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Application of Multivariate Statistical Methods to the Hydrochemical Study of Groundwater Quality in the Sahel Watershed, Algeria

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ABSTRACT

The quality of groundwater is characterized by several numbers of physical and chemical parameters, which determine the use of water (water supply, irrigation, industry). This search paper is a contribution made to know the hydrochemical characteristics of groundwater in the Sahel sub-catchment which belongs to the large Soummam North basin of Algeria. Different multivariate statistical techniques were used such as principal component analysis (PCA), Hierarchical Cluster Analysis (HCA) and Diagram Analysis. These analyses are exercised to a dataset formed from 37 boreholes with 12 chemical variables over the entire surface of the watershed. The samples were collected in 2016. The 37 boreholes are one of the main water resources that supply the wilaya of Bouira with drinking water and irrigation. The analysis of water quality using different methods (ACP, HCA and Diagram) resulted in two chemical kinds: (Chloride, calcium sulfate and magnesium), and (Bicarbonate calcium and magnesium). The results have shown that 74% of the boreholes were contaminated, the rest of boreholes were characterized by a good quality and they have not suffered any contamination and can be consumed without any risk.

Keywords: hydrochemical analysis, water quality, groundwater, principal component analysis, hierarchical cluster analysis, Sahel watershed.

INTRODUCTION

The groundwater is considered a guaranteed source for water supply and protection from dryness, in the most regions of the world (Calow et al., 2010). In northern Algeria, and particularly, in the region of the Sahel sub-watershed which belongs to the large Soummam basin, groundwater is intended for water supply and irrigation. Indeed, it is soft and of good quality compared to that of surface. Regardless of the importance of groundwater, these last can be damaged owing to several factors which affect its chemical composition leading to affecting its multiples uses. These factors include, among others, the geology and lithology, contact time of the water with the rocks, the ambient temperature, the pH, the quantity of water available in the aquifer, and its circulation rate (Akoteyon, 2013). This study aim the using multivariate statistical techniques such as Principal Component Analysis (PCA), and Hierarchical Cluster Analysis (HCA) to understand the hydrochemical processes that govern groundwater in the Sahel sub-basin region north of Algeria using 37 boreholes to carry out the analysis of 12 physicochemical parameters for each borehole. After data treatment, only 34 boreholes were representative and used to realize the study.

MATERIALS AND METHODS

Study area presentation

The Sahel sub-watershed is located between altitudes 36°11' and 38°26' North and longitudes

3°55' and 3°97'. It belongs to the large watershed of the Soummam bearing the number 15 in accordance with the nomenclature adopted by the National Water Resources Agency (NWRA). It is situated in the central northern part of Algeria and covers 9125 km² as shown the Figure 1. This area is irregularly elongated in shape (Belkhiri et al., 2011; Djafer khodja et al., 2017; Rezig et al., 2021), its approximate limits are:

- In north, the mountains of Djurdjura.
- In south, the Hodna Mountains and the Setifien plateau.
- In west, the Bouira plateau.
- In east, the Mediterranean.

Geology and hydrogeology of the region

In this watershed there are ancient soil types of paleo-swampy formation which are characterized

by well accentuated formations. The soil map of the Soummam basin was extracted from the soil map of Algeria (Figure 2). These soils generally have a light texture and are therefore permeable. Along the wadis, the existing soils are alluvial deposits called alluvial soils (Boudiaf et al., 1999).

In the southern of Sahel watershed, carbonate, marl, carbonate-terrigenous and terrigenous terrains from the Triassic, Upper Cretaceous and Paleogene are recognized. The continental facies represent loose and weakly cemented Pleistocene-Holocene formations. This zone corresponds to the Saharan Atlas, it is separated from the Tellian domain by the great North Atlas.

Measurements and samples

A sampling campaign was carried out in 2016 by the laboratory team of Algerian Direction of



Figure 1. Geographic location of the study area



Figure 2. Soil map of the Sahel and Soummam watershed (soil map of Algeria 1954)

Water in Bouira in order to get representative data on the spatial variability of the groundwater quality in the aquifer studied.

