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Using the Linear Least Square Method in determining the relationship between salinity, electrical conductivity, density and pH for water in some parts of Nigeria.

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Abstract

This study was aimed at generating a mathematical relationship connecting four quality parameters of water, namely salinity, electrical conductivity, density and pH. Samples of surface water and ground water were collected from eight major towns in Delta State, Nigeria. Measurements of the parameters were carried out using digital meters and the data analysed using the linear least square method of fitting a straight line to data points. The analysis of the data yielded a mathematical equation showing the relationship between the four measured parameters. This generated equation was subjected to test for reliability by the determination of the standard deviation. The result reveals that the standard deviation of the calculated values of salinity using the generated equation from the measured values for surfaces water is 2mg/l while that of ground water is 4mg/l. This shows an error of less than 2% and hence the equation can be relied upon.

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1.0 Introduction

Water quality may be described in a variety of ways which include physical, chemical and biological [1]. However, four physical parameters namely salinity, electrical conductivity, density and pH which are considered in this study are very important in describing the quality of water used for domestic purposes.

Salinity in an ideal situation should be the sum of all dissolved salts in grams per kilogram of sea water. In practice, this is difficult to measure. It however allows the determination of salt content through the measurement of a substitution quantity and calculation of the total of all materials making up the salinity from that measurement [2].

Furthermore, salinity has been defined as the total amount in grams of dissolved substances contained in one kilogram of sea water if all carbonates are converted into oxides, all bromides and iodides into chlorides, and all organic substances oxidized. The relationship between salinity and chloride was determined through a series of fundamental laboratory measurements based on sea water samples from all regions of the world ocean and was given as

$$S(^{o}/_{oo}) = 0.03 + 1.805\ Cl\ (^{o}/_{oo})$$

The symbol $^{o}/_{oo}$ stands for “part per thousand”. A salt content of 3.5% is equivalent to 35 $^{o}/_{oo}$, or 35 grams of salt per kilogram of sea water.

The fact that the equation gives a salinity of 0.03 $^{o}/_{oo}$ for zero chlorinity is a cause for concern. it indicates a problem in the water samples used for the laboratory measurements. The United Nations Scientific, Education and Cultural Organisation (UNESCO) decided to repeat the base determination of the relation between chlorinity and salinity and introduced a new definition, known as absolute salinity [2].

$$S(^{o}/_{oo}) = 1.80655\ Cl\ (^{o}/_{oo})$$

These two equations that define salinity give identical result at a salinity of 35 $^o/_{oo}$ and do not differ significantly for most applications.

The definition of salinity was reviewed again when techniques to determine salinity from measurements of electrical conductivity, temperature and pressure were developed. Since then, the practical salinity scale defines salinity in terms of a conductivity ratio.

The practical salinity, symbol S, of a sample of sea water, is defined in terms of the ratio K of the electrical conductivity of a sea water sample at 15^0C and at pressure of one standard atmosphere, to that of a potassium chloride (KCl) solution, in which the mass fraction of KCl is 0.0324356, at the same temperature and pressure. A K value exactly equal to one corresponds, by definition, to a practical salinity equal to 35. The corresponding formula is [2]

$$S = 0.0080 - 0.1692K^{1/2} + 25.3853K + 14.0941K^{3/2} - 7.0261K^2 + 2.7081K^{5/2}$$

where K is the conductivity.

Note that in this definition, salinity is a ratio and ($^o/_{oo}$) is therefore no longer used, but the old value of 35 $^o/_{oo}$ corresponds to a value of 35 in the practical salinity.

The relationship between salt concentration (C) and electrical conductivity (EC) is approximately C = 640 EC. The approximate relationship between the electrical conductivity of irrigated water (EC_i) and soil salinity is $EC_e = 1.5\ EC_i$, if about 15 percent of the applied water is drained from the crop root zone [3]. However, in the paper measuring the salinity of water, it was noted that the relationship between salinity and electrical conductivity for natural Victorian waters is [4]

$$\text{Salinity} = \text{Electrical Conductivity} \times 0.6.$$

Other parameters also may be relevant in describing water quality. One is pH, which is a measure of the acidity or alkalinity of the water. The pH of water is inversely related to acidity. The higher the pH, the more saline the water will be. Water that is neither acid nor alkaline has a pH of 7. For health reasons, concentrations of certain bacteria may also be monitored in drinking water supplies.

