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Standard Guide for Displaying Results of Chemical Analyses of Groundwater for Major Ions and Trace Elements—Diagrams Based on Data Analytical Calculations¹

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1. Scope

1.1 This guide covers methods that graphically display chemical analyses of multiple groundwater samples, discrete values and also those reduced to comprehensive summaries or parameters. Details required by the investigator to fully use the methods are found in the listed references. The methods included in this guide are many of the graphical procedures that were not discussed in two previous guides, Guides **D5738** and **D5754**.

NOTE 1—The graphic methods in this guide apply to both raw and transformed data, for example, unaltered medians, maximums, and minimums and transformed means, square-roots, frequency distributions, and so forth. The methods are often computational intensive, requiring the use of a digital computer. Some graphical methods illustrate the results of the statistical analysis of a sample data set. For example, box plots are graphical portrayals of the maximum, minimum, median, 25th percentile, and 75th percentile of one variable, such as the chloride ion from a group of chemical analyses.

Besides chemical components, other variables that may be plotted to show an interdependence with water chemistry include time, distance, and temperature.

1.2 This guide on diagrams based on data analytical calculations is the third of several documents to inform the hydrologists and geochemists about traditional graphical methods for displaying groundwater chemical data.

NOTE 2—The initial guide described the category of water-analysis diagrams that use two-dimensional trilinear graphs to display, on a single diagram, the common chemical components from two or more analyses of natural groundwater.

1.2.1 The second guide described the category of water-analysis diagrams that use pattern and pictorial methods as a basis for displaying each of the individual chemical components determined from the analysis of a single sample of natural groundwater.

1.3 This guide presents a compilation of diagrams that allows for transformation of numerical data into visual, usable forms. It is not a guide to selection or use. That choice is program or project specific.

1.4 Many graphic techniques have been developed by investigators to illustrate the results of the data analytical computations to assist in summarizing and interpreting related data sets. In this guide, selected graphical methods are illustrated using groundwater chemistry data.

1.5 The basic or original format of each of the graphical techniques given in this guide has been modified in several ways, largely depending upon the data analytical techniques used by the investigators. Several minor modifications are mentioned, some significant revisions are discussed in more detail.

1.6 Notations have been incorporated within many diagrams illustrated in this guide to assist the reader in understanding how the diagrams are constructed. These notations would not be required on a diagram designed for inclusion in a project document.

NOTE 3—Use of trade names in this guide is for identification purposes only and does not constitute endorsement by ASTM.

1.7 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.*

1.8 *This guide offers an organized collection of information or a series of options and does not recommend a specific course of action. This document cannot replace education or experience and should be used in conjunction with professional judgment. Not all aspects of this guide may be applicable in all circumstances. This ASTM standard is not intended to represent or replace the standard of care by which the adequacy of a given professional service must be judged, nor should this document be applied without consideration of a project's many unique aspects. The word "Standard" in the title of this document means only that the document has been approved through the ASTM consensus process.*

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2. Referenced Documents

2.1 ASTM Standards:²

- D596 Guide for Reporting Results of Analysis of Water
D653 Terminology Relating to Soil, Rock, and Contained Fluids
D1129 Terminology Relating to Water
D5738 Guide for Displaying the Results of Chemical Analyses of Groundwater for Major Ions and Trace Elements—Diagrams for Single Analyses
D5754 Guide for Displaying the Results of Chemical Analyses of Groundwater for Major Ions and Trace Elements—Trilinear Diagrams for Two or More Analyses

3. Terminology

3.1 Definitions:

3.1.1 Except as listed as follows, all definitions are in accordance with Terminology **D653**:

3.1.2 *adjacent values (statistics)*—values that fall between the quartile and one step beyond the quartile position, where the interquartile range is from the 25th to 75th percentile of a sample, and a step is equal to **1.5** times the interquartile range (**1**).³ The same definition applies to hinges (**2**).

3.1.3 *anion*—an ion that moves or would move toward an anode; thus nearly always synonymous with negative ion.

3.1.4 *cation*—an ion that moves or would move toward a cathode; thus nearly always synonymous with positive ion.

3.1.5 *equivalent per million (epm)*—for water chemistry, an equivalent weight unit expressed in English terms, also expressed as milligram-equivalent per kilogram. When the concentration of an ion, expressed in ppm, is multiplied by the equivalent weight (combining weight) factor (see explanation of *equivalent weight factor*) of that ion, the result is expressed in epm.

