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Graphical Techniques of Presentation of Hydro-Chemical Data

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Abstract

Water is vital to man's existence and early human civilizations centered on springs and streams for their day to day activities with water which is vital for survival. Throughout history, people around the world have used groundwater as a source of drinking water and even today, more than half of the world's population depends on groundwater for survival. Pure water does not exist in nature due to various interactions between the geologic Formation as well as atmospheric gases such as Carbon dioxide and Oxygen, hence the need for chemical analysis of water. Determination of concentration of various ions is one major form of chemical analysis. Because of the number of ions involved, it is usually more convenient to present the results in graphical forms for easy understanding of the water samples analyzed. There are several methods of graphical presentation which includes Bar Chart, Pie Chart, Stiff Diagram, Schoeller Diagram, Piper Diagram and Scattered Plots. For instance Bar chart, Pie Chart, Stiff Diagram are good for small numbers of chemical data, whereas the Schoeller, Piper Diagrams and Scattered Plots are suitable for presentation of results for large numbers of chemical data.

Keywords: Groundwater, Hydrochemistry, Graphical, Molality and Water type

INTRODUCTION

Natural waters are never pure; they always contain at least small amounts of dissolved gases and solids, because of the interactions with both atmosphere as well as the geological formations. For most of it's used the chemical properties and available quantity. Water constitutes about two third of the earth volume, while the rest is covered by land surface. Water occurs in three places in the earth. It occurs in the atmosphere in form of condense vapors, in lithosphere that is pore spaces in both inter/intra granular spaces in sedimentary rocks and fractures and veins in both igneous and metamorphic rocks. Whereas in hydrosphere in oceans, streams, rivers and lakes. An important task in groundwater investigation is the compilation and presentation of chemical data in a convenient manner for visual inspection, for these purpose several commonly used graphical methods are available. Among these is the bar chart (Freeze and Cherry 1979). Water in these various environments or area is characterized by unique concentration of organic, inorganic and bacteriology constituent tend to define the usability of the water. But it is worth noting that acceptable concentration limit is control by the purpose for which the water is used. Since there is no pure water in nature, there is need for chemical and biochemical constituent determination. Its suitability for utilization in the industry, it is therefore very necessary to undergo geochemical studies in water. Complete chemical analyses of a water sample include the determination of concentration of the inorganic constituent present, radiological and organic parameters are normally of concern only where human being influence the pollution that affect the quality.

Dissolved salts in water of normal salinity occur as dissociated ions plus other minor constituents are present and reported in elemental form. Chemical impurities in water can cause many health hazards. The analysis also include physical parameter such as pH and electrical conductivity, depending on the purpose for water quality investigation, partial analysis of only particular constituent will at time suffice. In a chemical analysis of water, concentration of different ions are expressed by weight or by chemical equivalence, some properties of the water properties evaluated in a physical analysis include colour, odour, temperature, taste and turbidity.

HYDROCHEMISTRY

Hydrochemical composition of water is as important as any other properties of water. The chemical components of water did not only indicate the quality of water, but also help to infer the geology of the area. Hydrochemistry is concerned with the chemical analysis of water, which involves determination of the concentration of the in-organic constituents present. In describing units and expressions for water quality, standard exist that are used to interpret the quality for suitability for a particular purpose. Concentrations of different ions are expressed in by chemical equivalent or weight.

UNITS OF REPORTING RESULTS

The results of chemical analyses are always presented or reported in concentration units. Various types of concentration units are in used.

CONCENTRATION BY WEIGHT

The concentrations of the common ions found in groundwater are reported by weight per volume units of milligrams per litre (mg/l).

CHEMICAL EQUIVALENCE

Positively charged cations and negatively charged anions combine and dissociate in definite weight ratio. By expressing ion concentrations in equivalent weights, these ratios are readily determined because one equivalent weight of a cation will exactly combine with one equivalent weight of an anion. The combining weight of an ion is equal to its formula weight divided by its charge.

MAJOR CATIONS AND ANIONS WITH THEIR CONVERTION FACTORS FOR CHEMICAL EQUIVALENCE (After Todd. 2004)

CATIONS ION						**CONVERSION FACTORS**
Calcium Ca^{2+}						0.0499
Magnesium Mg^{2+}						0.08226
Sodium Na^+						0.0435
Potassium K^+						0.02557
ANIONS ION						**CONVERSION FACTORS**
Bicarbonate $HC0_3^-$						0.01639
Sulphate SO_4^{2-}						0.02082
Chloride Cl^-						0.02821

MOLARITY

Is defined as the number of solutes in $1m^3$ of a solution. The unit for molarity is designated as mol/m^3.

