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Modeling and Optimization the Effect of Some Anions on the Water Conductivity

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Abstract: The implementation of natural water for public supply drinking water still requires a physicochemical treatment, more or less pushed, for the extraction of total or partial of the impurities are in suspension, colloidal or dissolved in water. After use and when it's rejected without pretreatment, it obviously contains pollutants and other elements that are irritating especially that which affects mineral composition, this composition is determined by the conductivity, the latter is an indication of mineralization of water and a function not only of the quantity of ions present, but as well their specific charge, mobility and the temperature of the water. The object of this study is to follow and optimize, in the first time, the variation of conductivity depending on the factors studied (chlorides, sulfates, nitrates and bicarbonates), in the second time, to found a correlation between the conductivity of these anions at different concentrations in three waters: ultra pure water, water intended for human consumption and waste water.

Key words: Water, anions,conductivity, optimization, correlation,principal component analysis.

INTRODUCTION

Several hydro chemical studies were made (Dahmani, B., 2003; Bchitou, R., 2006; Krimissa, S., 2004; Zerki, N., 2011) on the mineralization of the waters to assess the quantity of salts dissolved in water, and obtain valuable information to characterize these waters.Mineralization of most waters is dominated by some substances dissolved in water as electrically charged ions (major ions), which are:calcium, magnesium, sodium, potassium, chloride, sulfates, nitrates and bicarbonates.

However, determining the concentration of these ions in water directly from the conductivity appears complex due to the high variation in the concentration of these ions.

The conductivity measurement can reveal pollution, seepage areas, or mixed (Laftouhi, N., 2003). The conductivity is also a way to validate the physical and chemical analysis of water.

The objective of this study is to follow the variation in concentrations of some anions (chlorides, sulfates, bicarbonates and nitrates) on the conductivity of the water and determine the correlation between conductivity and mineralization in three types water (ultra pure, intended for human consumption, waste) by physicochemical analysis and statistical processing of analytical results collected.

MATERIALS AND METHODS

2.1. Chemical Analysis:

We studied the effect of some anions on thewater conductivity to select factors (anions) that influence this physicochemical parameter.For this purpose a synthetic preparation of solutions was made based on chlorides, sulfates, nitrates and bicarbonates at different concentrations were prepared sequentially from NaCl, $MgSO_4$, $NaHCO_3$, $NaNO_3$, each in 1 liter of ultra pure water to avoid any kind of contamination by the following equations:

$NaCl \longrightarrow Na^+ + Cl^-$
$MgSO_4 \longrightarrow Mg^{2+} + SO_4^{2-}$
$NaHCO_3 \longrightarrow Na^+ + HCO^-_3$
$NaNO_3 \longrightarrow Na^+ + NO^-_3$

To measure the conductivity, the electrode is immersed in the solution and we read the value.The measurement result is shown in µS/cm. the conductivity is measured by the unit CONSORT C831, has a temperature of 21 °C.

2.2. Statistical Analysis:

In order to determine the different correlations between conductivity and different anions, statistical method was applied which is the principal component analysis.This method reduces the number of variables called

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principal components (Fatah, N., 2007). This will lead to the fact that the cloud of individuals projected onto the new principal planes is the least distorted effort to make the total inertia of the cloud projected maximum (Legendre, L. and P. Legendre,1979). This gives a representation of variables in the principal planes which the coordinates are the correlation values of original variables with principal components (Saporta, G., 1978; Foucart, T., 1982). This was achieved on 10 variables centered reduced, which represent the concentrations of the anions studied in ultra pure water, water intended for human consumption and wastewater.

RESULTS AND DISCUSSION

In order to study the correlation between conductivity and anions in water, we characterized in ultra pure water the following anions: chlorides, sulfates, nitrates and bicarbonates.