3.1.5.1 *Discussion*—For a completely determined chemical analysis of a water sample, the total epm value of the cations will equal the total epm value of the anions (chemically balanced). The plotted values on the water-analysis diagrams described in this guide can be expressed in percentages of the total epm (although all illustrations are in milliequivalent per litre) of the cations and anions of each water analysis. Therefore, to use the diagrams, analyses must be converted from ppm to epm by multiplying each ion by its equivalent weight factor and determining the percent of each ion of the total cation or anion.

3.1.6 *equivalent weight factor*—the equivalent weight factor or combining weight factor, also called the reaction coefficient, is used for converting chemical constituents expressed in ppm to epm and mg/L to meq/L (see explanation of *epm* and *meq/L*). To determine the equivalent weight factor, divide the formula weight of the solute component into the valence of the solute component:

$$(\text{equivalent weight factor}) = \frac{(\text{valence solute component})}{(\text{formula weight solute component})} \quad (1)$$

Then to determine the equivalent weight (meq/L) of the solute component, multiply the mg/L value of the solute component times the equivalent weight factor, as follows;

$$(\text{meq/L solute component}) = (\text{mg/L solute component}) \times (\text{equivalent weight factor}) \quad (2)$$

For example, the formula weight of Ca²⁺ is 40.10 and the ionic charge is 2 (as shown by the 2 +), and for a value of 20 mg/L Ca, the equivalent weight value is computed to be 0.9975 meq/L:

$$(0.9975 \text{ meq/L Ca}) = (20 \text{ mg/L Ca}) \times \frac{(2)}{(40.10)} \quad (3)$$

3.1.6.1 *Discussion*—Many general geochemistry publications and water encyclopedias have a complete table of equivalent weight factors³ for the ions found in natural groundwater (**3**, **4**).

3.1.7 *far-out values (statistics)*—values that fall beyond the two-step range (see outside values) (**1**, **2**).

3.1.8 *hinge (statistics)*—as used by Tukey (**2**), the upper and lower values of a ranked sample that, along with the median, divide the number of data values into four equal parts. The data at the hinge position includes interpolated values.

3.1.8.1 *Discussion*—Tukey (**2**) used the hinge system for his box and whisker plots and for his hinge plot and related summaries. The hinge method of division is similar to the use of quartiles.

3.1.9 *interquartile or hinge range (statistics)*—the difference between the values at the quartile or hinge extremes (**2**).

3.1.10 *maximum or sample maximum (statistics)*—the value of the variable having the greatest value in a data set (sample).

3.1.11 *milliequivalent per litre (meq/L)*—for water chemistry, an equivalent weight unit expressed in metric terms, also expressed as milligram-equivalent per litre. When the concentration of an ion, expressed in mg/L, is multiplied by the equivalent weight factor (see explanation of *equivalent weight factor*) of that ion, the result is expressed in meq/L.

3.1.11.1 *Discussion*—For a completely determined chemical analysis of a water sample, the total value of the cations will equal the total value of the anions (chemically balanced). The plotted values on the water-analysis diagrams described in this guide are expressed in percentages of the total meq/L of the cations and anions of each water analysis. Therefore, to use the diagrams, analyses must be converted from mg/L to meq/L by multiplying each ion by its equivalent weight factor and determining the percent of each ion of the total cation or anion.

3.1.12 *milligrams per kilogram (mg/kg)*—for water chemistry, a weight-per-weight unit expressed in metric terms. The number of milligrams of solute (for example, Na) per kilogram of solution (water). For example, a 10 000-mg/kg solute is the same as 1% solute in the total 100 % solution. The mg/kg unit is equivalent to ppm according to Matthes (**5**).

3.1.13 *milligrams per litre (mg/L)*—for water chemistry, a weight-per-volume unit expressed in metric terms. The weight

² For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

³ The boldface numbers given in parentheses refer to a list of references at the end of the text.

in milligrams (10^{-3} g) of the solute within the volume (litre) solution. The weight can be also expressed in micrograms (10^{-6} g). The use of the mg/L unit is the worldwide standard for the analysis and reporting of water chemistry.