MOLALITY

Is also defined as the number of moles of solutes dissolved in a kilogram mass of a solution. The unit is mol/kg. Therefore one mole of a compound is the equivalent of one molecular weight.

MASS CONCENTRATION

Is also defined as mass of solute dissolve in a specified unit volume of solution. The unit is also in kg/m^3. Gram per litre (g/l) is a permitted unit, but the most common mass concentration unit reported in the groundwater literature is milligrams per litre i.e. (mg/l).

There are many other non concentration units used in groundwater literature are parts per million (ppm) equivalent per litre (epl), equivalent per million (epm) are all very important unit of reporting because in chemical reactions equivalent of anions. Therefore if cations and anions are expressed in (meq/l) it is possible to check the accuracy of the analysis, by comparing the equality of the cations and anions. Because natural water contains a variety of ionic and undissociated species, conductance cannot be simply related to total dissolved solids, conductance is easily measured and gives results that are convenient as a general indication of dissolved solid. Results of analyses of chemical quality of water samples are most conveniently presented in graphical form. The purposes are stated below:

- ✓ Display purpose
- ✓ Comparing analyses
- ✓ Emphasizing similarities and differences

These graphical representation also aid in detecting the mixing of water difference composition and identifying chemical process occurring as water move. A great number of naturally occurring minerals poses the ability of exchanging one ion for another, such processes usually involve cations. The cations which are most common are calcium, magnesium and sodium and the exchange actually takes place when ions absorbed in mineral grain surface are not the same as those in the water. The process of exchange terminates when equilibrium is established between the cations of the matrix and the cation in the water. Obviously, such phenomenon has a great bearing upon the chemical composition of water for instance zeolites. These constitutes a group of hydrous, aluminium silicate possessing calcium and sodium as important component when water traverses such minerals, sodium ions exchange with calcium and magnesium ions in the water and thus reduce its hardness, this process is therefore term the evolution of ions.

HYPOTHETICAL RESULTS USED IN THE GRAPHICAL PRESENTATIONS

Cations							**Anions**			
Sample A	Ca^{2+}	Mg^{2+}	Na^+	K^+			Hco_3^-	So_4^{2-}	Cl^-	
Mg/l	36.7	14.6	40.1	8.2	Total		22.7	29.5	7.2	Total
Meq/l	1.83	1.2	1.74	0.21	4.98		0.37	0.61	0.2	1.18
Percentage	36.7	24.1	34.9	4.2	100		31.4	51.7	16.9	100
Degree	66.1	43.4	62.8	7.6	180		56.5	93	30.4	180
Cations							**Anions**			
Sample B	Ca^{2+}	Mg^{2+}	Na^+	K^+			Hco_3^-	So_4^{2-}	Cl^-	
Mg/l	14.4	3.9	20.5	7.1	Total		101	9.9	3.4	Total
Meq/l	0.72	0.32	0.89	0.18	2.11		1.66	0.21	0.1	1.97
Percentage	34.1	15.2	42.2	8.5	100		84.3	10.7	5.1	100
Degree	61.4	27.4	76	15.3	180		151.7	19.3	9.2	180
Cations							**Anions**			
Sample C	Ca^{2+}	Mg^{2+}	Na^+	K^+			Hco_3^-	So_4^{2-}	Cl^-	
Mg/l	26.6	6.2	4.5	8.2	Total		44.6	6.6	3.1	Total
Meq/l	1.33	0.51	0.21	0.21	2.26		0.73	0.14	0.09	0.96
Percentage	58.8	22.6	9.3	9.3	100		76	14.6	9.4	100
Degree	105.8	40.7	16.7	16.7	180		136.8	26.3	16.9	180
Cations							**Anions**			
Sample D	Ca^{2+}	Mg^{2+}	Na^+	K^+			Hco_3^-	So_4^{2-}	Cl^-	
Mg/l	27.3	4.5	16.6	12.9	Total		81	35.2	7.1	Total
Meq/l	1.36	0.37	0.72	0.33	2.78		1.33	0.73	0.2	2.26
Percentage	48.9	13.3	25.9	11.9	100		58.8	32.3	8.8	100
Degree	88	23.9	46.6	21.4	180		105.8	58.1	15.8	180

