaternary sands of the Great Oriental Erg [11]. The Oued Righ area accompanied almost tectonic phases as the Algerian Sahara [16], while that post-Eocene may have an impact on water reservoirs. This area includes three (3) aquifers which are: (1) the confined aquifer called the Continental Intercalaire (CI) with a thickness that can reach 1000 m, containing sandy and sandstone lithology and usually attributed to Albian age. (2) The second aquifer is a multilayer called Terminal Complex (CT) contains two units exhibiting different lithologies: the former is deeper and mainly confined. It is characterized by limestone and is aged of Senonian-Eocene, whereas, the latter is called the Mio-Pliocene of sandy, gravel and sandstone lithologies. The CT has relatively low thickness comparing to CI with an average of about 200 m [27]. (3) Phreatic aquifer is formed mainly by sand and evaportic formation (Fig. 2).

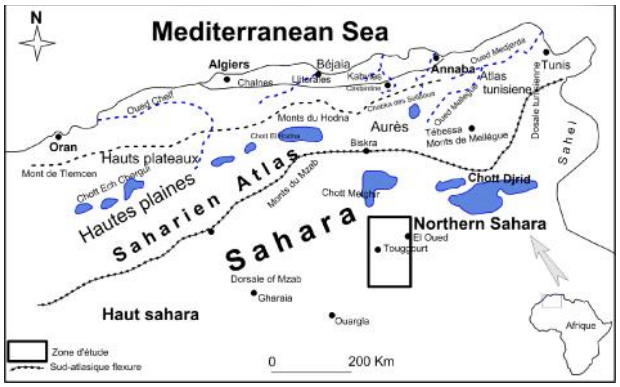

Fig. 1. Localization of the study area regarding the general disposition of main structural units in North Africa [7].

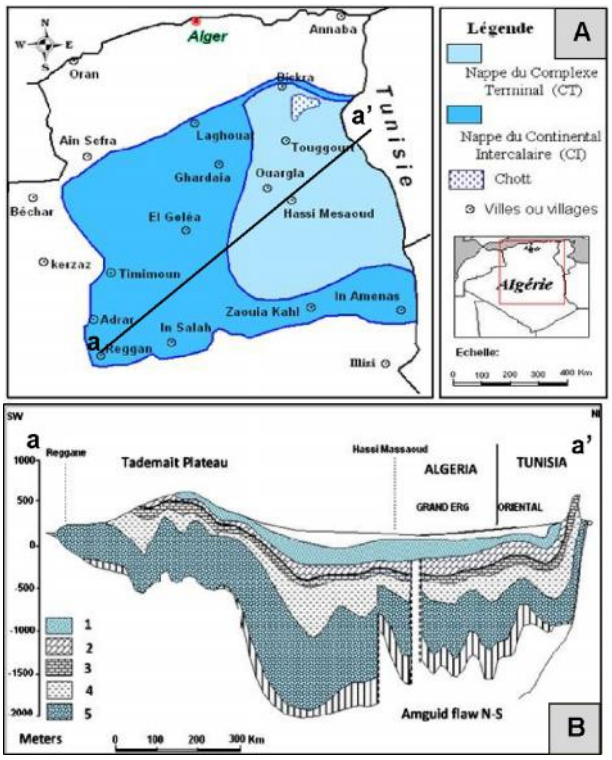

Fig. 2. Hydrogeology framework. (A) Lateral extention of CI and CT aquifers. (B) Synthetic hydrogeological section (a, a') across the septentrional Sahara: 1. Continental terminal aquifer, 2. Lower Senonian, 3. Turonian evaporates, 4. Cenomanian, 5. Continental intercalaire aquifer [24].

IV. DATA AND METHODS OF PROCESSING

A. Data set

About sixty three (63) wells were sampled by the help of ANRH-Ouargla services during the 2016-2017 periods from the three aquifers (Fig. 3). Excepting some parameters such electrical conductivity (Ec), temperature and potential of Hydrogen (pH) that have been measured "in situ" directly after sampling using a multiparameter, the other physicochemical analyses were carried out using the methods of Rodier (1996) [22] in the laboratory of the national agency of water resources (ANRH) - Ouargla. Ca, K, Na were analysed by flame spectrophotometry. Cl, HCO_3, SO_4 were recorded by DR2000 spectrophotometer and Mg determined by titration technique.