Manufacturers have tried very hard with little success in trying to produce a single instrument to measure most parameters that describe the quality of water. One such success is the PSC digital pH meter which is capable of measuring both pH and temperature. This paper therefore considers the mathematical relationship between the parameters under study and tries to generate a general relationship between them using the least square method. The use of the linear fit is as a result of the fact that the data acquired in this study are all having linear relationships as shown in figure 1 and figure 2. The outcome of this study will help Engineers/Manufacturers to manufacture a single instrument which will be capable of measuring these four parameters to a high accuracy. It will also be useful to programmers in the development of soft ware needed in the computation of these quality parameters of water if any one of them is known.

2.0 Method of data collection

Surface and ground water were collected from eight towns in Delta State, Nigeria, namely Warri, Sapele, Abraka, Ogharaeki, Ughelli, Patani, Oleh and Ozoro. The surface water was collected from existing streams in the areas and the ground water was collected from wells. Well water is best taken prior to any purification or treatment process. This is because chlorination, filters, softeners and other treatment may chemically alter the water quality. Samples were therefore taken prior to any treatment process. The samples were collected into different containers which were rinsed three times with the sampled water before the samples were collected into the containers. The containers were all labelled to indicate the point of collection and were taken to the laboratory where the different physical parameters were determined.

The electrical conductivity for both the surface and ground waters were determined using the YSI 85 conductivity meter and the TD Scan 10 meter while the test for salinity was carried out using the TDScan 20 digital meter which is widely used for salinity test [5].

The density was determined by first weighting an empty beaker and the weight noted. Then $250cm^3$ of the sampled water was measured into the empty beaker and the mass determined. The mass of the water sample in the beaker was determined by subtracting the mass of the beaker when empty from the mass of both beaker and water. This mass was divided by the volume of the sample which is 250cm^3. The values obtained are recorded as the density of the water sample.

The pH of the water samples was determined using a PHM 201 portable pH meter.

3.0 Mathematical background

Linear least squares fittings in which the fitted expression is linear, may be regarded as a special case of least squares methods for general expressions. We shall find, however, that its special feature makes it worthy of detailed study in its own right. Perhaps the most important of these features is that we are able to obtain an explicit formula for the fitted parameters.

It is normally assumed that the input data have the form [6]

$$(x_i, y_i \pm \sigma_i),\ i = 1, 2, \ldots, N$$

For each observation y_i, there is associated an uncertainty σ_i which can be estimated in relation to the experimental procedure. The x_i values distinguish different observations and are presumed to be known exactly.

Linear least squares fitting is based on the presumption that a set of function $f_\alpha(x_i)$ can be found such that the expression for y is linear in a set of $M(<N)$ parameters a_α i.e.

$$y(x) = \sum_{\alpha=1}^{m} f_\alpha(x) a_\alpha \tag{3.1}$$

Note that the number m of parameters a_α is less than the number of data values y_i.

Explicit formulae can be found for the a_α values if we minimise the sum of squares of deviations between the data values y_i and the $y(x_i)$ given by the fitting formula shown in equation 1 of reference [6].

Let the deviation between the data and the function y be written as;

$$\Delta = Y_i - Y(x) = y_i - \sum_{i=1}^{N} f(x_i) a_\alpha \tag{3.2}$$

The sum of squares to equation (3.2) gives

$$\sum_{i=1}^{N} \Delta^2 = \sum_{i=1}^{N} \left[y_i - \sum_{i=1}^{N} f(x_i) a_\alpha \right]^2 \equiv f(a,b) \tag{3.3}$$

The least squares fit is obtained by minimising the weighted sum of squares of deviations, hence we require that $\frac{\partial f}{\partial a} = \frac{\partial f}{\partial b} = 0$, i.e.

$$\frac{\partial}{\partial a} \sum_{i-1}^{N} \{ y_i - (ax_i + b) \}^2 = -2 \sum_{i-1}^{N} \{ y_i - (ax_i + b) \} x_i = 0$$

Re-arranging the above yield equation 3.4 below

$$\sum_{i-1}^{N} y_i x_i = a \sum_{i-1}^{N} x_i^2 + b \sum_{i=1}^{N} x_i \tag{3.4}$$

$$\frac{\partial}{\partial b} \sum_{i-1}^{N} \{ y_i - (ax_i + b) \}^2 = -2 \sum_{i-1}^{N} \{ y_i - (ax_i + b) \} \cdot 1 = 0$$

Again, rearranging the above will yield equation (3.5)

$$\sum_{i-1}^{N} y_i = a \sum_{i-1}^{N} x_i + b \sum_{i=1}^{N} i \tag{3.5}$$

Equations (3.4) and (3.5) will now be used to determine the relationship between;

(i) Salinity and Electrical Conductivity
(ii) Salinity and Density
(iii) Salinity and pH
for both surface and ground water using the data obtained in this study.