The parameters concerned by the measurements carried out in situ are: pH, temperature, and conductivity. The water analyses concerned the determination of the contents of the major elements $(Ca^{2+}, Mg^{2+}, Na^+, K^+, Cl^-, SO_4^{-2-}, HCO_3^{--}, NO_3^{--})$. To determine the concentration of the chemical elements, two methods were used:

- Volumetric method for the elements (Ca²⁺, Mg²⁺, Cl⁻, HCO₃⁻);
- Atomic Absorption Spectrophotometry (using a Dr 6000 spectrophotometer (HACH)) for the elements (Na⁺, K⁺, SO₄²⁻, NO₃⁻).

The study of the reliability of the data consists of a verification of the ion balance. It should be remembered that theoretically, the water is neutral electrically. Thus, the chemical equivalents sum of cations must be equal to the anions (Semar et al., 2013). Knowing that a chemical analysis of water is only considered representative when the ionic balance is less than or equal to 10%.

The calculation of the ionic balances is based on the following relationship:

$$BI = 100 * (\Sigma[Cations] - \Sigma[Anions]/(\Sigma[Cations] + \Sigma[Anions])$$
(1)

where: BI – ionic balance expressed as a percentage, Σ [Cations] – the cations sum (units in meq/l), Σ [Anions] – the anions sum (units in meq/l).

Figure 3 represents the ionic balance which is calculated for each water in the 37 boreholes 70% of the boreholes have -5% < BI < 5%, the quality of analyses is acceptable. 92% of boreholes have -10% < BI < 10%, this balance is high but nevertheless remains within a tolerable value range. This is expressed by the reliability of the results obtained. Only 3 samples correspond to 3 boreholes that exceed the BI range as indicated on the histogram, these analyzes are considered doubtful.

The analysis with BI values < 10% were retained and they are given in Table 1, and the analysis that present BI values > 10% were systematically eliminated from this study.

RESULT AND DISCUSSION

Multivariate statistical analysis

Principal component analysis

In this study, the principal component analysis was carried out on a data set of 64 individuals and 12 variables (hardness, pH, EC conductivity, T°c, Mg^{2+} , Ca^{2+} , K^+ , Na^+ , Cl^- , SO_4^{-2-} , HCO_3^{--} , and NO_3^{--}), the first step of the principal component analysis (PCA) consists of calculating the correlation matrix of parameters, they are given in Tables 2, and Table 3. It represents the level of variability commonly shared between individual pairs of water quality variables (Laura et al., 2018). The electrical conductivity EC also indicates a strong positive correlation (0.76, 0.66, 0.79 and 0.75) with, Ca^{2+} , Mg^{2+} , Na^{2+} , and salinity. This reflects the contribution of these elements in the gain of the salinity of groundwater in the region.

The correlation of Mg^{2+} with TH, Na⁺, and salinity was strong and positive (0.64, 0.71, and 0.45, respectively), by definition of total hardness TH, the correlation of this with Mg^{2+} is obvious. Mg^{2+} and Ca^{2+} were found to be linearly correlated with the TH values, indicating major contributors to groundwater salinity. TH further indicates a strong positive correlation (0.88, 0.89, and 0.82)