3.1. The Effect of Some Anions on the Conductivity:
a - Effect of Chloride on the Conductivity:

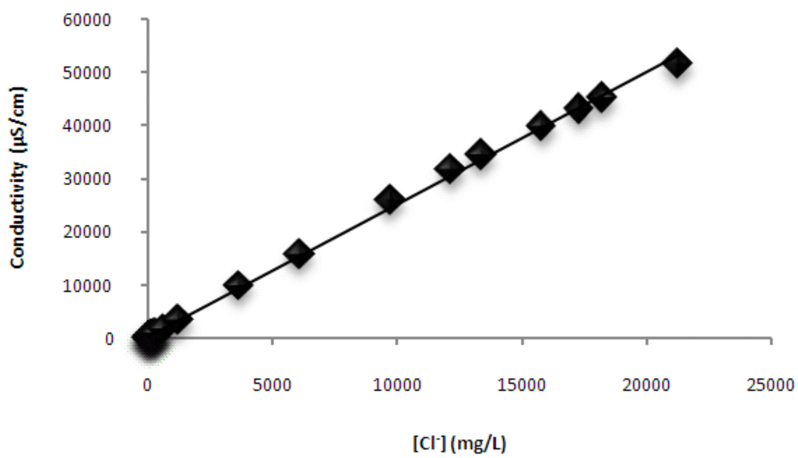

Fig. 1: Conductivity of ultra pure water depending on the concentration of chlorides.

Indeed, as shown in Fig. 1 which shows conductivity in terms of the concentration of chloride ions, the conductivity is strongly proportional to the concentration of these ions, with a correlation coefficient of r = 0,998 and for a concentration guideline 750 mg/L, the conductivity corresponds to the standard that is set at 2700µS/cm.

b - Effect of Sulphate on the Conductivity:

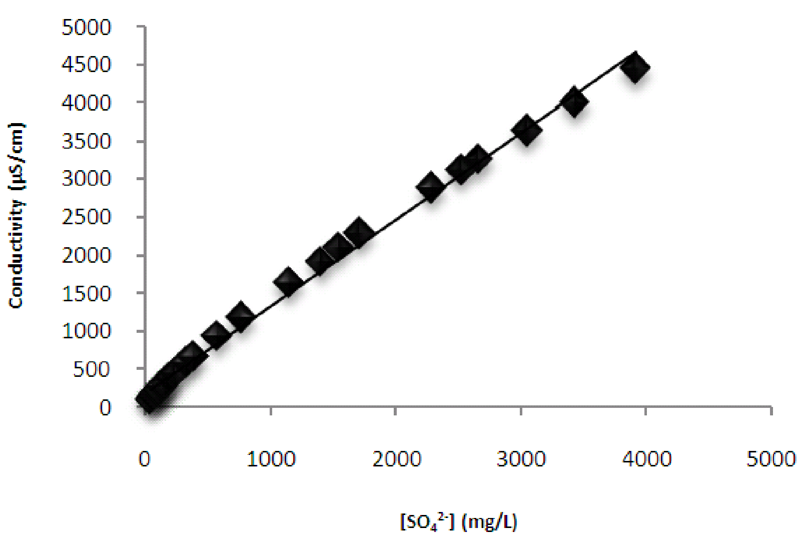

Fig. 2: Conductivity of ultra pure water depending on the concentration of sulfate.

The Fig.2 shows that the sulfate ions have little effect on conductivity since for concentration of 400 mg/L of sulfate, conductivity does not exceed than 1000 µS/cm.

c - Effect of Bicarbonates on the Conductivity:

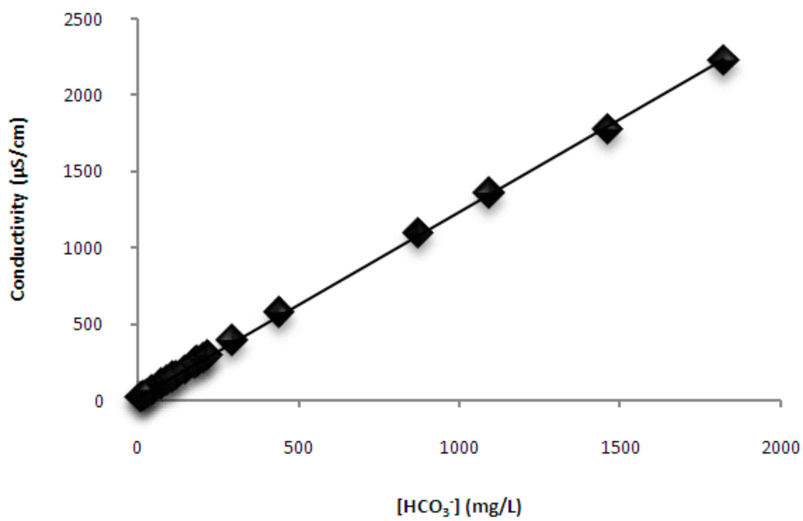

Fig. 3: Conductivity of ultra pure water depending on the concentration of bicarbonates ions.

These results show the bicarbonates ions have little effect on conductivity as a directive concentration of 150 mg/L to bicarbonates; the conductivity does not exceed 200 µS/cm.

In fact, as shown in Fig. 3 which shows conductivity depending of the concentration of bicarbonates ions, the conductivity increases with the concentration of these ions, with a correlation coefficient of r = 0,999.

d - Effect of Nitrates on the Conductivity:

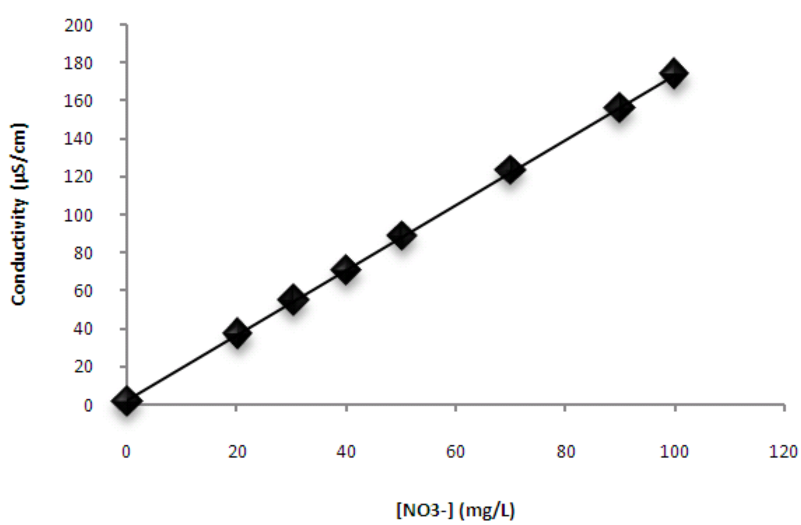

Fig. 4: Conductivity of ultra pure water depending on the concentration of nitrate ions.

The Fig. 4 shows that the conductivity increases with the concentration of nitrate, with a correlation coefficient of r = 0,999 and that these ions have no effect on the conductivity of ultrapure water since for a concentration of 50 mg/L nitrate; the conductivity is 80 µS/cm.The study results of the anions effect (chloride, sulfates, nitrates and bicarbonates) on the ultrapure water conductivity showed that level increasing of each of these four anions causes an increase in the water conductivity.Certainly, the effect of chloride ions is remarkable compared to other elements and the contribution of nitrate is negligible compared to other elements.

3.2. Study of the Correlation and Optimization of the Conductivity of Water:
a - Optimization of conductivity:

To understand the influence of certain chemical elements on the conductivity of water, we determined the curves of isoresponses of conductivity depending of several factors (Table 1), using JMP software [10]. The factors studied are the same mentioned above: chlorides, sulfates, nitrates and bicarbonates (the most influential factors). The response studied is the conductivity of ultrapure water, water intended for human consumption and waste water:

-The optimization of the conductivity in pure water (Fig. 5): isoresponses surfaces show that the optimum is a sulfate concentration less than 397.5 mg/L and a chloride concentration less than 744 mg/L for bicarbonates concentration fixed at 175 mg/L and nitrate at 50 mg/L.