4.0 Results and calculations

The measurement of the four physical parameters for surface water is presented as table 1 while table 2 contains the measurements obtained for ground water in all the eight locations. All the quality parameters measured, as shown in tables 1 and 2, were compared with each other using spearman rank order statistics to determine which variables significantly correlated with one another [7]. Very strong positive correlations between variables were found between all four parameter as shown in tables 3 and 4. Based upon this fact, a mathematical relationship was determined between the measured parameters.

4.1 Relationship between salinity and electrical conductivity for surface water

Using the experimental data for salinity and electrical conductivity for surface water, equations 3.4 and 3.5 transform to

$$\sum SK = a\sum K^2 + b\sum k \qquad (4.1)$$

$$\sum S = a\sum k + b\sum_i \qquad (4.2)$$

where S is the salinity and K the electrical conductivity.
Equations (4.1) and (4.2) become

$$3748924 = 5856649a + 5896b \qquad (4.3)$$

$$3774 = 5896a + 8b \qquad (4.4)$$

which can be reduced to

$$635.842 = 993.326a + b \qquad (4.5)$$

$$471.750 = 737.000a + b \qquad (4.6)$$

and hence 164.092 = 256.326a with $a = \frac{164.092}{256.326} = 0.6401$.

Substituting the value of 'a' into (4.5) we obtain the value for 'b' as follows

$$471.750 = 737 \times 0.6401 + b, \text{ and } b \approx 0$$

Hence the relationship between salinity and electrical conductivity for surface water in the area under study is given as;

Salinity = 0.64 x Electrical Conductivity (4.7)

4.2 Relationship between salinity and density for surface water

Equations (3.4) and (3.5) transform to

$$\sum S\rho = a\sum \rho^2 + b\sum \rho \qquad (4.8)$$

$$\sum S = a\sum \rho + b\sum_i \qquad (4.9)$$

where ρ is the density of the water samples, and equations (4.8) and (4.9) become

$$4139.468 = 9.206a + 8.575b \qquad (4.10)$$

$$3774.000 = 8.575a + 8.000b \qquad (4.11)$$

This reduces to

$$482.737 = 1.0736a + b \qquad (4.12)$$

$$471.750 = 1.0719a + b \qquad (4.13)$$

From (4.12^I) and (4.13^I) we get $a = \frac{10.987}{0.0017} = 6463$

Substituting the value of 'a' into (4.12), we obtain the value for 'b' as follows

$$482.737 = (1.0736 \times 6463) + b, \text{ and } b = -6456$$

Hence the relationship between salinity and density for surface water in the areas under study is given as;

Salinity = 6463ρ - 6456 (4.14)

4.3 **Relationship between salinity and pH for surface water**

Equations (3.4) and (3.5) transform to

$$\sum S(\text{pH}) = a\sum(\text{pH})^2 + b\sum \text{pH} \quad (4.15)$$

$$\sum S = a\sum(\text{pH}) + b\sum_i \quad (4.16)$$

and equations (4.15) and (4.16) become

$$30765.96 = 495.219a + 62.81b \quad (4.17)$$

$$3774.00 = 62.810a + 8.00b \quad (4.18)$$

This reduces to

$$489.826 = 7.884a + b \quad (4.19)$$

$$471.750 = 7.851a + b \quad (4.20)$$

From (4.19^I) and (4.20^I) we get $a = \dfrac{18.076}{0.033} = 548$.

