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A METHOD OF DIFFERENCES TO SOLVE TRANSCENDENTAL EQUATIONS,

WITH APPLICATIONS TO SANITARY ENGINEERING PROBLEMS

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DISSERTATION

A METHOD OF DIFFERENCES TO SOLVE TRANSCENDENTAL EQUATIONS, WITH APPLICATIONS TO SANITARY ENGINEERING PROBLEMS

In many engineering problems equations arise in which one or more parameters are to be determined using as data sets of observations. In some instances such parameters are implicit in more or less complicated transcendental equations, so that the trial and error method, or methods involving the use of graphs drawn on special scales, or tables, have been generally used to find the desired solutions. These methods are specific to each particular problem, not linear in nature, and time consuming. In this thesis, a brief review of these types of equations and their corresponding traditional methods of solutions are presented, and the method of differences is used to develop corresponding linear forms from which the respective parameters can be estimated in a more convenient way; the method is applied to a number of problems related to the field of sanitary engineering, and the results are compared with those obtained while using the traditional methods of solution. The results obtained from the application of the method of differences prove to be superior to those obtained using the traditional methods.

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To the memory of my parents, to my brothers and sisters, to my wife, Irma, and to my sons, Rodolfo, Waldo, Alfredo, and Pepito, I humbly dedicate this work.

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CHAPTER I

INTRODUCTION

1.1 General Concepts and Objectives

In sanitary engineering, as well as in other branches of engineering and science, the problem of finding the parameters of a given model or equation occurs quite frequently. For instance, in chemistry, it may be desired to know the rate at which a given reaction proceeds; in physics it could be of interest to determine the rate at which a certain gas dissolves in water; in demography, it may be necessary to determine the saturation limit of a growing population; and, in sanitary engineering, it may be required to determine the parameters of the so-called equation of self-purification, in order to plan the beneficial use of a certain stream.

In all the examples cited, as well as in many other cases, the determination of the parameters of the equations used to represent each particular phenomenon is based on sets of observations obtained, as necessary, in the laboratory under controlled conditions or in the field under natural conditions. Fortunately, in many cases the model equations used in engineering and science present their parameters in an explicit form so that the determination of their values can be readily obtained through the application of the method of least squares or any other method suitable to this purpose. This is the case of the straight line and polynomial models. In other cases, however, the model presents its parameters not explicitly, but involving exponential, logarithmic, or trigometric forms; this type of equations, called "transcendental," may be solved more or less easily if its parameters are explicit in the exponential forms, since in such a case the equation may be transformed logarithmically. Finally, the case in which the parameters of a transcendental equation appear in an implicit form present the most serious difficulties, so that special methods of solution have been developed for only a few of them, among these methods it is worthwhile to mention the method of Thomas-Snow, applicable to the first order chemical reaction equation, the method of Verhulst used to solve the logistic equation, and the method of Theis, used to determine the value of the formation constants of aquifers.

The purpose of this thesis is to present a general method to reduce transcendental equations to algebraic forms to which the method of least squares, or any other suitable method of solution, can be applied in order to find the parameters of the original equation. Although the method is general in character, its applications in this thesis will be restricted to the case of transcendental equations with non-explicit parameters.

1.2 Definitions

A model, as defined in this thesis, is a mathematical relationship between one or more independent variables and a single dependent variable. Such variables represent the different entities of a phenomenon, and the given relationship of the phenomenon as a whole.

The parameters of the model or equation are the constants involved in the mathematical relationship, whose values are unknown but can be estimated considering sets of corresponding values of all the variables inherent to the model.

A simple example of such a model is given by the equation of the straight line

$$y = a + bx \tag{1.1}$$

when used to represent the population "y" of a given city, at different times "x." In this model, "x" and "y" are the variables, independent and dependent respectively, and "a" and "b" are the parameters whose values can be estimated when a set or sets of paired data (x,y) are known.

A model can result from theoretical considerations related to a phenomenon, as normally occurs in the physical sciences, or may be chosen empirically to try to represent the phenomenon under consideration, as happens, for instance, when a normal distribution is used to represent the occurrences of annual precipitation in a given region. In every model there are implicit assumptions related to the way in which the corresponding phenomenon is supposed to occur, for instance, in equation 1.1 the assumption is made that the population is directly proportional to time, or that the rate of increase of population is constant since

$$\frac{dy}{dx} = b \tag{1.2}$$

A model is a compromise between simplicity and reality, in which the proper selection of the variables of relevance in the phenomenon represented, as well as the assumptions in regard to the relations in between these variables, and the precision with which the parameters are estimated, determine the quality of the model.