GRAPHICAL METHODS

Constituents in solution in water may be viewed as a chemical system with cations and anions in equilibrium with each other. In discussing graphical methods of presentation for this system, Piper (1944) noted the abundance of the cations calcium, magnesium, sodium and potassium and anions bicarbonate, sulphate and chloride. He proposed that ionic solutions of water be treated as though they contained three cations groups and three anion groups. The less abundant cation and anion constituents are summed with the major constituents in accordance with common physical properties and are therefore accounted for in the plotting method. To convert the result of chemical analysis into a suitable form for graphical interpretation, all result in milligram per liter is converted to milli equivalent per liter by multiplying it with a conversion factor. For a complete analysis the total equivalent weight of cations and anions in solution must be equal or same, to the extent that natural water can be treated in terms of 3 cation constituents and 3 anion constituents, the chemical character can be shown graphically by a single point on a conventional Piper diagram. There are several varieties of graphical techniques that have been developed for the presentation of chemical components of water. The major chemical constituents are usually used for the presentation. An important task of water investigation is the compilation and presentation of chemical data in a convenient manner for visual inspection. Graphs are used in comparing the similarities and differences in the concentration of the chemical constituents in each water sample analyzed. Graphs are also used in detecting mixing of water of different composition and identifying chemical processes occurring as water passed through the aquifer system. For this purpose, a variety of data presentation techniques have been developed for showing the major chemical constituents over the year and these include:

✓ Bar Charts
✓ Pie Charts
✓ Stiff Diagrams
✓ Scattered Plots
✓ Schoeller Diagrams
✓ Piper Diagram

BAR CHARTS

The bars are plotted with concentration values in milli equivalent per liter. It is widely used in portraying chemical quality. Each analysis appears as a vertical bar having a height proportional to the total concentration of anions or cation. These graphs show the relative and total concentration of dissolved constituents present. Bar charts show the similarities or difference between water from their concentration ranges and it also show clearly the chemical constituent of total cations are plotted to the left of vertical bar and anions to the right. These segments are divided horizontally to show the concentration of major ions or groups of closely related ions and identified by distinctive shading pattern.

ADVANTAGES OF BAR CHARTS

- It gives an idea of the overall concentration of cations and anions.
- Visually strong.
- Can easily compare two or three data set.

DISADVANTAGES OF BAR DIAGRAM

- It is not suitable for large water samples.
- It does not give clear water type characteristics.
- Use only with discrete data.

PIE CHARTS

Represent the total concentrations of major cations and anions of water sample by means of circle. The segments of the circle are indicative of the percentage composition, i n degree. The diagrams of this type are probably most useful for indicating the composition of water on a geologic section or column.

ADVANTAGES OF PIE CHARTS

- Visually appealing.
- Shows percent of total for each category.
- It provides quick visual comparison of individual chemical analyses.

DISADVANTAGE OF PIE CHARTS

- It is not suitable for large graphical presentation of analyses.
- Hard to compare 2 data sets.
- Use only with discrete data.

STIFF DIAGRAM

Stiff (1951) proposed another way of presenting chemical analysis data, in which he used four parallel axes and one vertical axis for representing the chemical analysis. The procedure as proposed by Stiff (1951) is such that four cation concentrations are plotted to the left of the vertical zero axis and four anions to the right, all value are in milli equivalent per liter. The resulting point, when connected form an irregular polygonal pattern, waters of a similar quality define a distinctive shape from other of different quality. Stiffs method may be useful in making comparison of water, especially highly mineralized ones, is simple to use and can be varied to suit the water being studied. !t is more applicable to groundwater data that are interrelated than to miscellaneous surface water analyses. Stiff patterns are useful in making a rapid visual comparison between water from different sources. The use of the lower horizontal bar with ion of carbonate is optional as in much water they are close to zero. The larger the area of polygon shapes the greater the concentrations of the various ions.

ADVANTAGES OF STIFF DIAGRAMS

- It is relatively simple to construct.
- It gives a clear pattern for ions of the same water type.
- It gives a direct picture of the water type by means of shapes.

DISADVANTAGES OF STIFF DIAGRAM

- It is not convenient for large samples analysis.
- It does not give the concentration of ions present in direct form.

SCATTERED PLOTS

The scattered plot enables us to see the relationship between the two variables at once. It can be used to determine the relationship between two set of data. The measure of this relationship between any of these two variables (variables mean things taking different values or forms) is called *correlation*. Therefore calculating correlation coefficients is the calculation of the measure of relationship which gives the indication of the size or magnitude of the relationship. When we plot the values or points on the rectangular coordinate axes (our usual graph paper) indicating x and y axes, the resulting picture is the *scattered plot*.

ADVANTAGES OF SCATTERED PLOTS

- Shows a trend in the data relationship.
- Retains exact data values and sample size.
- Shows minimum/maximum and outliers.

DISADVANTAGES OF SCATTERED PLOTS

- Hard to visualize results in large data sets.
- Flat trend line gives inconclusive results.
- Data on both axes should be continuous.