Substituting the value of ‘a’ into 4.13^I, we obtain the value for ‘b’ as follows

$$489.826 = (7.884 \text{ x } 548) + b, \text{ and } b = -3831$$

Hence the relationship between salinity and pH for surface water in the area under study is given as;

$$\text{Salinity} = 548\text{pH} - 3831 \quad (4.21)$$

This is valid for all positive values salinity

The above three equations showing the relationship between salinity and electrical conductivity, salinity and density, and Salinity and pH (i.e. equations 4.7, 4.14 and 4.20) can be added together as;

$$\text{Salinity} = 0.64K + 0 + 0$$
$$\text{Salinity} = 0 + 6463\rho - 6456 + 0$$
$$\text{Salinity} = 0 + 0 + 548\text{pH} - 3831$$
$$3 \text{ x Salinity} = 0.64K + 6463\rho - 6456 + 548\text{pH} - 3831$$
$$= 0.64K + 6463\rho + 548\text{pH} - 6456 - 3831$$
$$= 0.64K + 6463\rho + 548\text{pH} - 10287$$

$$\text{Salinity } (S_{SW}) = 0.213K + 2154.33\rho + 182.67\text{pH} – 3429 \quad (4.22)$$

Equation (4.22) is the mathematical relationship between salinity, electrical conductivity, density and pH for surface water in the area under study

4.4 **Relationship between salinity and electrical conductivity for ground water**

Using equations (4.1) and (4.2), we have that

$$6310392 = 9857868a + 7696b \quad (4.23)$$

$$4926 = 7696a + 8b \quad (4.25)$$

which can be reduced to

$$50483136 = 78862944a + 61568b \quad (4.26)$$

$$37910496 = 59228416a + 61568b \quad (4.27)$$

From (4.26) and (4.27^I) we get

$$12572640 = 19634528a, \text{ and } a = 0.6403 \approx 0.64$$

Substituting the value of ‘*a*’ into 4.25, we obtain the value for ‘*b*’ as follows

$$4926 = 7696 \text{ x } 0.64 + 8b, \text{ and } b = 0.07 \approx 0$$

Hence the relationship between salinity and electrical conductivity for ground water in the area under study is given as;

$$\text{Salinity} = 0.64K \quad (4.28)$$

4.5 **Relationship between salinity and density for ground water**

Using equations (4.8) and (4.9) we have that

$$5532.636 = 9.576a + 8.742b \quad (4.29)$$

$$4926.000 = 8.742a + 8b \quad (4.30)$$

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This reduces to

$$632.880 = 1.0954a + b \qquad (4.31)$$

$$615.750 = 1.0928a + b \qquad (4.32)$$

From (4.31^I) and (4.32^I) we get

$$17.13 = 0.0026a, \text{ and } a = 6589$$

Substituting the value of a into (4.31), we obtain the value for '*b*' as follows

$$4926 = (8.742 \times 6589) + 8b, \text{ and } b = -6584$$

Hence the relationship between salinity and density for surface water in the area under study is given as;

$$\text{Salinity} = 6589\rho - 6584 \qquad (4.33)$$

4.6 Relationship between salinity and pH for ground water

Using equations (4.15) and (4.16) we have that

$$41911.93 = 532.24a + 62.04b \qquad (4.34)$$

$$4926 = 65.04a + 8b \qquad (4.35)$$

This reduces to

$$644.167 = 8.1685a + b \qquad (4.36)$$

$$615.750 = 8.1163a + b \qquad (4.37)$$

From (4.34^I) and (4.35^I) we get

$$28.417 = 0.0522a, \text{ and } a = 544$$

Substituting the value of '*a*' into (4.36), we obtain the value for '*b*' as follows

$$644.167 = (8.1685 \times 544) + b, \text{ and } b = -3800$$

Hence the relationship between salinity and pH for surface water in the area under study is given as;

$$\text{Salinity} = 544\text{pH} - 3800 \qquad (4.38)$$

This is valid for all positive values of salinity.

The three equations showing the relationship between salinity and electrical conductivity, salinity and density and salinity and pH for ground water (i.e. equations 4.28, 4.33 and 4.38) can be added together as;

$$\text{Salinity} = 0.64K + 0 + 0$$

$$\text{Salinity} = 0 + 6589\rho - 6584 + 0$$

$$\text{Salinity} = 0 + 0 + 544\text{pH} - 3800$$

$$3 \times \text{Salinity} = 0.64K + 6589\rho - 6584 + 544\text{pH} - 3800$$

$$= 0.64K + 6589\rho + 544\text{pH} - 6584 - 3800$$

$$= 0.64K + 6589\rho + 544\text{pH} - 10384$$

$$\therefore \text{Salinity } (S_{GW}) = 0.213K + 2196.33\rho + 181.33\text{pH} - 3461 \qquad (4.39)$$

Equation 4.26 is the mathematical relationship between salinity, electrical conductivity, density and pH for ground water in the area under study