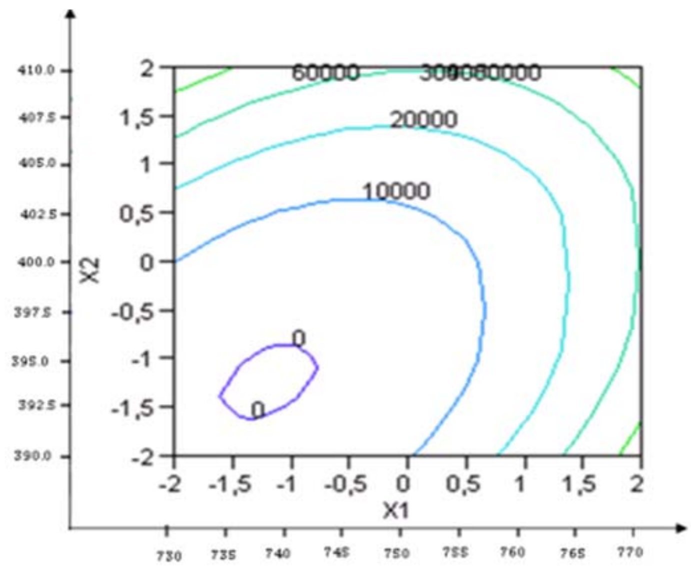

Fig. 5: Curve of isoresponses conductivity of ultrapure water depending on the concentration of chlorides (X1), and sulfates (X2), ($[HCO^-_3]$ = 175 mg/L and $[NO^-_3]$ = 50 mg/L).

-The optimization of the conductivity in the water intended for human consumption: The geometric representation of the isoresponses surfaces in Fig. 6 allowed us to deduce that the optimum value of conductivity can be obtained when the chloride concentration less than 753 mg/L and sulfate concentration less than 408 mg/L for bicarbonates concentration fixed at 125 mg/L and nitrate concentration fixed at 46 mg/L.

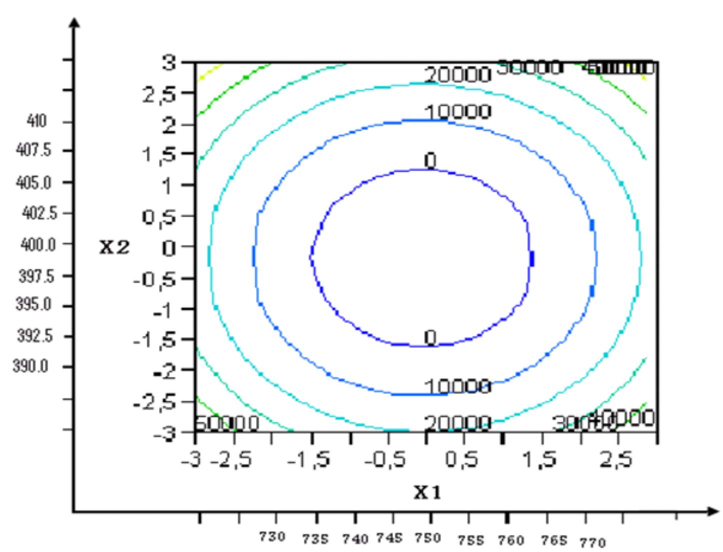

Fig. 6: Curve of isoresponses conductivity of surface water depending on the concentration of chlorides (X1) and sulfates (X2). ($[HCO_3^-]$ = 125 mg/L, $[NO^-_3]$ = 46 mg/L).

-The optimization of the conductivity in wastewater: the geometric representation of curve of isoresponses in Fig. 7 shows that the optimum is by the side of chloride concentration less than 770 mg/L and a sulfate concentration less than 407 mg/L, the concentration of bicarbonates fixed at 175 mg/L and nitrate at 48mg/L.