SCHOELLER SEMILOGARITHMIC DIAGRAM

Schoeller (1962) proposed the use of semi logarithmic graph paper to plot the concentration of anions and cations. The concentrations are plotted in milli equivalent per liter. That type of diagram allows us to make a visual comparison of the composition of different water. They are plotted on six equally spaced logarithmic scales in the arrangement. The points plotted are joined by straight line. This type of graph shows not only the absolute value of each ion but also the concentration differences among various groundwater analyses. Because of the logarithmic scale, a straight line joining the points A and B of two ions in a water sample is parallel to another straight line joining the point A and B of the same ions in another water sample the ratio of the ions in both analyses is equal.

ADVANTAGES OF SCHOELLER DIAGRAM

- It is widely used for comparing water analyses.
- It can be adapted to determine the degree of saturation in water.
- It shows the concentration difference among various water analyses.

DISADVANTAGE OF SCHOELLER DIAGRAM

- It does not show the water type directly.
- Use only with continuous data.

PIPER DIAGRAM

This method was developed by Arthur M. Piper. (1944). Diagram reveals similarities and differences among large number of groundwater samples because those with similar qualities will tend to plot together as groups. The following are steps for plotting a Piper diagram.

1. Calculate the concentration of the analysed major ions (Na^+, K^+, $Mg^{2+,}$ Ca^{2+}, Cl^-, HCO_3^-, CO_3^{2-}, and SO_4^{2-}) in milli equivalent per liter.
2. Calculate the percentage milli equivalent of anions and cations respectively, combining Na^+ and K^+, $CO_3^{2-}$and HCO_3^-.
3. Plot each value in the cations - anions triangle at the base of the central diamond shape field.
4. Extend the point by dotted lines into the central diamond field.
5. According to total dissolved solids concentration point of intersection of the extended dotted lines from both cations and anions triangles might be enlarged or circled.

The total dissolved solids concentrations are often not important in the first stage of geochemical interpretation and points are often sufficient and allow larger number of samples to be plotted. By the use of Piper diagram chemical relationship among waters may be brought out in more definite terms than is possible with any other plotting graphical procedure. Piper plotting is a very useful interpretative tool in groundwater chemistry.

ADVANTAGES OF PIPER DIAGRAM

- It is most useful for representing and comparing water quality because it reveals the similarities and difference among water samples.
- It directly gives you the various water types.
- It can handle results of many samples of water within the same graph.

DISAVANTAGES OF PIPER DIAGRAM

- It is not good for a few data sets that's make it hard to be compared.

WATER TYPES

From the chemical analysis and graphical techniques used in these paper presented, the following water types were obtained;

SAMPLE A	*Ca-Na-Mg*
SAMPLE B	*Na-Ca-*HCO_3
SAMPLE C	*Ca-Mg-*HCO_3
SAMPLE D	*Ca-Na-*HCO_3-SO_4

DISCUSSION OF RESULTS

The general dominance of calcium bicarbonate and sulphate in the water samples analysed is related to the rocks minerals which released these ions into solution after their weathering. Feldspars and micas when K^+, Mg^{2+}, and Ca^{2+} are leached out leaving clay minerals such as Kaolinite, Elite, Montmorilonite etc. Most carbonate and bicarbonate in groundwater are derived from the carbon dioxide in the atmosphere, soil and solution of carbonate rocks. Sodium bicarbonate water can be concentrated by evaporation in the soils and desert basins. Despite a relatively large amount of sulphur mostly in form of sulphate in water and sedimentary rocks, Sulphates are derived from the solution of sulphate minerals in sedimentary rock particularly organic shale may also yield large amount of sulphate through the oxidation of marcasite and pyrite. Considering both the Bar and Pie charts (see sample d & a) in figure 4 and 5 in appendix. Ca^{2+} is the most dominant cation followed by alkali of Na^+ + K^+ and the least is the Mg^{2+}.

While on the anions species, HCO_3^- is the most dominant followed by SO_4^{2-} and the least Cl^- ion which is a strong acid. The plots of the chemical compound from water samples (a) and (b) seems to be scattered within the diamond field showing a different characteristic, the other plotted sample (c) and (d) points together as a group within the diamond field in the Piper diagram (see figure 9) in the appendix which indicates similar water type of same characteristics. The plots from the schoeller diagram (see figure 10) in the appendix indicate no particular trends in the water samples analyzed. The haphazard arrangement support different water types in sample (a) and (b) and a closer look at both sample (c) and (d) seems to be closely related as indicated by the Piper (1944) diagram. The Stiff diagram (see figure 11, 12, 13 & 14) in the appendix shows differences in shapes of the water sample analyzed. These differences in shapes in form of hexagons in sample (a) and (b) shows different water types, that is to say no mixing of water and the similarity of hexagonal shape in sample (c) and (d) indicate water of similar characteristics. Therefore both the Bar, Pie and Stiff diagrams are all easier to construct and provide quick visual comparison of individual chemical analyses and they are good in plotting small number of water samples, for large number of chemical data analysis the Piper (1944) diagram is more suitable.