3.1.13.1 *Discussion*—The ppm and mg/L values of the constituents in natural groundwater are nearly equal (within anticipated analytical errors) until the concentration of the dissolved solids reaches about 7000 mg/L. For highly mineralized waters, a density correction should be used when computing ppm from mg/L (3).

3.1.14 *minimum or sample minimum (statistics)*—the value of the variable having the smallest value in a data set (sample).

3.1.15 *natural groundwater*—is water positioned under the land's surface, which consists of the basic elements, hydrogen and oxygen (H_2O), and numerous major dissolved chemical constituents, such as calcium (Ca), magnesium (Mg), sodium (Na), potassium (K), carbonate (CO_3), bicarbonate (HCO_3), chloride (Cl), and sulfate (SO_4).

3.1.15.1 *Discussion*—Other major constituents, in special cases, can include aluminum (Al), boron (B), fluoride (F), iron (Fe), nitrate (NO_3), and phosphorus (PO_4). Minor and trace elements that can occur in natural groundwater vary widely, but can include arsenic (As), copper (Cu), lead (Pb), mercury (Hg), radium (Ra), and zinc (Zn). In addition, natural groundwater may contain dissolved gases, such as hydrogen sulfide (H_2S), carbon dioxide (CO_2), oxygen (O_2), methane (CH_4), ammonia (NH_3), argon (Ar), helium (He), and radon (Rn). Also maybe included are neutrally charged mineral species, such as silicate (SiO_2), naturally occurring organics, such as tannic acids, colloidal materials, and particulates, such as bacteria viruses and naturally charged pollen spores.

3.1.15.2 *Discussion*—Most of the natural groundwater is a part of the hydrologic cycle, that is the constant circulation of meteoric water as vapor in the atmosphere as a result of evaporation from the earth's surface (land and ocean), liquid and solid (ice) on and under the land as a result of precipitation from the atmosphere, and as liquid returned to the ocean from the land. A small amount of the groundwater may be magmatic water originating from rocks deep within the crust of the earth. Other groundwater is connate in that it is trapped in sediments and has not actively moved in the hydrologic cycle for a period measured in geologic time.

3.1.15.3 *Discussion*—While moving through the hydrologic cycle, chemical elements in the water undergo ion exchange, adsorption/desorption, precipitation/dissolution, oxidation/reduction, and other chemical reactions in response to changes in temperature, hydraulic pressure, biological agents, and chemical composition of the water. The chemical composition of natural groundwater ranges from that similar to distilled water with a minor amount of dissolved solids to brines with at least 100 000 mg/L dissolved solids (natural occurring brines have been analyzed with more than 300 000 mg/L dissolved chemical solids) (6).

3.1.16 *outlier (statistics)*—observations whose values are quite different from others in the sample (far-out values fall

into this category). These may be the most important values in the data set and should be investigated further (1). In the case of a single deletion, the relationship between the change in mean and the deleted observation is linear, whereas, the relationship between the change in standard deviation and the deleted observation is nonlinear or approximately quadratic for the total number of sample observations considerably larger than the standardization variable squared (7). Values as described by Sara (8) as unusually high, low, or otherwise unexpected values within the sample.

3.1.16.1 *Discussion*—Outliers (8) can be attributed to a number of conditions, including: extreme, but accurately detected, conditions or environmental conditions; sampling errors or field contamination; analytical errors or laboratory contamination; recording or transcription errors; and faulty (water) sample preparation or preservation, or shelf-life exceedance.

3.1.17 *outside values (statistics)*—values that fall between one and two steps beyond the interquartile range (see adjacent values) (1, 2).

3.1.18 *parts per million (ppm)*—for water chemistry, a dimensionless ratio of unit-of-measurement per unit-of-measurement expressed in English terms. One part per million is equivalent to one milligram of solute in one kilogram of solution. For example, if the total weight of the solution (one million ppm) has 99 % solvent and 1 % solute, this is the same as 990 000 ppm solvent and 10 000 ppm solute in the one million parts of solution.

3.1.19 *polar smoothing (statistics)*—this type of smooth, as used on a scatterplot or Piper diagram, improves the visualization of multiple groups of data sets by enclosing a fixed percent (50 or 75 %) of each group with a mathematically determined ellipse (1, 9, 10, 11, 12, 13).

3.1.20 *population (statistics)*—a well-defined set (either finite or infinite) of elements (14).