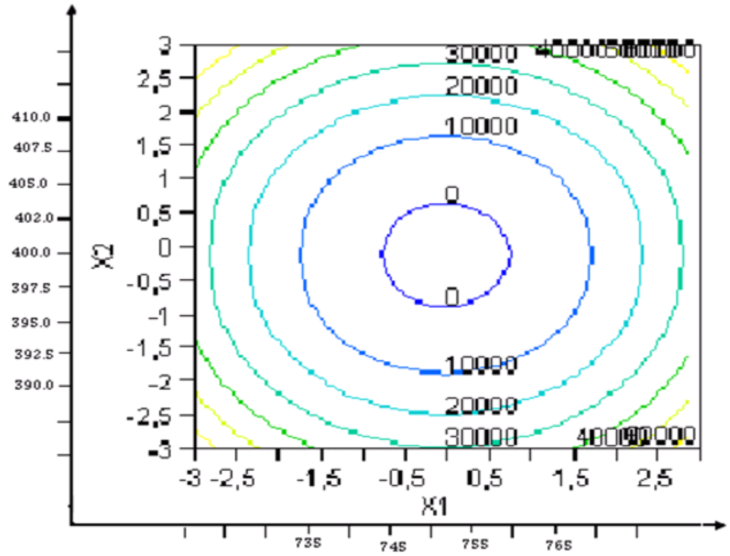

Fig. 7: Curve of isoresponses of the conductivity of wastewater depending on the concentration of chlorides (X1), and sulfates (X2), ($[HCO_3^-]$ = 175 mg/L, $[NO_3^-]$ = 48 mg/L).

b - Correlation Between the Anions at Different Concentrations in the Waters Studied:

For the range of concentrations from 40 to 5000 of Cl^-, SO_4^{2-}, HCO_3^- and NO_3^-, we measured the conductivity of each element at 21 °C. The results of this mathematical analysis are summarized in Tables 1 and 2, and Fig. 8.

Table 1: Conductivity(µS/cm) of selected anions at different concentrations (mg/L) in the three types of water.

		40	50	100	200	600	1000	1400	2000	4000	5000
Ultra pure water	$[Cl^-]$	130	161	313	608	1723	2860	3950	5550	10770	13270
	$[SO_4^{2-}]$	98	117	215	390	960	1456	1481	2580	4510	5390
	$[HCO_3^-]$	72	762	141	271	767	1238	1696	2410	4600	5650
	$[NO_3^-]$	70	91	175	339	986	1584	2220	3110	6010	7400
Water intended for human consumption	$[Cl^-]$	441	477	624	907	2030	3130	4220	5860	11050	13430
	$[SO_4^{2-}]$	404	422	507	662	1207	1688	2717	2810	4720	5590
	$[HCO_3^-]$	380	392	453	576	1044	1498	1946	2650	4790	5830
	$[NO_3^-]$	398	412	491	653	1277	1860	2490	3370	6270	7700
Waste water	$[Cl^-]$	814	841	980	1261	2380	3460	4560	6120	11330	13780
	$[SO_4^{2-}]$	763	778	862	1010	1540	2050	2070	3130	5020	5920
	$[HCO_3^-]$	744	756	818	933	1404	1833	2320	3000	5110	6330
	$[NO_3^-]$	831	851	929	1082	1673	2320	2920	3780	6640	8060

Table 2: Correlation Matrix between conductivity and the factors studied at different concentrations.