Once a model and the appropriate variables have been established to represent a given phenomenon, the problem of determining the parameters involved in the model arises. To solve this problem, it is a generalized practice, when possible, to linearize the model by means of functional transformations of the original equation; the parameters of the straight line are then estimated, and from them, the parameters of the original equation are obtained. For instance, the geometric model of population growth

$$y = ae^{bx} \tag{1.3}$$

in which "y" and "x" represent population and time respectively, is linearized taking natural logarithms on both sides of the equation, so that

$$\ln y = \ln a + bx \tag{1.4}$$

In many cases, after the functional linearization of the model, some parameters of the original equation may appear combined with one or more variables in a functional form. Consider, for instance, the equation

$$y = a(1 - e^{-bx}) \tag{1.5}$$

used to represent the amount of substrate "y" remaining at time "x" in a first order reaction equation. After linearization, this equation becomes

$$\ln (a - y) = \ln a - bx \tag{1.6}$$

in which case the parameters "a" and "b" cannot be determined using the linear form because, "a" being unknown, it is impossible to calculate the values of ln (a - y). An equation containing exponential, logarithmic, or trigonometric terms is called a transcendental equation, for instance equations 1.4 and 1.5

A transcendental equation which after functional linearization shows its parameters in a non-explicit form, as in the case of equation 1.6, will be referred to in this thesis as a transcendental equation with non-explicit parameters. Some transcendental equations with non-explicit parameters have been solved by different methods; in most cases the method requires the use of graphs drawn with special functional scales. For some models, several methods exist, approximate or exact, but in general, these methods of solution are specific to the given equation and consequently they lack generality.

In Chapter III of this thesis a survey of the traditional methods of solution of the transcendental equations with implicit parameters listed in Chapter II will be presented. In Chapter IV, which constitutes the principal aim of this thesis, the method of differences to solve this kind of problem will be explained, and in Chapter V the method will be applied to solve several numerical examples. In Chapter VI the advantages of the method of differences are explored. In Chapter II an attempt is made to present the meaning of some equations used in sanitary engineering. In the remainder of the present chapter, the main mathematical tools used to estimate parameters of linear equations is summarized, and finally, in Chapter VII a method of interpolation of missing data is presented and illustrated with examples.

In the appendix, Chapter VIII, a summary of the transcendental equations and the linear forms developed in Chapter IV will be found, as well as other useful equations of this type and their respective nomenclature.

1.3 The Least Squares Method

Once a transcendental equation has been reduced to a non-transcendental form, the problem of determining its parameters remains. Among the several methods available, the method of least squares is considered to be the most frequently used on account of its many statistical advantages.

First, consider the case in which after plotting a set of data (x,y), the resulting "scattered diagram" shows that there exists some linear relationship between both variables. If the values of "x" are known precisely, then, for a given value of "x" several different values of "y" may occur, so that

$$y = a + bx + e \qquad (1.7)$$

where "e" is the error, or difference in between the observed value of "y" and the corresponding ordinate of the straight line

$$y' = a + bx \qquad (1.8)$$

which is called the "regression curve of y on x.

In order to find the "line of best fit," the sum of the squares of the errors is minimized. From equations 2.1 and 2.2

$$\Sigma e^2 = \Sigma(y - a - bx)^2 = \min \qquad (1.9)$$

where the summation is taken for all the set of "n" corresponding observations (x, y).

Equation 1.9 is satisfied when the partial derivatives with respect to "a" and "b" vanish. After derivation and reordering of terms, the following equations, called "normal," are obtained.

$$\Sigma y = an + b\Sigma x$$
$$\Sigma xy = a\Sigma x + b\Sigma x^2 \qquad (1.10)$$

from which the values of "a" and "b" are easily determined.

The method of least squares can be applied to non-linear equations by direct differentiation, however, it is commonly preferred to use the normal equations of the corresponding linear transform. For instance, in the case of equation 1.3, whose linear transformation is

$$\ln y = \ln a + bx$$

equations 1.10 are applied to the "n" pairs of values (x, ln y) to obtain estimates of ln a, and b.

Finally, in the case of multiple regression, which deals with "n" (r + 1) - tuples of data (x_1, x_2, x_3, . . . y), where the x's are known without error, the method of least squares is applied to obtain estimates of the parameters in equation

$$y = b_0 + b_1x_1 + b_2x_2 + \ldots b_rx_r \qquad (1.11)$$

whose corresponding normal equations are

$$\Sigma y = nb_0 + b_1\Sigma x_1 + b_2\Sigma x_2 + \ldots b_r\Sigma x_r$$
$$\Sigma x_1y = b_0\Sigma x_1 + b_1\Sigma x_1^2 + b_2\Sigma x_1x_2 + \ldots b_r\Sigma x_1x_r \qquad (1.12)$$
$$\Sigma x_ry = b_0\Sigma x_r + b_1\Sigma x_1x_r + b_2\Sigma x_rx_2 + \ldots b_r\Sigma x_r^2$$

Since the set of equations 1.10 will be frequently applied in Chapter V, the solution of this set is

$$I = \frac{\Sigma Y}{n} - P\frac{\Sigma X}{n}$$
$$P = \frac{n\Sigma XY - \Sigma X\Sigma Y}{n\Sigma X^2 - (\Sigma X)^2} \qquad (1.13)$$

The change of notation from small to capital letters is done to avoid confusion with the notation of the linear forms to be presented in Chapter IV. "P" now stands for the slope of a straight line, and "I" for its intercept.

1.4 Other Methods of Solution of the Linear Model

Method of Averages

A "quick method" to estimate the values of the parameters "a" and "b" from equation

$$y = a + bx \tag{1.1}$$

consists in dividing the set of "n" data into two groups, one containing "k" data and the other the remaining "n - k," and adding up the corresponding data in each group, to obtain the two simultaneous equations

$$\begin{aligned} \sum_{1}^{k} y &= ka + b\sum_{1}^{k} x \\ \sum_{n-k}^{n} y &= (n - k)a + b \sum_{n-k}^{n} x \end{aligned} \tag{1.14}$$

The solution yields the desired values of "a" and "b."