3.1.20.1 *Discussion*—For groundwater quality data the infinite population is actually the finite sampled population, as it would be impossible, and certainly impractical, to obtain and chemically analysis all of the groundwater from an aquifer.

3.1.21 *quantile (statistics)*—the data point corresponding to a given fraction of the data. Similar to percentile, which is the data point corresponding to a given percentage of the data (15).

3.1.22 *quartile (statistics)*—the upper and lower values of a ranked sample that, along with the median, divides the number of data values into quartile percentages or four equal parts (>0 to ≤ 25 , > 25 to ≤ 50 , > 50 to ≤ 75 , and > 75 to ≤ 100 %). The data at the quartile position includes interpolated values.

3.1.23 *sample mean (statistics)*—an arithmetic average of a series of values of a data set (sample) (16).

$$\bar{X} \text{ (sample mean)} = \sum_{i=1}^n \frac{X_i}{n} \quad (4)$$

3.1.24 *sample median (statistics)*—the value of the middle variable in a data set (sample) arranged in rank order (16).

Also, the 50th percentile or the central value of the distribution when the data are ranked in order of magnitude (1).

3.1.24.1 *Discussion*—For an odd number of observations, the sample median is the data point which has an equal number of observations both above and below it. For an even number of observations, it is the average of the two central observations (1).

3.1.25 *sample size (n) (statistics)*—the number of data observations in the sample.

3.1.26 *sample (statistics)*—a subset of elements taken from a population (14). Also, called sampled population, sample data set or data set. The part or subset of a statistical population that if properly chosen may be used to estimate parameters (16).

3.1.26.1 *Discussion*—If the sample is representative of the entire population, important conclusions about the population can often be inferred from analysis of the sample (15). For groundwater quality data, the sample is a finite subset of data elements from an infinite population.

3.1.27 *smoothing (statistics)*—smoothing techniques are methods of fitting a line through a number of related data values to enhance the perception of understanding the relationship of one variable (Y) to another (X). By use of mathematical computations, another set of points (X_i, Y_i) are determined (several methods are used) and plotted, these are termed the smoothed values. For this guide, the two types of smoothing discussed are line (1, 9, 10, 11) and polar (1, 9, 10, 11, 12, 13).

3.1.28 *standard deviation or sample standard deviation (statistics)*—the square root of the average of the squares of deviations about the mean of a set of data (16).

$$s \text{ (sample standard deviation)} = \sqrt{s^2} \quad (5)$$

3.1.29 *statistical analysis*—the art of reducing numerical data and their interrelationships to comprehensible summaries or parameters (16).

3.1.30 *variance or sample variance (statistics)*—the square of the standard deviation (16). The expected value of the square of deviations of the variable from its expected value (17):

$$s^2 \text{ (sample variance)} = \sum_{i=1}^n \frac{(X_i - \bar{X})^2}{(n - 1)} \quad (6)$$

3.1.31 *water analysis*—a set of data showing the concentration of chemical ions and measure of physical properties determined from a water sample. In this guide, the water analysis normally includes the common constituents and project-dictated parameters as found in natural and human-influenced groundwater (see *natural groundwater*).

3.1.32 *water-analysis diagram*—for purposes of this guide, a diagram for graphically displaying water-quality analyses and related parameters. These diagrams can be used to assist in the scientific interpretation of occurrence of cations and anions in natural and human-influenced groundwater, for example, the interrelationship of a number of water samples within the studied area.

3.1.33 *water sample*—in this guide, a water sample refers to a carefully collected specimen of natural or human-influenced

groundwater obtained from the aquifer for analyzing the chemical constituents in the water.

3.1.33.1 *Discussion*—In this guide on analytical calculations, a water sample is one element in the entire sample or data set with a sample size of n from the entire population. (See *population (statistics)*, *sample (statistics)*, and *sample size (n) (statistics)*.)

4. Summary of Guide

4.1 The significance and use present the relevance of the water-analysis diagrams that pictorially display the results of data analytical computations of chemical constituents and related parameters from natural and human-influenced groundwater sources.

4.2 A summary of the recommended checks for accuracy (quality control of the data) is presented.

NOTE 4—Most of the graphical methods presented in this guide use one or two chemical constituents from each of many analyses. However, several methods require the use of complete analyses. The measure of the quality confidence of the analyses used for these methods must follow the same level of evaluation as that outlined in Guides D5738 and D5754.