SUMMARY AND CONCLUSION

This work shows the different techniques used in presenting hydrochemical data of water samples. These techniques include the Bar charts, Pie charts, Scattered plots, Stiff diagrams, Schoeller semi logarithmic diagram and the Piper diagram. The first four techniques are only suitable for smaller numbers of chemical data; the last two are suitable even for a larger numbers of chemical data.

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APPENDIX

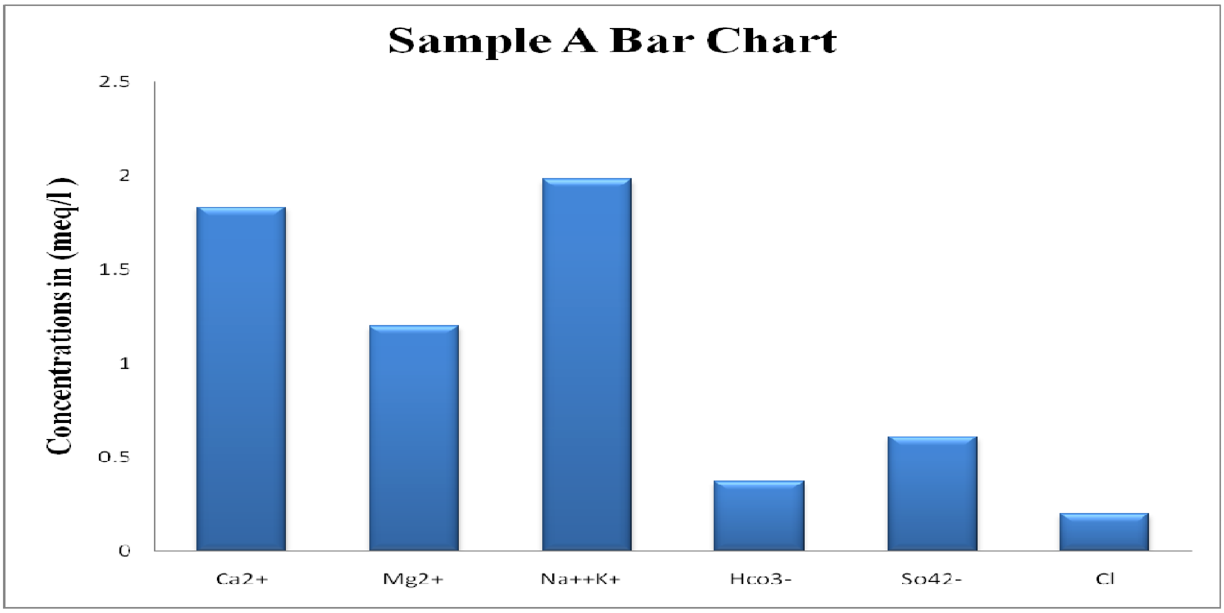

Fig. 1

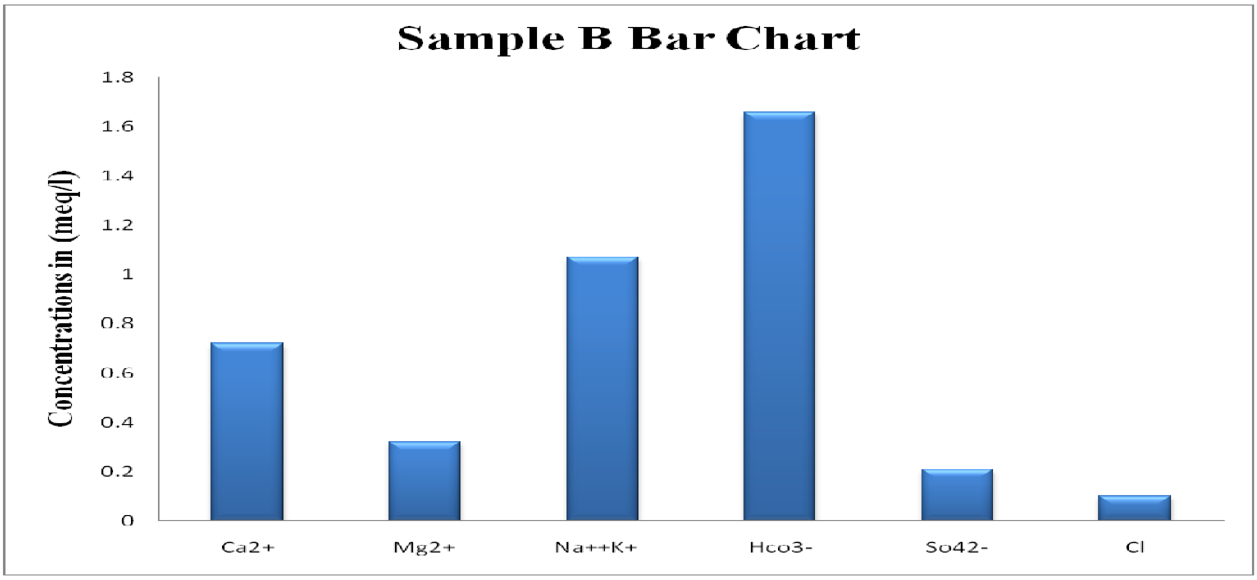

Fig. 2

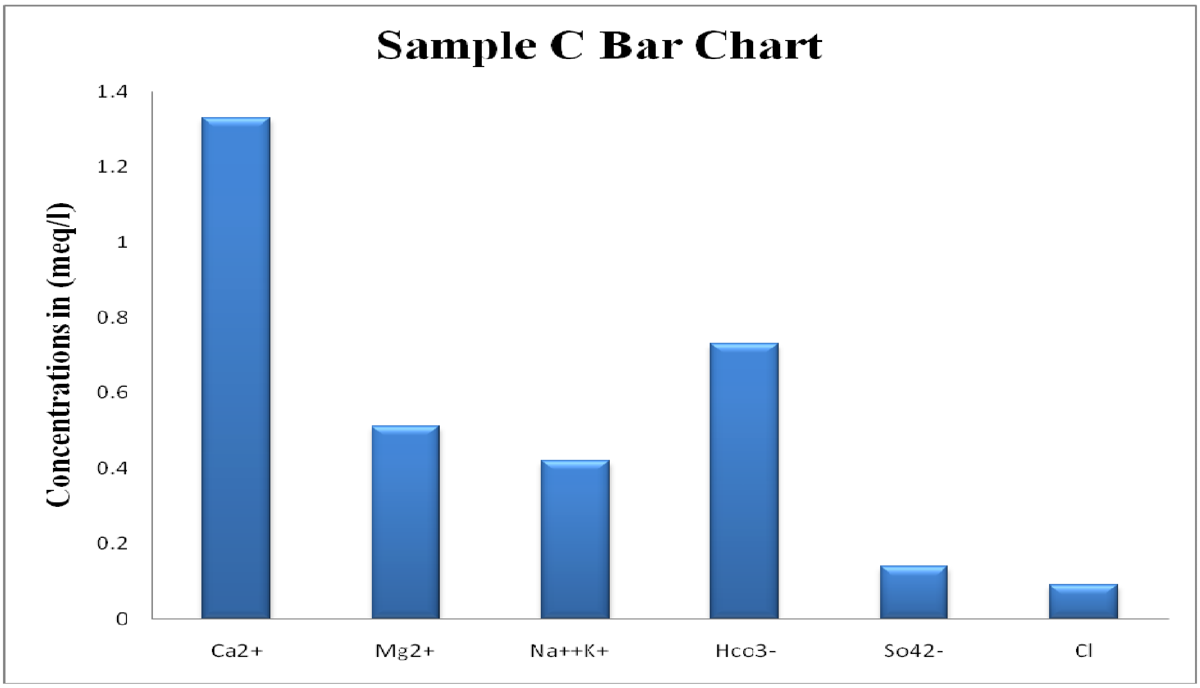
Sample C Bar Chart
Concentrations in (meq/l)
1.4
1.2
1
0.8
0.6
0.4
0.2
0
Ca2+
Mg2+
Na++K+
Hco3-
So42-
Cl