Graphical Method

The graphical determination of the parameters of the linear equation 1.1 is, maybe, the method most frequently used in solving engineering problems, mainly when functional forms of the variables are involved. The procedure consists of simply plotting the data and passing a straight line through the average values of all the "x's" and "y's," spinning the line until a line of "best fit" is obtained by eye. The values of the slope "b" and the intercept "a" are then obtained by measuring directly on the graph.

1.5 Method Selection

Obviously, the selection of a method to determine the parameters from a given equation is a matter depending on the quality of the model, the reliability of the data, and the accuracy desired in the determination. These factors relate to each other, so that there may not be any advantage, for instance, in applying the least squares method to a set of data that does not conform to a straight line, or when the scatter diagram is so disperse that nothing more than a "trend" can be obtained, or when no more than a rough estimate of the parameters is necessary to be known. In all these cases the application of such a method will represent time wasted, and no real benefits. In this respect, engineering good judgment and experience are the best tools available.

CHAPTER II

MODEL EQUATIONS USED IN SANITARY ENGINEERING

2.1 Model Equations

Sanitary engineering is a complex and fastly evolving branch of engineering. Although its bases lie in the laws of mathematics, physics, chemistry, and biology, there remains a good deal of empiricism in its methods and practices. New categories such as air pollution, noise control, radiological health, etc., have been added to the traditional ones of water supply and waste water disposal. This growth has made sanitary engineering so extensive that a reorganization of its contents is being carried out in order to allow the future sanitary engineers to meet their functions in operation, management, design, planning, etc. Repackaging of material common to several disciplines appears now in courses such as unit operations and processes, systems analysis, systems design, etc. [1]

From the new tools used in engineering, perhaps the "systems approach" is the most striking, for it considers models as mathematical or quantitative descriptions of problems. The model is the item that changes the problem from one of intuition into one to be solved mathe-

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[1] G. W. Reid, "Graduate Programs in Sanitary Engineering," a report to the University of Mexico, 1973.

TABLE 2.1

SOME TRANSCENDENTAL MODELS USED IN SANITARY ENGINEERING

Models arising from ordinary differential equations	
Equation	Applications
Chemical first order reaction equation	Biochemical oxygen demand Rate of absorption of gases Rate of stabilization of new reservoirs Flood routing Population growth Biokinetics
Chemical second order reaction equation: Autocatalytic, Logistic	Anaerobic decomposition Population growth
Rate of purification	Biological treatment units design Bacterial self-purification
Models arising from partial differential equations	
Molecular diffusion	Diffusion of dissolved substances
Theis	Formation constants of aquifers
Empirical model	
Rainfall	Intensity of storms precipitation

matically, as precisely as possible. Even more, just as it is possible for a phenomenon to be represented by several different models, the same model is frequently applicable to many kinds of phenomena. This property gives unity to apparently unrelated concepts used in sanitary engineering and allows for repackaging. For instance, the compound interest model used to compute internal rates of return in economy is often applied in specific studies, such as rates of growth, in bacterial populations. The methods used at the present to solve these two problems are different, but much time of teaching could be saved by contemplating both problems through the same model.

Model equations used in sanitary engineering can be classified in different ways. They may be theoretical or empirical; discrete or continuous; deterministic or probabilistic; exact or approximate, etc., with regard to their mathematical characteristics. They may also be classified in accordance to their origin, since they may arise from the fields of physics, chemistry, biology, hydraulics, hydrology, demography, etc. However, although the importance of having a good classification is recognized in the study of model equations, this job is left for further research, since the scope of this thesis is restricted to the presentation of a method of solution, irrespective of the origin, characteristics, etc. of the equations to be considered. So, in the remaining part of this thesis, these properties will be considered with the purpose of identification rather than classification; in this way, generality would not be lost and clarity would be gained.

Table 2.1 presents a list of the non-explicit transcendental equations applied in sanitary engineering that will be covered in this thesis.

The shape graphs of the transcendental equations listed in Table 2.1 are depicted in Figure 2.1. Their mathematical expressions and the way in which they are used in sanitary engineering is as follows.

2.2 Chemical First Order Reaction Equation

Chemical reaction kinetics studies the time dependence of reactions that proceed at slow rates. The type equation in this kind of study is