B. Methods

Many methods are used to classified groundwater and to recognize the typology of each water type (eg. [22], [8] and other). Here, we investigate the use of multivariate statistical analysis that are related to factorial methods such as: Principal Component Analysis (PCA) and Factorial Descriminant Analysis (FDA)

The PCA was initiated and developed for the first time by Pearson (1901) [20] and Hotelling (1933) [14] to explore analyses of multidimensional space having the R^p structure (*P* dimensions and data as *n* points). PCA help the reduction of information and transforms a high-dimensional data into reduced-dimensional sub-space in terms of component scores (factor scores) and loadings. In other word, PCA allow the identification of variable associations towards selected new factorial axis as well as group of observations [23]. The FDA is also a factorial method but in contrary to PCA, it searches the separation between groups of observations and therefore it helps a classification of the samples based on *n* quantitative *p* qualitative variables [15], i.e, the FDA the use qualitative variable in addition to quantitative variables.

Furthermore, the FDA is a multidimensional method that suggests a comparison between statistical populations ranging within predefined groups named *a priori,* while the variance of a given character can be divided into two: the interclass variance that represents the dispersion of gravity centers called barycenters which are previously defined and the interclass variance which originated from the dispersion of samples (observations) around their barycenters. By measuring distance between observations of a group and the gravity centers of all groups defined as *a priori* allows putting in perspective each observation [19]. If an observation is close to the barycentre of its group membership it called well classified if the contrary or the observation is near to another barycentre, it considered as misclassified and it therefore assigned to another group called assignment group. This is to say that method helps the match verification of each observation to predefined groups.

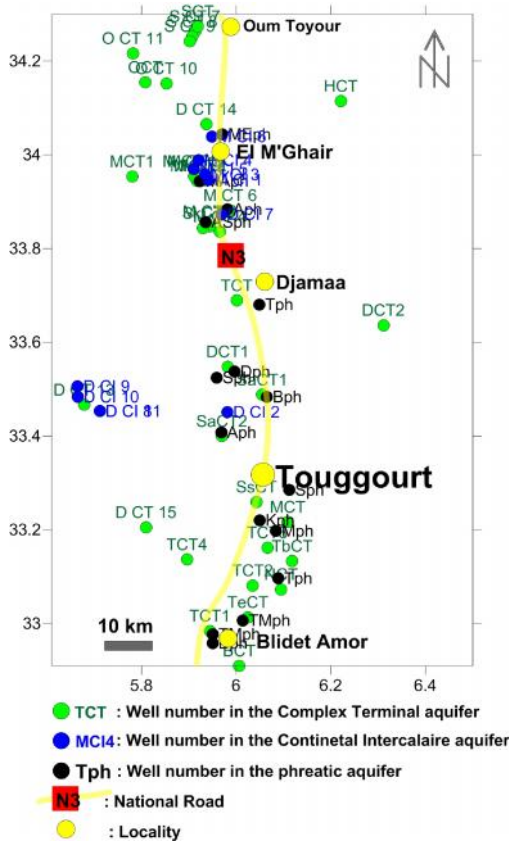

Fig. 3. Inventory of water samples point for this study.

V. RESULTS AND DISCUSSION

A. *Elementary statistics*

The elementary statistics on analysed physico-chemical parameters are given separately for each aquifer (Table 1-3). They show that all groundwaters are highly mineralized.

The phreatic aquifer is higher in Ce regarding the other aquifers (min = 2.67 ms/Cm, max = 11.20 ms/Cm). It is noticed that waters show the influence of lithology in acquiring mineralization and is represented mainly by evaporates.

The CI aquifer shows the lower mineralization among the three aquifers with conductivities varying between 2.52 ms/Cm and 5.58 ms/Cm (standard deviation = 1.16 ms/Cm)

Table 1. Elementary statistics of physico-chemical parameters from CI groundwater.

	N	*Min.*	*Max.*	*Mean*	*S.D (n)*
Ca^{2+} (mg/l)	11	155.00	237.50	183.76	28.90
Mg^{2+} (mg/l)	11	115.20	266.20	158.60	46.87
Na^{+} (mg/l)	11	140.00	542.50	259.32	130.51
K^{+} (mg/l)	11	11.50	35.00	28.91	7.72
Cl^{-} (mg/l)	11	265.00	775.00	463.68	178.54
SO_4^{2-} (mg/l)	11	503.00	1375.00	824.00	285.25
HCO^{-}_3 (mg/l)	11	179.95	271.45	214.89	28.03
Ce (ms/cm)	11	2.52	5.58	3.48	1.16
pH	11	7.19	8.43	8.00	0.32

Table 2. Elementary statistics of physico-chemical parameters from CT groundwater.