	40	50	100	200	600	1000	1400	2000	4000	5000
40	1,000									
50	0,782	1,000								
100	0,991	0,746	1,000							
200	0,941	0,677	0,978	1,000						
600	0,634	0,387	0,732	0,856	1,000					
1000	0,447	0,234	0,562	0,719	0,974	1,000				
1400	0,330	0,150	0,444	0,608	0,908	0,959	1,000			
2000	0,260	0,090	0,383	0,562	0,906	0,977	0,967	1,000		
4000	0,160	0,020	0,284	0,469	0,852	0,946	0,954	0,993	1,000	
5000	0,148	0,014	0,272	0,457	0,843	0,939	0,950	0,990	1,000	1,000

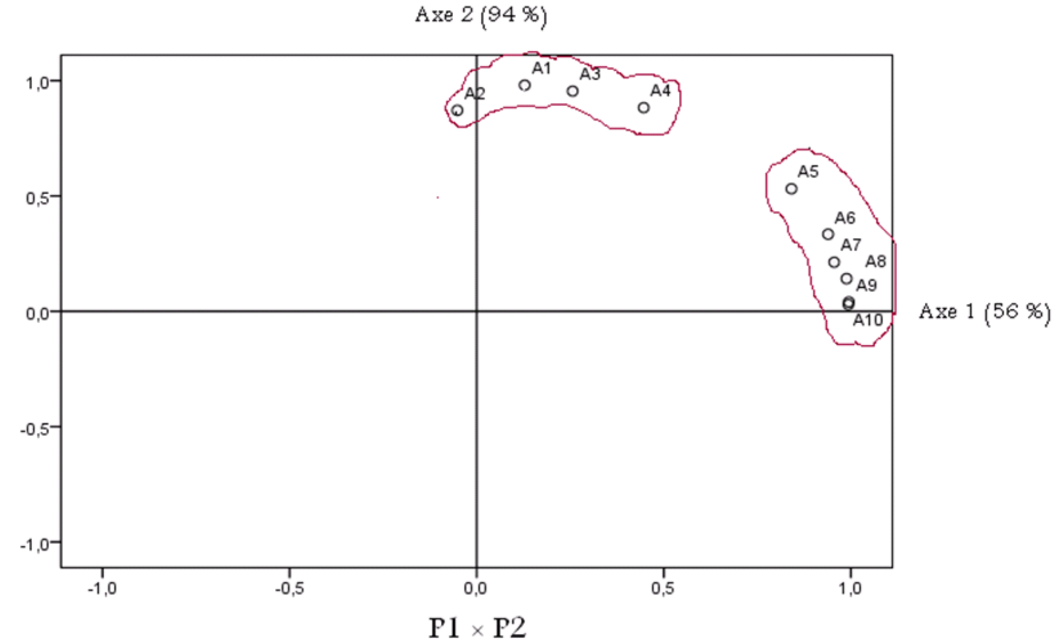

Fig. 8: Plot in the plane P1xP2 of principal component analysis of normalized factors studied at different concentrations in the three types of water.

Where A1, A2..., A10 represent the concentrations of 40 mg / L, 50 mg/L,..., 5000 mg / L.

For the principal component analysis, two axes were selected, which the respective contributions to the total inertia of the cloud are: Axis 1: 56%, Axis 2: 94%.

The plot obtained in the plane P1×P2 represents the formation of two groups:

-The first group formed by concentrations of the factors studied between 40 and 200 mg/L, in this group there is a strong correlation between these factors and the conductivity of water studied with the same character as the axis P1.

-The second group formed by concentrations of the factors studied above 600 mg/L in this group the correlation between these factors and the conductivity is low along the axis P2.

Certainly, as well as the concentration of factors studied is higher; make conductivity correlation of three waters is low.

4. Conclusion:

The factors effect studied (chlorides, sulfates, bicarbonates and nitrates) on the conductivity of ultra pure water, allowed us to select the factors influencing this physicochemical parameter that is chlorides and sulfate and to remove nitrate ions which have feeble effect. For determining the correlation between conductivity and different concentrations of the factors studied in three types of water, a statistical method which is the principal component analysis is used. This method allowed us to distinguish two groups well represented in the P1xP2 plan.

In fact, as well as the concentration of factors studied is higher; make conductivity correlation of three waters is low.

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