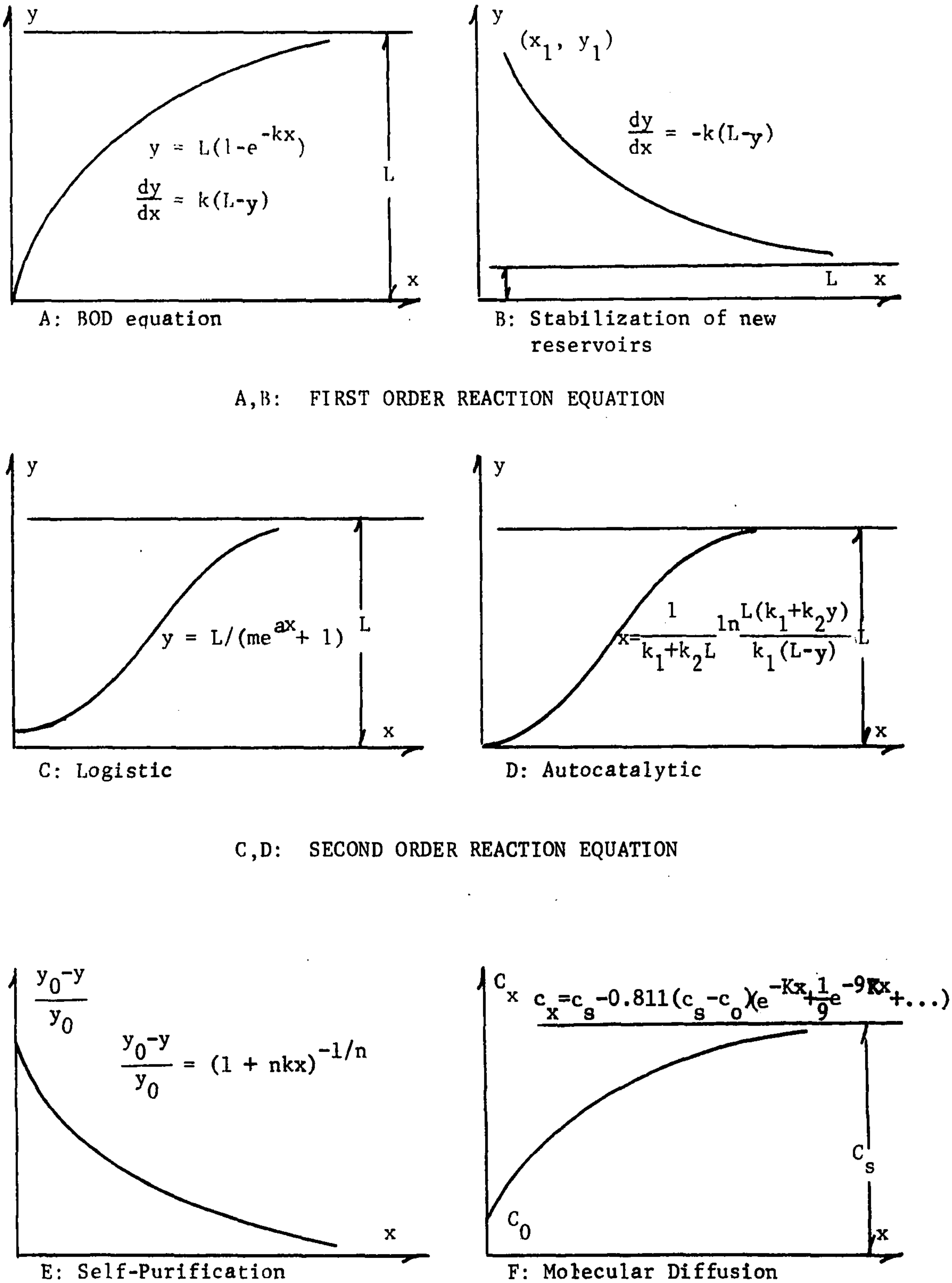
$$\frac{dc}{dx} = kf(R) \tag{2.1}$$

where "c" represents the concentration at time "x" of the material of interest, "k" the specific reaction rate constant, and "f(R)" a function of the concentrations of the substances concerned in the reaction.

The order of a reaction equation is defined by the order of "f(R)." If f(R) is a linear function of the concentration of a single reacting substance, the equation is of the first order; if "f(R)" is a function of the square of the concentration of a single substance, or the product of the concentrations of two different substances, the equation is of the second order, etc.

The BOD Equation

The progress of decomposition of organic matter in water and sewage due to the action of aerobic bacteria is reflected in the gradual consumption of the oxygen in solution in the sustaining medium. The rate at which oxygen utilization occurs is called "biochemical oxygen demand" (BOD), which at the present time provides the best means to identify the pollutional status of water by indirectly measuring the amount of decomposable matter in water or sewage. Exertion of BOD in



A: BOD equation

B: Stabilization of new reservoirs

A,B: FIRST ORDER REACTION EQUATION

C: Logistic

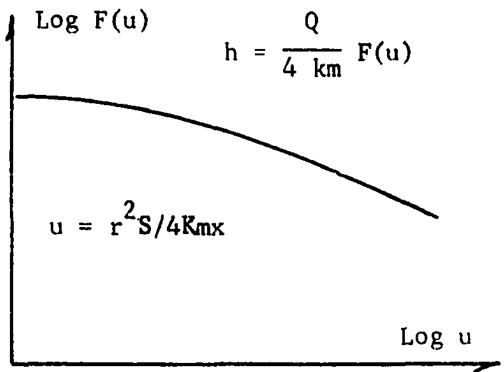
D: Autocatalytic

C,D: SECOND ORDER REACTION EQUATION

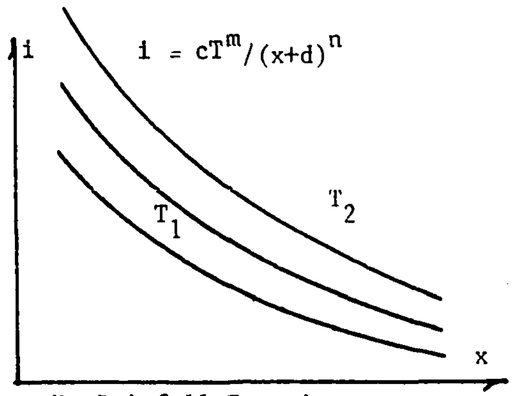
E: Self-Purification

F: Molecular Diffusion

FIGURE 2.1: SHAPE GRAPHS OF SOME TRANSCENDENTAL EQUATIONS



G: Theis Equation



H: Rainfall Equation

FIGURE 2.1: Continued

freshly polluted water takes place in two stages during which oxygen is consumed. In the first stage the carbonaceous matter is oxidized, and in the second stage the nitrogenous substances are attacked and nitrification takes place. Multiple experiments have shown that during the second stage the reaction rates are practically constant, and that during the first stage the rate of the reaction depends on the concentration of the oxidizable organic material present. If the temperature is maintained constant the equation representing the first stage is