	N	*Min.*	*Max.*	*Mean*	*S.D (n)*
Ca^{2+} (mg/l)	36	221.30	480.00	328.20	76.06
Mg^{2+} (mg/l)	36	115.20	563.20	265.67	91.95
Na^{+} (mg/l)	36	305.00	1177.50	687.01	213.56
K^{+} (mg/l)	36	12.30	71.30	28.22	14.99
Cl^{-} (mg/l)	36	400.00	2588.00	1076.29	527.59
SO_4^{2-} (mg/l)	36	815.00	2375.00	1789.72	331.84
HCO^{-}_3 (mg/l)	36	140.30	219.60	180.21	17.36
Ce (ms/cm)	36	2.44	8.18	5.66	1.35
pH	36	7.65	8.49	8.16	0.20

Table 3. Elementary statistics of physico-chemical parameters from the phreatic aquifer.

	N	*Min.*	*Max.*	*Mean*	*S.D (n)*
Ca^{2+} (mg/l)	16	116.00	776.00	373.50	167.64
Mg^{2+} (mg/l)	16	145.00	579.00	293.50	144.79
Na^{+} (mg/l)	16	367.00	1420.00	678.00	304.06
K^{+} (mg/l)	16	10.00	33.00	24.13	6.53
Cl^{-} (mg/l)	16	525.00	2431.00	1169.00	553.33
SO_4^{2-} (mg/l)	16	1180.00	4150.00	1781.00	721.07
HCO^{-}_3 (mg/l)	16	98.00	136.00	117.00	8.70
Ce (ms/cm)	16	2.76	11.20	5.58	1.92
pH	16	7.70	8.30	7.91	0.17

Min : Minimum; Max: Maximum, S.D: Standard Deviation.

B. *PCA analysis*

The PCA is aimed at interpreting in multidimensional space the correlations between investigated variables. The extraction of PCA components was performed on a correlation matrix of seven (7) variables versus fifty-eight (63) observations from all aquifers.

Results show that the two main components PC1 and PC2 gather a cumulative variance of 70.73 % (PC1 = 54.62 %, PC2 = 16.11 %).

The PC1 displays the highest variance. This component represents the mineralization axis while the PC2 show strong positive loading to K+ and may represent the hydrolysis of silico-clastic material.

The projection of individuals (observations) on the PC1 versus PC2 highlights a good classification of groundwaters according their mineralization. The CT and the phreatic aquifer show higher mineralization than the CI aquifer (Fig. 4).

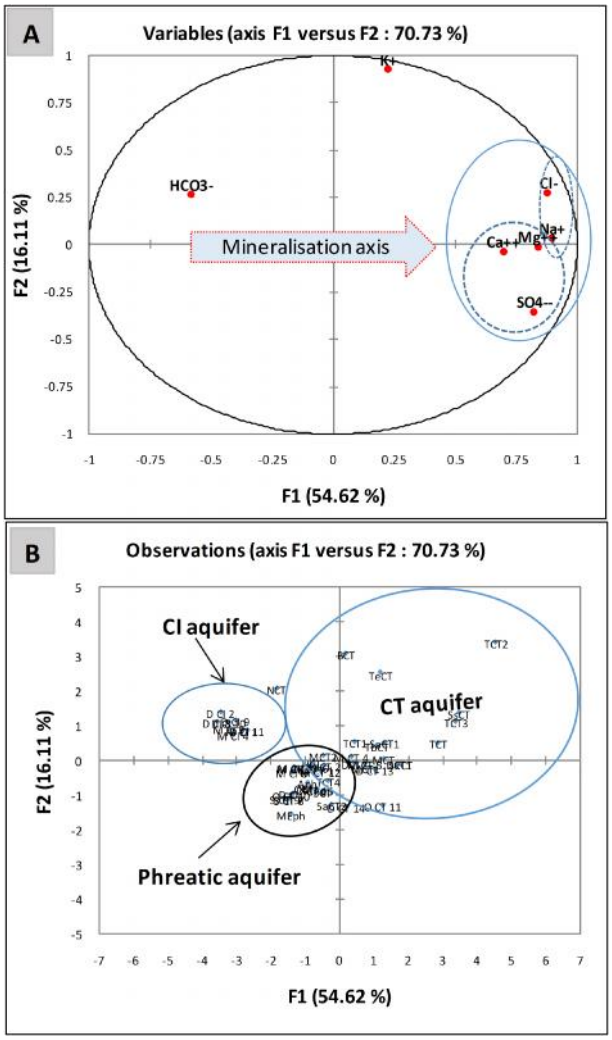

Fig. 4. Loading the PC1 versus PC2 factors from the Principal Components Analysis (PCA):

(A) Physicochemical parameters showing the mineralization axis (B) Plotted individuals (samples) into PC1 versus PC2 showing different groups of individuals

FDA analysis

This method has been successfully used to check the origin of pollution at Berahal (NE Algeria) by Khelfaoui et al. (2012) [17].