Fig. 3

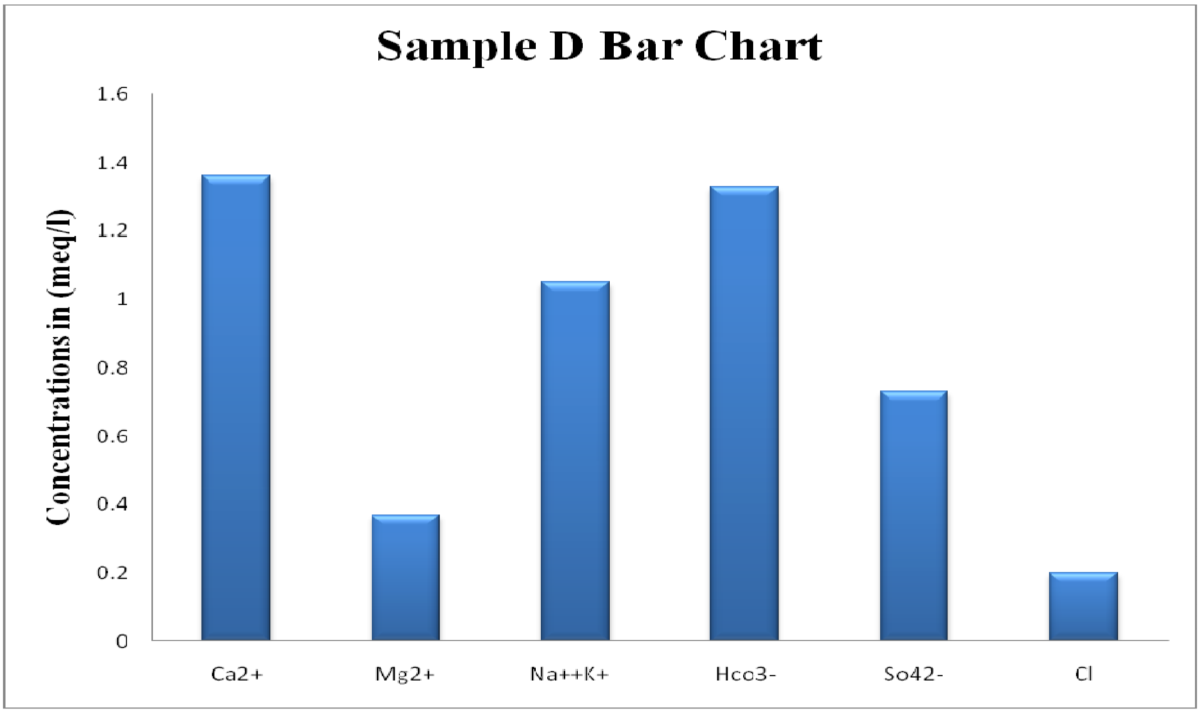
Sample D Bar Chart
Concentrations in (meq/l)
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
Ca2+
Mg2+
Na++K+
Hco3-
So42-
Cl