Figure 3. Presentation of the ionic balances of drillings in the Sahel watershed

Drilling	Name	Dureté	PH	cond	T°C	Ca ²⁺	Mg ²⁺	Na⁺	K⁺	Cl-	SO42-	HCO ³ .	NO ₃ -
F1	F1 Chorfa	44.3	7.31	1236.5	16.35	120.4	39.15	55.4	2.1	123.86	77.835	275.72	2.755
F2	F3 Chorfa	35.6	7.22	917.5	15.8	88.8	32.26	26.6	2.1	82.285	81.3	262.3	8.92
F3	F4 Chorfa	36.7	7.22	943.5	16.6	77.6	56.7	32.6	1.8	83.565	109.975	261.69	7.947
F4	F51 Mchedellah	58	7.09	1450	17.9	120	67.685	57.2	2.3	185.31	207.825	322.07	14.24
F5	F1 adjiba	32.3	7.71	996	16.65	63.6	39.65	56.4	4	102.595	103.68	248.88	0.73
F6	F2 Adjiba	49.6	7.13	911	20.5	102.4	58.32	56.8	2.5	157.38	153.8	301.34	5.98
F7	F3 Semmache	33.7	7.9	1028.5	17.25	72	37.905	38.6	2.9	96.915	119.21	255.59	3.545
F8	F1 Haizer	43.5	7.2	1055	18.2	75.2	60.015	20.8	1.5	67.75	50.325	346.48	14.71
F9	F2 Haizer	38.3	7.325	935.5	18.7	70.4	50.3	19.4	1.9	54.315	43.07	319.64	10.01
F10	F5 Haizer	29	7.35	763	19.05	56.4	36.2	23.8	1.4	60.35	61.105	261.08	8.46
F11	F3 Taghzout	27.6	7.25	795	20.5	47.2	38.39	28.6	1.7	76.68	18.12	272.06	10.76
F12	F4 Taghzout	30.8	7.37	785	20.8	50.4	44.22	28.8	1.1	41.18	38.22	264.74	5.93
F13	F7 Taferka	52	7.23	1764	21.2	83.2	75.81	107.18	2.27	298.2	42.06	335.5	2.165
F14	F12 Taferka	52	7.23	1764	21.2	83.2	75.81	107.18	2.27	298.2	42.06	335.5	2.165
F15	H12 taghzout	40	7.27	1404.5	20.95	84	75.33	56.8	1.7	195.83	42.945	314.76	15.64
F16	H17 taghzout	40	7.27	1404.5	20.95	84	75.33	56.8	1.7	195.83	42.945	314.76	15.64
F17	F16 Sidi Ziane	44.6	7.09	1092.5	17.5	103.2	45.04	44	1.4	145.905	68.71	289.14	6.005
F18	Puit Ain El Beida	68	7.05	1767	17.4	225.6	28.18	53.2	0.6	230	236.25	245.22	110.75
F19	Puit Ouled Zidane	58	7.05	1288	17.6	177.6	33.04	31.5	1.3	138.27	162.8	172.02	110.75
F20	F Guelta Zarga	50.4	7.73	1111.33	19.9	133.6	41.305	40	0.7	101.875	184.8	268.4	18.935
F21	F Bekouche	45.4	7.67	1002	14.8	125.6	31.36	21.8	0.8	48.28	153.6	279.38	12.75
F22	F21 Sidi Ziane	56	7.05	1448	20.6	172.8	31.1	37.6	1	276.9	76.52	242.78	39.0726
F23	F1 SidiZiane	38.3	7.11	1020	18.6	99.2	32.525	37.6	1	134.545	69.065	248.27	25.295
F24	F8 Harket	40.8	7.135	1141.5	18.05	114.4	29.36	42	0.9	129.93	69.66	242.78	11.82
F25	F1 Said Abid	19.4	7.24	854	21.6	56.8	12.63	29.2	1.3	32.66	48.72	140.3	8.46
F26	F2 Said Abid	20.8	7.31	856	21	64.8	11.17	23.8	1.3	39.05	61.94	115.9	12.09
F27	F11 Ouadhia	45.2	7.115	1158.5	19.4	110.4	43.445	50.8	1	191.345	50.57	261.105	15.99
F28	F2 Al Asnem	39.2	7.08	1096	17.1	129.6	16.52	44.4	1.3	127.09	39.12	292.8	91.03
F29	F3 Al Asnam	50.8	6.84	1445	13.8	147.2	33.6	44.4	1.3	149.8	71.54	372.1	19.66
F30	F Djaada	54.2	7.06	1396	16	151.2	39.61	46	0.9	192.375	39.15	340.38	52.8
F31	F1 Guemgouma	43.9	7.025	1173.5	15.85	121.2	32.745	45.2	1.3	125.655	41.37	317.8	66.45
F32	Puit Tarfa	120	7.235	2515	23.35	281.6	119.64	120	2.3	172.885	1101.9	366.97	8.57
F33	F Oued El Berdi	46.2	7.33	1219.5	19.6	104	37.415	37.1	1.2	130.285	110.73	223.26	35.26
F34	Source El Mesdour	21.2	7.82	684.5	23.25	42.8	25.37	54	3.3	66.74	113.835	198.86	1.17

Table 1. Physico-chemical data of borehole water in the Sahel sub-basin region (2016)

Note: data in (mg /L) except (TH, EC, pH and T).

with EC, Ca^{2+} , and SO_4^{2-} . From the study of PCA technique, it can be said that there were seven factors given superior than 70% of the total variance of parameters. As shown in Table 2, the Kaiser standard was used to decide the absolute number of important factors (Khelif et al., 2018).