In this study, The FDA analysis was used to classify the water from the three aquifers according their chemical characteristics. Samples were divided into three classes and results show that waters are well classified and each water aquifer has a distinguished chemical typology excepting four (4) wells from the CI and phreatic aquifer (Table. 4; Fig. 5).

Table 4. Results of confusion matrix of cross-validation.

From\ To	CI	CT	Phreatic	Total	% correct
CI	8	3	0	11	72.73%
CT	0	35	1	36	97.22%
Phreatic	0	1	15	16	93.75%
Total	8	39	16	63	92.06%

The figure 5 shows that the classification using FDA indicates a significant distinction between the three groups of water. In other word, each aquifer has a water chemical behavior which is not similar in respect with other aquifers. The barycenter of samples from the phreatic unsaturated aquifer, is located away the other barycenters regarding the factorial projection.

The only four (4) wells are misclassified. It is about three (3) wells from the CI aquifer (MCI 3, MCI 6, MCI 7) which are *a posteriori* classified nearby CT aquifer behavior and one well from the CT aquifer (MCT) which is also misclassified and is nearby the phreatic aquifer. All these wells are situated in the El M'Ghair locality to the northern of the studied area. This locality is nearby the Sebkha and chotts which can consist of an outlet of groundwater. Therefore, we suggest a possible exchange locally between aquifers (CT-Phreatic) need to be confirmed with other tools such isotope geochemistry. Furthermore, drilling problems may occur and are probably at the origin of exchanges. The evolution of chemical characteristics of waters nearby the outlet zones could be also the cause of CI misclassified samples. The obtained results allow evidencing a chemical typology for each aquifer.

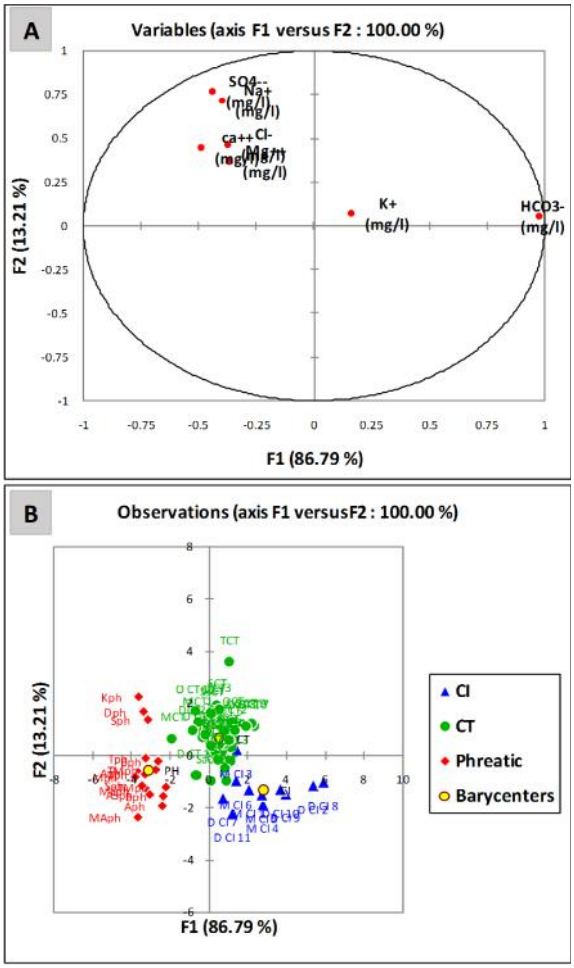

Fig. 5. Discriminat factorial analysis. (A) Physicochemicalparameters (B) Plotted individuals showing the classification groups.

VI. Conclusion

The present study investigates the groundwater typology from the three aquifers (CI, CT and phreatic) according their chemical behavior. Therefore, chemical parameters (Ca^{2+}, Mg^{+2}, Na^{+}, K^{+}, Cl^{-}, SO_4^{2-}, HCO_3^{-}) of samples from these aquifers were used to perform some statistical analysis (PCA and FDA). This study reveals a well classifying of water according to their aquifer membership for almost wells. Each aquifer has a distinguished typology regarding their chemical composition. The few misclassified wells, are locally founded in El M'Ghair city and should be treated with caution. They otherwise can hold proxies of local exchanges between aquifer (CT and phreatic) due drilling problems or other structural factors such as faults on a one hand and the evolution of waters nearby the outlet zones.

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