4.3 Descriptions and comprehensive illustrations are given for the following water-analysis diagrams.

4.3.1 *Diagrams for a Single Set of Data:*

4.3.1.1 Frequency histogram diagram (1, 3, 8, 14, 18, 19, 20, 21, 22, 23, 24, 25),

4.3.1.2 Relative frequency histogram diagram (14, 19, 23, 26),

4.3.1.3 Rootogram diagram (27),

4.3.1.4 Stem and leaf plot (1),

4.3.1.5 Dot and line or error plot (1, 8),

4.3.1.6 Hinge plot, five-number summaries, and fenced summaries (2, 27),

4.3.1.7 Box and whisker or range plots (1, 2, 8, 18, 20, 21, 27, 28, 29, 30, 31),

4.3.1.8 Frequency distribution diagram (17, 19, 20, 32),

4.3.1.9 Cumulative frequency distribution and quantile diagram (3, 17, 19, 20, 21, 29),

4.3.1.10 Cumulative percentage diagram (3),

4.3.1.11 Probability plot using percent (34), and

4.3.1.12 Probability plot using normal quantiles (1, 34, 40).

4.3.2 *Diagrams for Two Sets of Related Data:*

4.3.2.1 Simple scatterplot (scattergrams) (1, 3, 21, 22, 23, 25, 26, 29, 30, 36, 37, 38, 39, 40),

4.3.2.2 Scatterplot with samples (data sets) from two populations (1),

4.3.2.3 Scatterplot with moving medians or means smooth (1),

4.3.2.4 Scatterplot with LOWESS smooth (1, 10, 11, 41, 42),

4.3.2.5 Scatterplot with polar smooths of samples (data sets) from more than one population (1, 9),

4.3.2.6 Scatterplot with absolute differences versus the sample (data set) (1, 9, 11),

4.3.2.7 Scatterplot for correlation coefficient (1, 3, 14, 19, 26, 35, 43, 44),

4.3.2.8 Basic time-series plot (1, 3, 8, 9, 19, 24, 31, 32, 33, 45, 46, 47, 48, 49),

- 4.3.2.9 Time-series plot for multiple data sets (1),
- 4.3.2.10 Elapsed time plot (1, 8, 9, 50, 51, 52), and
- 4.3.2.11 Q-Q plots (1, 19, 41, 53).

4.3.3 *Other Diagrams of Interest :*

- 4.3.3.1 Schoeller nomograph or vertical scale diagram (3, 5, 38, 54, 56, 57, 58, 59),
- 4.3.3.2 Irrigation classification or salinity hazard diagram (3, 55, 59),
- 4.3.3.3 Piper diagram with polar smoothing (1, 9, 10, 11, 12, 13),
- 4.3.3.4 Three-variable pattern plot (60),
- 4.3.3.5 Three-dimension rotational plot (1, 60, 61),
- 4.3.3.6 Ropes three-dimensional diagram (62, 63, 64), and
- 4.3.3.7 Cluster analysis diagrams (1, 32).

4.4 Automated procedures (computer-aided graphics) for basic calculations and the construction of the water-analysis diagrams are identified,

4.5 Keywords, and

4.6 A list of referenced documents is given for additional information.

5. Significance and Use

5.1 Each year, many thousands of water samples are collected, and the chemical components are determined from natural and human-influenced groundwater sources.

5.2 An understanding of the relationship between the similarities and differences of these water analyses is simplified by use of data analytical methods and the display of the results of these methods as pictorial diagrams.

5.3 This guide presents a compilation of the diagrams used for illustrating the results of these methods.

5.4 This type of diagram summarizes data from a number of analyses to allow for an objective comparison between the chemical and related parameters.

5.5 The diagrams based on data analytical calculations described in this guide display the following; time and areal trends; maximums, minimums, and means; relationships between chemical and associated parameters; significant outliers; distributions; and a summary of a number of data parameters.

5.6 The objective interpretations of the origin, composition, and interrelationships of groundwater are common uses of the diagrams based on data analytical calculations.

5.6.1 The origin of the water may be postulated by the amount and the relationship of the chemical constituents in a sample of water analyses summarized on the diagrams.