4.7 Generalized Equations for both surface and ground water

The two equations derived for both surface and ground water (equations 4.16 and 4.26) show that the two equations coincide and there are infinitely many points of intersection from linear algebra. Therefore, the two equations S_{SW} and S_{GW} can be combined to give a single equation that can be used for either surface or ground water [8].

$$S = 0.213K + 2154.33\rho + 182.67\text{pH} - 3429$$

$$S = 0.213K + 2196.33\rho + 181.33\text{pH} - 3461$$

$$2S = 0.426K + 4350.66\rho + 364.00\text{pH} - 6890$$

$$\therefore S = 0.213 + 2175.33\rho + 182\text{pH} - 3445 \qquad (4.40)$$

Equation (4.40) is the generalized equation describing the relationship between salinity, electrical conductivity, density and pH for surface and ground water.

The determination of the standard deviation (*SD*) of the calculated values using the generalized equation and the measured values as shown in Tables 1 and 2 are carried out using equation (4.41) below [9].

$$SD = \sqrt{\frac{\sum (S_M - S_C)^2}{N}} \qquad (4.41)$$

where S_M is the measured values of salinity, S_C is the calculated value of salinity and N is the number of data points. The calculation reveals that the *SD* for surface water is 2mg/l while the *SD* for ground water is 4mg/l.

5.0 Discussion of Results

This study applies the linear least square method of fitting a straight line to a set of data point in determining the relationship between salinity, electrical conductivity, density and pH for both surface and ground waters in some parts of Nigeria. The linear relationship between the measured parameters as shown in figures 1 and 2 was the reason for adopting this method. Equations showing the relationship between the parameters were generated for surface water and also for ground water. These equations were then combined together mathematically to yield a single general equation as is seen in equation 4.27. This equation can be conveniently used for both surface water as well as for ground water. The calculation of the standard deviation of the calculated values of salinity from the measured values reveal that the standard deviation for surface water is 2mg/l while the standard deviation for ground water is 4mg/l.

6.0 Conclusions

It has been shown successfully through this study that a mathematical relationship exists between salinity, electrical conductivity, density and pH of water. This finding is very important to Engineers who are interested in building a single instrument capable of measuring these four parameters. This instrument can be referred to as 4 in 1 salinity meter. The study will also be beneficial to programmers who are interested in developing soft wares for the computation of water quality parameters using computer interactive techniques. This study has shown that the linear least square method can be used quite successfully in the determination of the relationship that exist between salinity, electrical conductivity, density and pH of water in the Delta area. The method yielded fairly reasonable result as the determination of the standard deviation reveals an error of less than 2% for both surface and ground waters.

Table 1: Summary of results obtained from surface water measurements.

LOCATIONS	Electrical Conductivity μS/cm)	Salinity (mg/l)	Density (gm/cm^3)	pH
Warri	1115	714	1.108	8.29
Sapele	1450	928	1.142	8.69
Abraka	260	166	1.026	7.29
Ughelli	581	372	1.056	7.67
Patani	1003	642	1.098	8.16
Oleh	244	156	1.024	7.27
Ozoro	257	164	1.025	7.29
Ogharaeki	987	632	1.096	8.15

Table 2: Summary of results obtained from ground water measurements.

LOCATIONS	Electrical Conductivity (μS/cm)	Salinity (mg/l)	Density (gm/cm^3)	pH
Warri	1215	778	1.116	8.40
Sapele	2140	1370	1.208	9.50
Abraka	360	230	1.036	7.42
Ughelli	779	500	1.076	7.91
Patani	1216	778	1.116	8.42
Oleh	449	287	1.044	7.49
Ozoro	449	287	1.044	7.52

Ogharaeki	1088	696	1.104	8.27

Table 3: Tables showing the correlation coefficient between measured parameters for surface water