The factor of the variables ($F_1 \& F_2$) represents about 65.34% of the total variance of the parameters, it is well correlated with relatively

high loads such as EC, Ca^{2+} , Mg^{2+} , TDS, SO_4^2 , turbidity, TH and salinity. This is probably, due to the reactions of mineral water in the region;, therefore, factor F_{11} can be named salinization factor. Factor F_2 represents more than 33.33%, this factor better explains the parameter of pH, temperature T and NO_3^- ; on the contrary, an inverse correlation is observed with the parameters EC, Cl⁻, SO₄²⁻, and HCO₃⁻. Indeed, F_2

Variables	TH	PH	EC	T°C	Ca ²⁺	Mg ²⁺	Na⁺	K⁺	Cl	SO42-	HCO ₃ -	NO ₃ -
TH	1											
PH	-0.309	1										
EC	0.883	-0.339	1									
T°C	0.067	0.195	0.148	1								
Ca ²⁺	0.892	-0.388	0.761	-0.128	1							
Mg ²⁺	0.639	-0.058	0.664	0.364	0.260	1						
Na⁺	0.623	-0.077	0.792	0.392	0.376	0.709	1					
K⁺	-0.077	0.463	-0.022	0.180	-0.309	0.314	0.383	1				
Cl	0.531	-0.418	0.747	0.149	0.446	0.457	0.707	-0.014	1			
SO4 2-	0.821	0.038	0.640	0.275	0.695	0.566	0.517	0.151	0.104	1		
HCO ₃ -	0.498	-0.259	0.501	-0.196	0.253	0.670	0.455	0.097	0.420	0.215	1	
NO ₃ -	0.258	-0.427	0.217	-0.291	0.546	-0.314	-0.125	-0.455	0.217	0.005	-0.129	1

Table 2. Correlation matrix of the physico-chemical parameters of the waters of the Sahel watershed (Pearson)

Table 3. Correlations between variables and factors

Parameter	F1	F2	F3	F4	F5	F6	F7	F8	F9	F10	F11	F12
ТН	0.940	0.144	0.216	-0.170	-0.048	0.009	-0.013	-0.057	-0.064	-0.046	-0.077	-0.054
pН	-0.348	-0.628	0.387	-0.193	0.257	0.476	0.072	-0.014	-0.001	-0.003	0.000	-0.001
EC	0.960	0.068	0.002	0.077	0.075	0.082	-0.087	-0.008	0.131	0.174	-0.008	-0.006
T°C	0.186	-0.537	0.316	0.665	-0.294	-0.016	0.178	0.052	-0.107	0.041	-0.013	0.006
Ca ²⁺	0.768	0.491	0.341	-0.134	0.075	0.033	-0.085	-0.014	-0.118	-0.003	-0.009	0.077
Mg ²⁺	0.760	-0.482	-0.162	-0.095	-0.246	-0.010	0.180	-0.199	0.132	-0.055	0.004	0.030
Na⁺	0.813	-0.390	-0.105	0.223	0.214	-0.002	-0.094	0.222	0.112	-0.093	-0.013	0.013
K⁺	0.041	-0.770	-0.042	-0.156	0.507	-0.328	0.070	-0.053	-0.074	0.041	-0.011	0.005
Cl	0.717	0.096	-0.409	0.428	0.246	0.156	-0.095	-0.127	-0.113	-0.032	0.045	-0.020
SO4 2-	0.718	-0.164	0.597	-0.248	-0.112	-0.133	-0.035	0.040	-0.006	-0.014	0.078	-0.029
HCO ₃	0.598	-0.108	-0.575	-0.430	-0.164	0.107	0.199	0.148	-0.113	0.036	0.011	-0.001
NO ₃ -	0.164	0.813	0.169	0.140	0.325	-0.020	0.392	0.024	0.059	-0.013	0.009	-0.008

presents the sodium bicarbonate factor. The F₃ factor expresses more than 16.67% of the parameters including: SO₄²⁻ and HCO₃⁻. The F₄ factor explains 8.33% of parameters total variance, this factor shows a positive and strong charge in HCO₂⁻ to moderate in Cl⁻. The disintegration of evaporite formations generates salinity of Cl-, while the origin of salinity is due to the presence of HCO_3^- . The F_5 factor explains the lowest parameter variance with 8.33%, where K⁺ gives the greatest contribution with a positive charge in addition to Na⁺. The presence of K⁺ is owing to the interaction between the water and the rock. A detailed explanation of previous five factors is presented in Table 2 and the Figure 4. The analysis of the projection for boreholes in the factorial plane $F_1 - F_2$ (Figure 4) shows that the measurement points can be subdivided into three groups:

- The first group: Characterized by strong mineralization in boreholes F_{32} , F_{13} , F_{14} (north of Oued Dhous sub-basin and south of Oued Zaiane sub-basin) and moderately strong in boreholes F_{42} , F_{62} , F_{13} , F_{16} . This mineralization has a rapport with the lithology of the aquifer presented.
- The second group: It includes the most polluted regions which represent high levels of nitrates correspond to the boreholes: F_{17} , F_{18} , F_{22} , F_{28} , F_{29} , F_{30} , and F_{31} on the Oued Zaiane and Oued Dhous sub-basins. The presence of nitrogenous compounds in the waters of the groundwater, testifies to an organic pollution resulting from the complete or incomplete



Figure 4. Diagram of individuals (Correlations between variables and factors)

degradation of the organic matter by microorganisms in the surface layers of the soil. The NO_3^{-1} is a good indicator of superficial contribution.

 The third group: These are the least mineralized waters, compared to the other groups, i.e. F₃, F₅, F₇, F₈, F₉, F₁₀, F₁₁, F₁₂, F₁₉, F₂₀, F₂₁, F₂₄, F₂₅, F₂₆, F₂₇, F₂₂, F₃₃, and F₃₄.

Hierarchical cluster analysis

The analysis of Hierarchical Cluster Analysis (HCA) was done to obtain a collection of groups of observations (Yiming et al., 2018; Ferhati et al., 2021). Ward's method in which the distance between two clusters denotes how much the sum of squares will increase when merged, also Euclidean distance which is the ordinary straight line distance between two points, were used for grouping the hydrochemical parameters from of the Sahel sub-basin. In this study, for statistical purposes, data have been classified in their

standard ranking. In this approach, 12 hydrochemical parameters are used: T, EC, pH, T, NO₃⁻, Cl⁻,SO₄⁻²⁻, Mg₂⁺, Na⁺, Ca₂⁺, K⁺, TDS, HCO₃⁻, NH₄⁺, and NO₂⁻; however, the last three parameters are relatively negligible.

The analysis of Figure 5 proves that there are two different families: blue and red starting from left to right. Visual investigation is the primary criterion for choosing classes in the dendrogram Figure 5a. The characterized Phenon line was taken at a dissimilarity of 100. At this separation, the groupings could be recognized as to their hydrochemical factors, as shown in Figure 5a. The 12 factors were classified into two groups, as shown in Figure 5b, these groups are:

- Group 1 (C1): hardness, conductivity, Ca₂⁺, Mg₂⁺, Na⁺, Cl⁻, SO₄⁻², HCO₃⁻, and NO₃⁻.
- Group 2 (C2): pH, T°, and K⁺.

After having summarized the hydrochemical parameters in two clusters, the authors worked with the water samples from all the boreholes studied,



Figure 5. Cluster dendrogram for variables: in twelve groups (a), and in two groups (b)

applying the same previous technique which is cluster analysis. More details on the pooled borehole analysis are shown in Figure 6. The investigation of the Figure 6 proves that there are three families of different holes: black, red and green, starting from left to right. There are three groups of boreholes with different chemical characterizations. The dendrogram of the individuals shown in Figure 6a and 6b allows three groups to be recognized as indicated by the degree of mineralization.

These groups are:

- Group 1: Borehole F₃₂.
- Group 2: Boreholes, F₁, F₂, F₃, F₅, F₇, F₈, F₉, $F_{10}, F_{11}, F_{12}, F_{13}, F_{20}, F_{21}, F_{25}, F_{26}, and F_{34}.$ Group 3: Boreholes $F_4, F_6, F_{14}, F_{15}, F_{16}, F_{17}, F_{18},$
- $F_{19}, F_{22}, F_{23}, F_{24}, F_{27}, F_{28}, F_{29}, F_{30}, F_{31}$, and F_{33} .