5.6.2 The chemical composition of the water can be scrutinized for distinct characteristics and anomalies by use of the diagrams.

5.6.3 A graphical comparison of distinct data sets of chemical analyses allows the investigator to evaluate the interrelationships of the groundwater from separate locations.

5.7 This is not a guide for the selection of a diagram for a distinct purpose. That choice is program or project specific.

NOTE 5—For many hydrochemical research problems involving the scientific interpretation of groundwater, the 'analytical water-analysis diagram' is only one segment of several methods needed to interpret the data.

6. Selection and Preparation of Data for Plotting on the Analytical Diagrams

6.1 For the data analytical graphical methods described in this guide, transformation of the raw data is often required before analysis. However, several methods, for example, some of the scattergrams, the transformation is accomplished by analytical smoothing of the curve after the data are plotted on the diagram.

NOTE 6—Helsel and Hirsch (1) on pages 253 through 255 discusses the subject of whether to transform or not to transform the response variable (y). The response variable may require transformation because the variance of the residuals is a function of x for much of the groundwater quality data and for hydrology in general. Helsel and Hirsch states that the decision of whether to transform y should generally be based on graphs.

6.2 *Minimum Data Requirements:*

6.2.1 The basic requirements for the analytical methods described in this guide are that the samples are randomly selected and of sufficient size to represent the sampled population and therefore, allow for a meaningful analysis (1).

NOTE 7—A truly random sample is impractical, as groundwater samples are from a subsurface population that only can be obtained from sources that intersect the water table, for example, wells, springs, and tunnels or caves. These sources are not likely to be distributed randomly in three dimensions throughout an aquifer. However, a more refined picture of the entire population is possible as the size of the random sample is increased (1).

6.3 *Recommended Checks for Accuracy of Data Parameters:*

6.3.1 For those methods described in this guide that use a sample (data set) from chemical analyses that are not complete, the individual data values must be carefully reviewed to avoid errors in the results.

NOTE 8—Some of these methods can use a data set consisting of a single constituent, for example, the evaluation of chloride by a histogram. Other methods use two parameters, for example, the evaluation of the relationship of nitrate and dissolved solids by a scattergram. Other methods, such as a ratio evaluation, use data sets consisting of more than two parameters, but less than complete analyses.

6.3.1.1 Erroneous values in a data set (sample) flagged as outliers, become more apparent when using graphical methods, as these values do not plot with the prevalent group of the data points.

6.3.1.2 Erroneous values that fall in the same numerical range as a typical value in the data set are difficult to detect, but are most likely found by a complete validation of the data set (sample) against the original data source.

NOTE 9—To reduce the chance of incorporating erroneous numbers into the data analytical evaluation, the original chemical analyses and related data must be carefully previewed as to proper collection and analytical procedures. In addition, take care to ensure that none of the numbers have been transposed during preparation of the data for the analytical evaluation.

6.3.2 For those methods described in this guide that use a sample (data set) that consists of complete chemical analyses (where all of the major chemical ions in the groundwater are

determined), a check of the chemical balance should be made to help in the detection of data errors.

6.3.2.1 The chemical balance or chemical equilibrium of a complete analysis is calculated by converting the ions from mg/L to meq/L values and adding the cations together and the anions together. The computation for percent balance is as follows, with 0 (zero) as the optimum percentage value (percentage is determined by multiplying the computed value times 100);

$$\begin{aligned} & \% \text{ chemical balance } (+/-) \qquad (7) \\ & = \frac{\text{total cations} - \text{total anions (meq/L)}}{\text{total cations} + \text{total anions (meq/L)}} \times 100 \end{aligned}$$

NOTE 10—Minor amounts of ions such as fluoride (F), nitrate (NO₃), iron (Fe), and barium (Ba), may occur in natural or human-influenced groundwater, but normally do not significantly influence the chemical balance. If any of these ions (for example, NO₃) occur in amounts that alter the chemical balance, they should be included in the computations. Other constituents may occur in minor amounts in a colloidal or suspended state, such as silica (SiO₂), iron hydroxide (Fe), and aluminum compounds (Al), and are not considered in the chemical balance because they are not dissolved constituents.

6.4 Required Calculations for Diagram Construction:

6.4.1 The data analytical methods described in this guide use a wide range of computations to analyze the data sets (samples) and to prepare the data for illustration on the various diagrams.