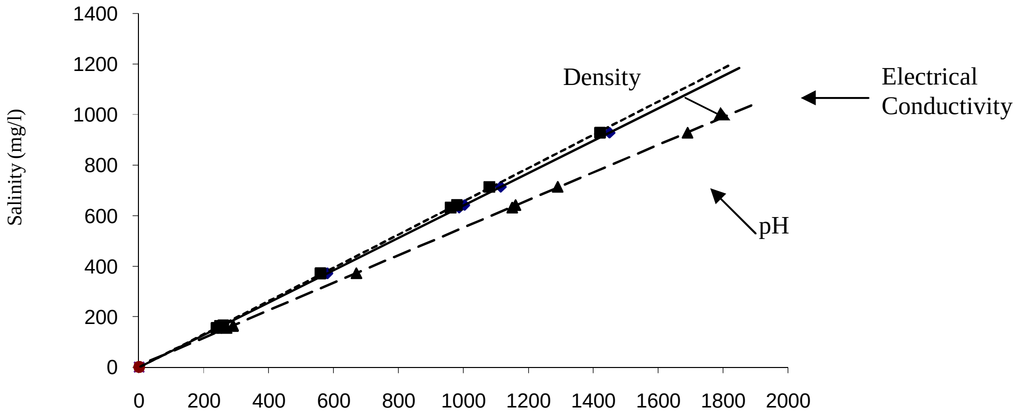
		Salinity	Electrical Conductivity	Density	pH
Salinity	Pearson Correlation Sig. (2-tailed) N	1.000 . 8	1.000** .000 8	1.000** .000 8	1.000** .000 8
Electrical Conductivity	Pearson Correlation Sig. (2-tailed) N	1.000** .000 8	1.000 . 8	1.000** .000 8	1.000** .000 8
Density	Pearson Correlation Sig. (2-tailed) N	1.000** .000 8	1.000** .000 8	1.000 . 8	1.000** .000 8
pH	Pearson Correlation Sig. (2-tailed) N	1.000** .000 8	1.000** .000 8	1.000** .000 8	1.000 . 8

** Correlation is significant at the 0.01 level (2-tailed)

Table 4: Table showing the correlation coefficient between measured parameters for ground water.

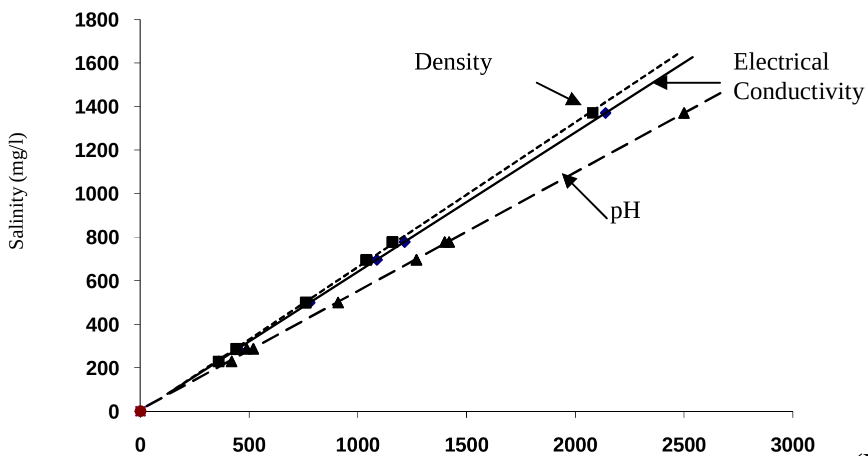
		Salinity	Electrical Conductivity	Density	pH
Salinity	Pearson Correlation Sig. (2-tailed) N	1.000 . 8	1.000** .000 8	1.000** .000 8	.999** .000 8
Electrical Conductivity	Pearson Correlation Sig. (2-tailed) N	1.000** .000 8	1.000 . 8	1.000** .000 8	.999** .000 8
Density	Pearson Correlation Sig. (2-tailed) N	1.000** .000 8	1.000** .000 8	1.000 . 8	.998** .000 8
pH	Pearson Correlation Sig. (2-tailed) N	.999** .000 8	.999** .000 8	.998** .000 8	1.000 . 8

** Correlation is significant at the 0.01 level (2-tailed)



= (K/μcm)
1 1.018 1.038 1.058 1.078 1.098 1.118 1.138 1.158 1.178 1.198 = (ρ /gm/cm^3)
7 7.22 7.46 7.70 7.94 8.18 8.42 8.66 8.90 9.14 9.38 = (pH)

Figure 1: The graph of salinity against electrical conductivity, density and pH of surface water in Delta State.



= (K/μcm)
1 1.048 1.096 1.144 1.192 1.240 1.288 = (ρ /gm/cm^3)
7 7.59 8.16 8.75 9.34 9.93 10.52 = (pH)

F**igure 2**: The graph of salinity against electrical conductivity, density and pH of ground water in Delta State.

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