Diagram

Piper diagram

The piper diagram was chosen to represent different chemical facies of a set of water samples. This kind of diagram has different uses, the most dominant is: to study the development of the water when the increasing of mineralization of water, to indicate the major kinds of anions and cations found in water, and to specify the groups of samples (Blake et al., 2016; Changchang et al., 2018).

The chemical analysis results representation of the water sampled from the 34 boreholes on the piper diagram is given in Figure 7; it indicates that the analyzed waters are characterized by two chemical facies, namely:



Figure 6. Cluster dendrogram: in 34 groups (a), and in three groups (b)



Figure 7. Classification of drillings in the Sahel watershed on the piper diagram (F1-F34)

- Chloride, sulfate, calcium and magnesium.
- Calcium and magnesium bicarbonate.

Knowing that calcium and magnesium are the major cations, and bicarbonates and chlorides are the major anions for all the samples studied. The chloride, sulfate, calcium and magnesium facies; represents 76.47% of the analyzed waters (F_1 , F_3 , F_4 , F_5 , F_6 , F_7 , F_{13} , F_{14} , F_{15} , F_{16} , F_{17} , F_{18} , F_{19} , F_{20} , F_{21} , F_{22} , F_{23} , F_{24} , F_{26} , F_{27} , F_{28} , F_{30} , F_{31} , F_{32} , F_{33} , and F_{34}). It considered the major facies in the studied zone. Usually, it represents waters the most mineralized. The location of this facies is near the fault crossing zones, they are characterized by a strong crushing and injections of Triassic red clays. Its existing is owing to the infiltration and dissolution of clayey-evaporitic Triassic rocks near the faults.

The bicarbonate, calcium and magnesium facies represents 23.53% of the analyzed waters (F_2 , F_8 , F_9 , F_{10} , F_{11} , F_{12} , F_{25} , and F_{29}), it represent least major facies. Usually, it gives waters least mineralized. Water source of this facies is the infiltrations from Liassic carbonate rocks.

Schoeller-Berkaloff diagram

The Schoeller-Berkaloff diagram is a representation semi-logarithmic. This diagram has shown effective results in the field of hydrochemistry. It has given very satisfactory results in Côte d'Ivoire, Ghana, India and Pakistan found by many researchers such as (Oga et al., 2009, Eblin et al., 2014; Loh et al., 2014; Siegel et al., 2015).

When there is a family of broken lines parallel to each other: it is a single group of water with variable mineralization but the proportions are the same for the different dissolved elements. When there are lines that cross: it is a change of chemical facies. The presentation of the water sampled from the 34 boreholes by the Schoeller-Berkaloff diagram is given in Figure 8; it confirms the predominance of the following two facies:

- Chloride, sulfate, calcium and magnesium;
- Bicarbonate, calcium and magnesium.

CONCLUSIONS

The present paper aimed to understund the hydrochemistry and the characteristics of groundwater in the Sahel sub-basin region from multivariate statistical analysis techniques (ACP and HCA) and the Diagram. The representation of the chemical results of the water sampled from the 34 boreholes is characterized by two chemical facies, namely: chloride and sulfated calcium and magnesium; calcium and magnesium bicarbonate.

Thus, it can be said that the waters of the boreholes of the Sahel watershed which are drinkable and respect the standards which are 16: F_1 , F_2 , F_5 , F_7 , F_{10} , F_{11} , F_{12} , F_{17} , F_{21} , F_{23} , F_{24} , F_{25} , F_{26} , F_{27} , F_{33} , and F_{34} . The rest of the boreholes should not be intended for the water supply.

The factors obtained from PCA explain more than 65.34% of the total variance of the data used, it is well correlated with relatively high loads such as EC, Ca_2^+ , Mg_2^+ , TDS, SO_4^{-2} , turbidity, TH and salinity. This is probably due to the reactions of the mineral water in the area. Therefore, this review



Figure 8. Classification of drillings in the Sahel watershed on the Schoeller-Berkaloff diagram (F1–F11), (F12–F22) and (F23–F34)

emphasizes that multivariate statistical techniques are an admirable exploratory tool for interpreting complex informational indices of water quality and for understanding spatial varieties, which are useful and compelling for sustainable and effective water management and water quality.

The found results are helpful for the authorities to planify the supply water to their populations, and rational use of groundwater resources.

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