$$\frac{dy}{dx} = k(L-y) \tag{2.2}$$

where "y" is the oxygen demand exerted in time "x," "L" the ultimate oxygen demand which represents the original amount of oxidizable matter in water, and "k" the rate of the reaction constant. Upon integration, considering that y = 0 at x = 0, the so-called BOD equation is obtained

$$y = L(1 - e^{-kx}) \tag{2.3}$$

Rate of Absorption of Gases

When a gas does not react chemically with water, its solubility is defined in terms of Henry's Law

$$c_s = k_s p \tag{2.4}$$

where "c_s" is the saturation concentration of the gas in water, "p" the partial pressure of the gas in the gas phase, and "k_s" the proportionality constant called "coefficient of absorption." The rate of absorption of a gas by water is proportional to its degree of undersaturation

$$\frac{dc}{dx} = K_g\ (c_s - c) \tag{2.5}$$

here, "c" is the concentration of the gas at a given temperature at time "x" and "K_g" is the constant of solution for the conditions of exposure.

The value of K_g depends on temperature and the degree of mixing of gas and liquid. When water is sprayed into the air in droplets, or when air is bubbled through water, K_g is equal to $k_g A/V$, where k_g is the "gas transfer coefficient," and A/V is the interfacial area per unit volume of the liquid.

Integration of the first order reaction equation 2.5, considering that $c = c_0$ at $x = 0$, yields

$$c_x - c_0 = (c_s - c_0)\ (1 - e^{k_g x}) \qquad (2.6)$$

which is exactly of the same form as equation 2.3.

Rate of Stabilization of New Reservoirs

When a reservoir area is flooded, the original vegetation and the top soil undergo decomposition. Odors, taste, and color are imparted to the water, and 10 to 15 years elapse before equilibrium is reached. The incoming water affects the general water quality of the reservoir. The process of stabilization takes place in accordance to the first order reaction equation

$$\frac{dy}{dx} = -k\ (L-y) \qquad (2.7)$$

where "y" represents the color, algal growth, or any other suitable index of pollution, "x" is time, and "L" the concentration of equilibrium. Integration of this equation, considering that $y = y_1$ at $x = x_1$, yields

$$y = L + (y_1 - L)e^{-k(x-1)} \tag{2.8}$$

2.3 Chemical Second Order Reaction Equation

A second order reaction equation is one in which f(R) in equation 2.1 is a function of the square of the concentration of a single substance, or a function of the product of the concentration of two different substances. Two important equations pertain to this group: the autocatalytic equation and the logistic equation.

Autocatalytic Equation

The progress of anaerobic decomposition of sludge can be measured by capturing the gases released during the decay of known amounts of putrescible matter. During the process of decomposition the production of enzymes plays an important role in catalyzing the reactions. The action of the enzymes determines an s - shaped curve when the gas production of a single batch of organic material is plotted against time.

Anaerobic decomposition proceeds at lower rates than aerobic decay. At 20°C the rate of gasification of seeded sludge solids is 8.4% per day compared to a rate of 32.3% per day for BOD at a "k" value of 0.39. Anaerobic decomposition takes place when the oxygen dissolved in water is exhausted by the aerobic organisms engaged in the stabilization of organic matter. Then, the predominate microorganisms are anaerobic rather than aerobic. This happens when streams or bodies of water are overloaded with waste materials, when solids settle from water and accumulate to a sufficient thickness to become anaerobic, or when sludges from municipal or industrial waste treatment plants are to be digested before final disposal. In formulating the autocatalytic equation, it is assumed that the rate of decomposition is a function of the amount of organic matter to be digested and the amount of material that has undergone decomposition.

$$\frac{dy}{dx} = k_1 \ (L-y) + k_2 y \ (L-y) \tag{2.4}$$

where "y" is the amount of gas produced of time "x," "L" is the total amount of gas which can be potentially produced, and "k_1" and "k_2" are the intensity factors.

Integration of equation 2.9, considering that y = 0 at x = 0, yields

$$x = \frac{1}{k_1 + k_2 L} \ln \frac{L(k_1 + k_2 y)}{k_1 (L-y)} \tag{2.10}$$

2.4 Logistic Equation

Experiments of bacterial growth accomplished by continually pumping fresh nutrients in the growing environment and at the same time allowing the waste products to be carried out from the environment are always alike in one feature. The growth is exponential at the beginning but after some time the rate of growth starts to decrease to finally produce a situation of equilibrium depending on the amount of nutrients provided and the general conditions of the medium. This condition is known as zero-growth. The sigmoid characteristics of the curve resulting when population is plotted against time comprise three different stages of growth: geometric for young populations, linear for intermediate, and "first order" for the mature populations.

Perhaps the first man to recognize the sigmoid character of the human population growth was Thomas Robert Malthus; however, his predictions that the growth period of the human population would come to and end during the nineteenth century turned out wrong, due mainly to technological advancements that occurred after his lifetime.