Fig. 4

Sample A to D Pie Charts

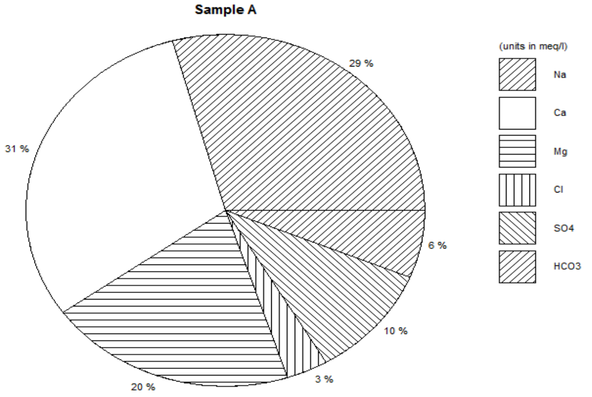
Sample A

Fig. 5

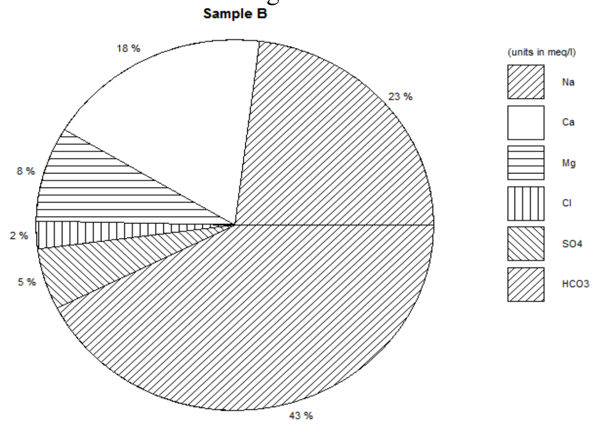
Sample B

Fig. 6

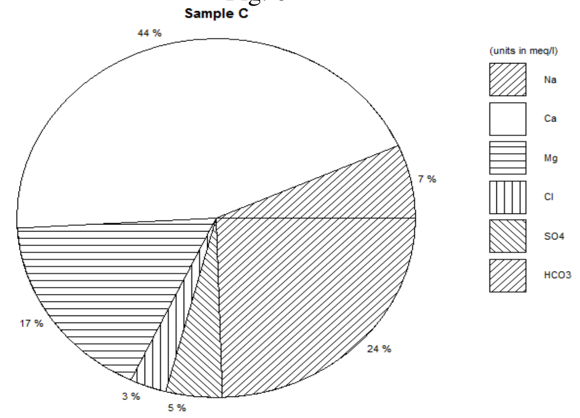
Sample C

Fig. 7

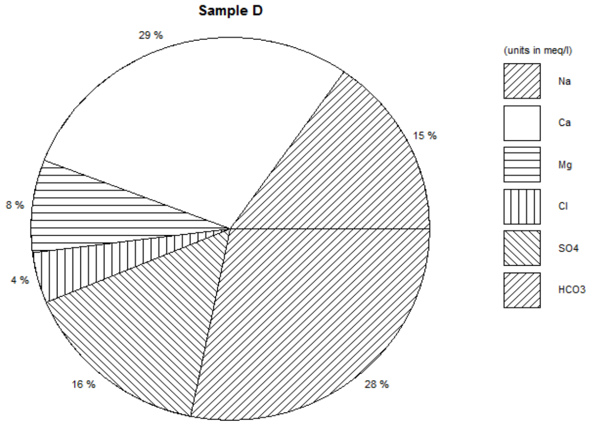
Sample D

Fig. 8

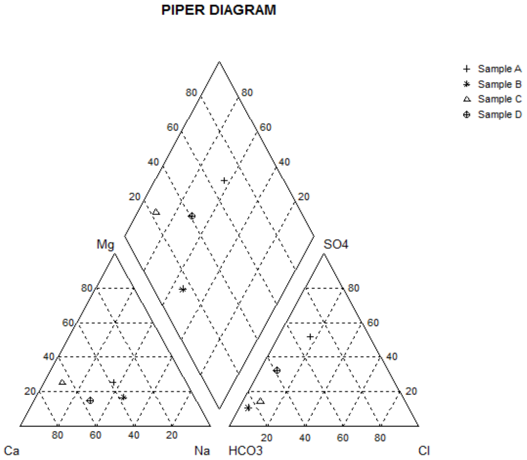
PIPER DIAGRAM
Sample A
Sample B
Sample C
Sample D
80
60
40
20
Mg
SO4
Ca
Na
HCO3
Cl

Fig. 9

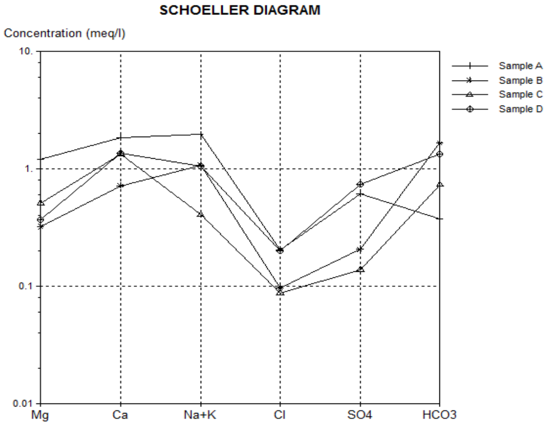
SCHOELLER DIAGRAM
Concentration (meq/l)
10.
1.
0.1
0.01
Mg
Ca
Na+K
Cl
SO4
HCO3
Sample A
Sample B
Sample C
Sample D

Fig. 10

Sample A to D Stiff Diagrams

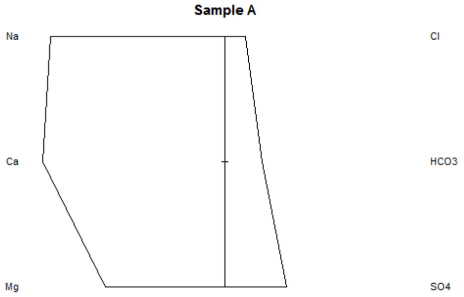

Fig. 11

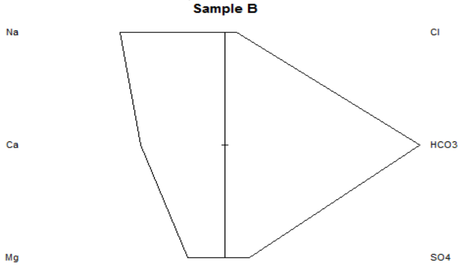

Fig. 12

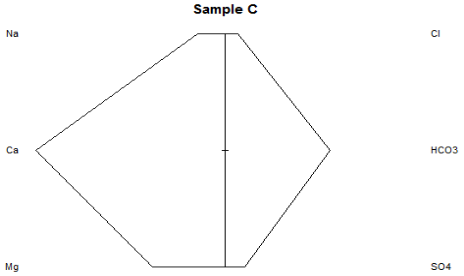

Fig. 13

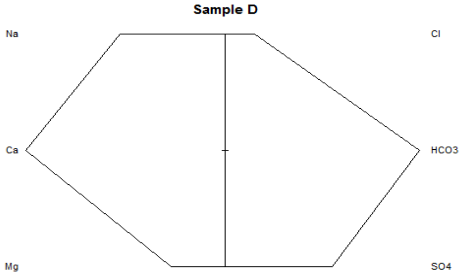

Fig. 14