6.4.2 Because of the many types of equations, they are presented or referred to with the first diagram that discusses the computational method and then cited when used in later diagrams.

7. Water-Analysis Diagrams

7.1 Introduction—This guide provides methods that furnish helpful graphical summaries of the results of data analysis of water samples. These methods include procedures that graphically display a single data set (sample), two sets of directly related data, and multiple sets of data.

7.1.1 Helsel and Hirsch (1), describe many of the data analytical methods for use in the study of water resources. The book explains many graphical procedures to illustrate chemical analyses and related groundwater data.

7.1.2 In the description by Helsel and Hirsch (1) they state one of the most frequent tasks when analyzing data is to describe and summarize those data in forms which convey their important characteristics.

7.1.3 Helsel and Hirsch also said that “Graphs are essential for two purposes: (1) to provide insight for the analyst into the data under scrutiny, and (2) to illustrate important concepts when presenting the results to others” (1).

NOTE 11—Many other excellent publications are available for the statistical study of natural groundwater; most of those are referred to in the text and listed in the bibliography.

NOTE 12—The criteria for the selection, error check of data values, and preparation of the data sets (samples) used for plotting on many of the data analytical diagrams is described in Section 6.

7.2 Diagrams for a Single Set of Data—These diagrams graphically illustrate the results of an analytical examination of a single set of data (sample) selected from a number of chemical analyses of natural and human-influenced groundwater.

7.2.1 Histograms—This type of diagram is a vertical bar-graph for showing the distribution of a variable. The length of the individual bars represents the frequency of the data values within each subdivision of the total parameter range.

7.2.1.1 Frequency Histogram Diagram—One type of diagram has the bars representing the occurrence numbers on the Y-axis plotted against the subdivided parameter values on the X-axis (see Fig. 1 and Table 1). The parameter values are subdivided so that there are no open or zero intervals (1, 3, 8, 14, 18, 19, 21, 22, 23, 24, 25).

7.2.1.2 Relative Frequency Histogram Diagram—The relative frequency histogram has the occurrence number (as shown on the frequency histogram) replaced by the percentage value to show the distribution of a ranked sample data set (see Fig. 2 and Table 1) (14, 19, 23, 26).

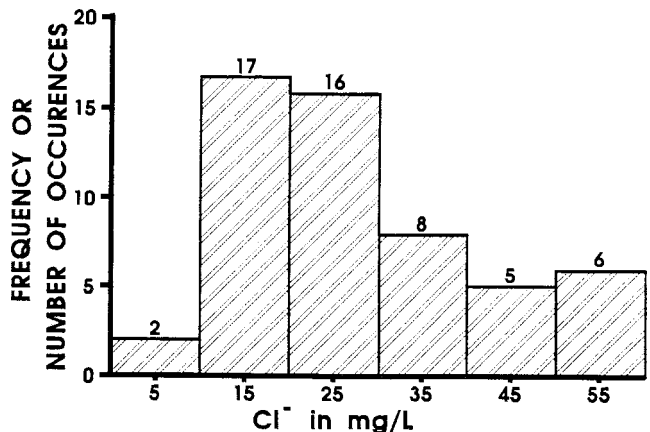
NOTE 13—The relative frequency percentages are computed as follows:
relative frequency = number of occurrences in interval/total sample size (8)

For example: on Fig. 2, from a sample data set of 54, six values are >50 and ≤60 and the relative frequency is 11.1 % (6/54).

7.2.1.3 Rootogram Diagram—The rootogram is a histogram where the frequency for each interval is plotted as square root (27). For example, the frequency or number of occurrences on Fig. 1 are shown as square root values on Fig. 3. This tends to make the interval differences look smaller than on the traditional histogram and is useful where some intervals have a lopsided large number of occurrences (see Fig. 3 and Table 1).

7.2.2 Stem and Leaf Plot—The stem and leaf plot is similar to a histogram rotated 90° (1). An advantage of this plot is that the real values are placed on the diagram (see Fig. 4 and Table 1).

7.2.3 Dot and Line or Error Plots—The dot and line plot is used to represent the mean and standard deviation (or standard error) of a sample (see Fig. 5 and Table 1) (1, 8).



NOTE 1—Analyses selected from Ref (67) . See Table 1.
FIG. 1 Histogram