Sigmoid curves can be described by a number of different equations that seek a rational basis for their selection. One of the best-known is the logistic curve of Verhulst, which is a particular case of the autocatalytic equation 2.9.

The logistic model supposes that the population rate of growth is proportional to the population "y" and to the difference between the saturation value "L" and the population, at time "x."

$$\frac{dy}{dx} = \frac{a}{L} y \ (L-y) \qquad (2.11)$$

Integration considering that $y = y_0$ at $t = 0$ yields

$$y = \frac{L}{me^{ax} + 1} \qquad (2.12)$$

where "a" and "m" are constants, and

$$m = \frac{L - y_0}{y_0} \qquad (2.13)$$

2.5 Rate of Purification Equation

Biological Treatment Units

The processes that take place in natural purification of water are similar to those taking place in a biological sewage treatment plant, to the extent that it has been suggested that a sewage treatment plant is like a river wound up in a small space.

The rate of activity in biological treatment units, measured by the removal of BOD, suspended solids, bacteria, etc. is greater at the beginning of the process because the most easily decomposable substances are removed first, and the concentration of removable substances is a decreasing factor. The rate of purification in this type of units is a function of the concentration of removable substances, and the removability of the constituent fractions as well.

$$\frac{dy}{dx} = k((y_0 - y)/y_0)^n \ (y_0 - y) \tag{2.14}$$

where "y" is the amount of substance removed at time "x" (or while a distance "l" has been traveled by sewage at time "x"), "k" the reaction velocity constant, "n" a coefficient that measures the non-uniformity of the rate of purification, and "y_0" the amount of removable substance present in the applied sewage.

When n = 0, equation 2.14 becomes a first order reaction equation similar to equation 2.2.

Integration of equation 2.14, considering that $y = y_0$ at $x = 0$, yields, for n>0

$$\frac{y}{y_0} = 1 - (1 + nkx)^{-1/n} \tag{2.15}$$

Bacterial Self-Purification

The discharge of sewage into a receiving body of water increases the number of bacteria essential to the processes of self-purification of water; when they reach a balance under the prevailing environmental conditions, their number and variate declines. The number of intestinal bacteria isolated from samples of water is observed to increase below a sewer outfall during the first 10 to 12 hours of flow. The presence of predators in polluted, natural waters, as well as the influence of biophysical factors, as sedimentation and biological coagulation and precipitation, determine that the pattern followed in the die-away of bacteria under natural conditions are different than results obtained in the laboratory, which conform to Chick's Law. The rate of purification equation should, therefore, apply to natural situations; to meet this purpose, equation 2.15 is rewritten in a more suitable form

$$\frac{N}{N_0} = (1 + nkx)^{-1/n} \qquad (2.16)$$

where N_0 is the modal number of bacteria at time of flow "x," below the point of modal density "N_0."

2.6 Molecular Diffusion Equation

Diffusion of Dissolved Substances in Water

The process of equalization of concentration of dissolvable substances throughout a given volume of water is called molecular diffusion. Fick's Law of diffusion is analogous to the law governing heat conduction. The rate of diffusion across an area A is proportional to the concentration gradient of the substance from a point of higher toward one of lower concentration.

$$\frac{\partial w}{\partial x} = k\ A\ \frac{\partial c}{\partial l} \qquad (2.17)$$

where "w" is the weight of dissolved substance, "x" is time, "A" the cross sectional area, "c" the concentration, "l" the distance, and "k" the "coefficient of diffusion." The solution to this partial differential equation, obtained by Black and Phelps, is as follows:

$$c_x = c_s - 0.811(c_s - c_0)(e^{-kx} + \frac{1}{9}\,e^{-9kx} + \frac{1}{25}\,e^{-25kx} + \ldots) \qquad (2.18)$$

where "c_s" is the saturation concentration of the dissolved substance; "c_0" and "c_x" the concentrations at time zero and "x" respectively; and

$$K = \frac{\Pi^2 k}{4\ell^2} \qquad (2.19)$$

2.7 Theis' Equation

The relationship known as Darcy's Law establishes that the velocity of water flowing through the porous medium is proportional to the hydraulic gradient, or loss of head per unit area of flow path.

$$v = Ks \qquad (2.20)$$

where "v" is the face or approach velocity of water, "s" the hydraulic gradient, and "K" the so-called "coefficient of permeability, represents the velocity of flow associated with a unit hydraulic gradient.

The "coefficient of transmissibility," "T" of an aquifer, is obtained by multiplying the coefficient of permeability by the full saturated height of the aquifer. The coefficient of transmissibility represents the amount of water that would flow through a unit width of aquifer at a unit of time, when the hydraulic gradient is unity. When water is pumped from a well, the original piezometric line of the aquifer is disturbed, producing the so-called "drawdown surface," this deepens and grows in extension until a condition of equilibrium is reached. The "storage coefficient," "S" of an aquifer, is the amount of water released by a column of aquifer of unit cross sectional area, when the drawdown level is depleted by one unit.

The basic equation showing the relationship between drawdown levels "h" vs. distance "r" from the center of the well, at time "x" is given in differential form, and polar coordinates by:

$$\frac{\partial^2 h}{\partial r^2} + \frac{1}{r}\frac{\partial h}{\partial r} = \frac{S}{T}\frac{\partial h}{\partial x} \tag{2.21}$$

C. V. Theis developed a solution to this equation based on an analogy to the flow of heat toward a sink, which can be written in the following form

$$h_0 - h = \frac{Q}{4\Pi T}\left(-0.5772 - \ln u + u - \frac{u^2}{2.2!} + \frac{u^3}{3.3!} + \ldots\right) \tag{2.22}$$

where "h_0-h" is the drawdown at time "x" and distance "r" from the well, "Q" is the uniform pumping rate, and

$$u = \frac{r^2 S}{4Tx} \tag{2.23}$$

2.8 Rainfall Equation

The "intensity" of rainfall is expressed by dividing the height of the rainfall accumulated in a standard pluviometer by the time it has taken for this accumulation to occur. The intensity is highest for short periods, and declines steadily as the period increases. The greater the intensity of the storms, the rarer is their occurrence or the smaller their "frequency." The frequency with which a given intensity occurs is obtained by dividing the number of years on record by the number of times the given intensity occurred in that period of years.

It has been found empirically that the intensity-duration-frequency relationships conform very well to equation

$$i = \frac{cT^m}{(x+d)^n} \tag{2.24}$$

where "i" is the intensity, "x" the duration of rainfall, and "T" its frequency of occurrence; "c," "d," "m," and "n" are parameters varying regionally according to prevailing hydrological conditions.

CHAPTER III

TRADITIONAL METHODS OF SOLUTION OF TRANSCENDENTAL EQUATIONS

3.1 General Description

Traditional methods used in the solution of transcendental equations vary in accordance to the equation under consideration. Practically all of the methods make use of graphs or tables in some stage of the solution process. In many cases, the corresponding graphs are drawn using special functional scales, while in other cases, conventional functional scales are used combined with a process of trial and error until a plotting of the data fits a straight line. In some instances, the original equation is approximated by a mathematical relationship that shows the unknown parameters in a more explicit form; some times, this yields to second or third degree equations whose parameters are determined by graphical methods.

A method commonly used, when applicable, consists in measuring the slopes from a plot of the original equation using arithmetic scales, after which a second plot is performed using the slopes as a dependent variable, to determine the paramenters by graphical means. A variation of this method consists in approximating the values of the slopes by the relations between the increments in the dependent and independent variables.

Obviously, the methods described above are applicable only to equations involving two unknown parameters. When more parameters are involved, elimination of the exceeding number of parameters is usually performed previously to the application of the most suitable method of solution.

In the remainder of this chapter a brief description of the most important traditional methods of solution of the equations listed in Table 2.a will be presented, starting with the chemical first order reaction equation in Section 3.2, following.

3.2 Chemical First Order Reaction Equation

BOD Equation

There have been proposed a number of methods to find the magnitudes of the parameters "L" and "k" in the BOD equation

$$y = L(1 - e^{-kx}) \qquad (2.3)$$

from which the "method of moments" developed by Moore, Thomas and Snow, and the "approximate graphical method" worked out by Thomas have proved to be most useful.

Method of Moments

In this method a set of graphs that relates the first two moments of equation 2.3 with the parameters "k" and "L" are drawn using arithmetic scales. In each graph two curves are plotted; one corresponding to the relation $\Sigma y/\Sigma yx$ vs. k, and one for the relation $\Sigma y/L$ vs. k. After the first two moments of the set of paired data are computed, the value of "k" is determined from the first curve, entering with the known relation $\Sigma y/\Sigma yx$. This value of "k" is then used to determine the value of $\Sigma y/L$ from the second curve, from which "L" is finally determined. Obviously, each set of curves corresponds only to a fixed number of paired observations, and to a given system of units previously selected, being also limited by the range of values shown in the coordinates.

The equations underlying this method are obtained taking the moments of order zero and one from equation 2.3.

$$\Sigma y = (n + 1)L - L\Sigma\ e^{-kx} \tag{3.1}$$

$$\Sigma yx = L\Sigma x - L\Sigma xe^{-kx} \tag{3.2}$$

Dividing equation 3.2 by equation 3.1 eliminates "L", to yield

$$\frac{\Sigma y}{\Sigma yx} = \frac{(n + 1) - L\Sigma e^{-kx}}{\Sigma x - \Sigma xe^{-kx}} \tag{3.3}$$

From equation 3.1, the relation $\Sigma y/L$ is obtained.

$$\frac{\Sigma y}{L} = (n + 1) - \Sigma e^{-kx} \tag{3.4}$$

In equations 3.1 through 3.4, the summations are taken from zero to "n", "n" being the number of paired data (x,y).

Approximate Graphical Method

This method is based on the fact that the expansion

$$(1 - e^{-kx}) = kx(1 - \frac{kx}{2} + \frac{(kx)^2}{6} - \frac{(kx)^3}{24} + \ldots) \tag{3.5}$$

is approximated by the expansion

$$kx(1 + \frac{kx}{6})^{-3} = kx\ (1 - \frac{kx}{2} + \frac{(kx)^2}{6} - \frac{(kx)^3}{21.6} + \ldots) \tag{3.6}$$

so that, equation 2.3 may be approximated by

$$y = Lx(1 + \frac{kx}{6})^{-3} \tag{3.7}$$

which may be written in the straight line form

$$(\frac{x}{y})^{\frac{1}{3}} = (kL)^{-\frac{1}{3}} + (k^{\frac{2}{3}}/(6L)^{\frac{1}{3}})x \tag{3.8}$$

from which, the values of "k" and "L" may be determined, analytically, or graphically as proposed by Thomas.

Rate of Absorption of Gases

Values of the constant "K_g" in equation

$$c_t - c_o = (c_s - c_o)(1 - e^{-K_g x}) \tag{2.6}$$

are not determined under field conditions, instead its values are computed from the relationship

$$K_g = k_g \frac{A}{C} \tag{3.9}$$

where A/C is the area of the interface per unit volume of liquid, and kg is the "gas transfer coefficient. Existing tables of values of k_g, obtained under controlled conditions of temperature and pressure are normally considered in the solution of problems related to the absorption of gases by water.

Rate of Stabilization of New Reservoirs
Trial and Error Method

In the determination of the constants "k" and "L" of equation

$$y = L + (y_1 - L)e^{-k(x - 1)} \tag{2.8}$$

the trial and error method is generally used. First, an equilibrium value for "L" is assumed, and then the percent values $\frac{y - L}{y_1 - L}$ are plotted logarithmically against time trying to obtain a fit to the straight line equation

$$\log \frac{y - L}{y_1 - L} 100 = (2 + k.\log e) - (k \log e)x \tag{3.10}$$

Once a straight line has been obtained, the value of "k" is determined from the slope of the line.

3.3 Chemical Second Order Reaction Equation

Autocatalytic Equation
Approximate methods

It is generally recognized that the evaluation of the parameters of the autocatalytic equation is difficult. Since the differential form of equation 2.10

$$\frac{dy}{dx} = k_1(L - y) + k_2\, y(L - y) \tag{2.9}$$

is in fact the summation of the rates of change in a first order reaction and in the logistic equations, it is assumed that anyone of these two equations can be used to fit the data conforming to the autocatalytic equation

$$x = \frac{1}{k_1 + k_2L} \ln \frac{L(k_1 + k_2y)}{k_1(L - y)} \tag{2.10}$$

When a first order reaction equation is used, a lag period at the beginning of the process has to be assumed, since this type of equation can represent only the part of the sigmoid curve in which the slope is decreasing. When the logistic model is used, departures on the upper part of the curve may be expected, although compensated by a modified value of "k_2", since the value of k_1 is not considered in the computations.

3.4 Logistic Equation

Several methods have been developed to determine the parameters of the logistic equation

$$y = \frac{L}{me^{ax} + 1} \tag{2.12}$$

McLean Method

The solution proposed by McLean considers the selection of three pairs of values $(0, y_0)$, (x_1, y_1), $(2x_1, y_2)$, that cover the range of censal data. The parameters are determined solving three simultaneous equations to yield:

$$L = \frac{2y_0y_1y_0 - y_1^2(y_0 + y_2)}{y_0y_2 - y_1^2} \tag{3.11}$$

$$m = \frac{L - y_0}{y_0} \tag{3.12}$$

$$n = \frac{1}{x_1} \ln \frac{y_0(L - y_1)}{y_1(L - y_0)} \tag{3.13}$$

Graphical Method

The graphical method attributed to Verhulst, is based in the construction of a logistic scale, built in a similar way as the one used to build a probability scale, to plot population against time represented on an arithmetic scale.

To plot the data, a value of "L" is first assumed, and the populations expressed as percentages of the saturation value; if the assumed value for "L" is correct, the plotting results in a straight line from which the parameters "m" and "a" can be obtained.

The equations underlying this method follows. From equation 2.12:

$$100 \frac{Y}{L} = \frac{100}{1 + me^{ax}} = P \tag{3.14}$$

where "P" is the population percent; taking natural logarithms, equation 3.14 becomes

$$\ln\left(\frac{100 - P}{P} \right) = \ln m + ax \qquad (3.15)$$

which is the equation of a straight line on the scales x, (1/P)ln(100 - P); the slope of the line is "a", and its intercept "ln m"

3.5 Rate of Purification Equation

Biological Treatment Units
Trial and Error Method

In the determination of the values of the parameters of equation

$$\frac{y}{y_0} = 1 - (1 + nkx)^{-\frac{1}{n}} \qquad (2.15)$$

use is made of a graph showing a family of curves for different values of "n", obtained by plotting the values $\frac{y - y_0}{y_0}100$ against corresponding values of kx. These graphs are generalized to fit different types of treatment units. First, a value of "n" is assumed and substituted in equation 2.15, from which as many values of "k" are obtained as pairs of data (x, y) are available in a given problem; an average value of "k" is then selected to compute the values of "kx"; from the graph new values of "y" are obtained and compared with the corresponding observed data. The procedure is repeated until the estimated values of "y" match the data.

Bacterial Selfpurification
Approximate Method

The determination of the parameters of equation

$$\frac{N}{No} = (1 + nkx)^{-\frac{1}{n}} \qquad (2.16)$$

is based on the approximate empirical relationship:

$$n = \frac{\ln x_2/x_1}{\ln \frac{N_1}{N_0} \frac{N_o}{N_2}} \qquad (3.16)$$

which holds for large values of "n" and "k." Equation 3.16 is applied to pairs of observed data, and the resulting values of "n" are averaged; using this value of "n," values of "k" are computed for each observation, taking the average "k" as the desired parameter. Since the values of "n" and "k" vary widely for different streams, in cases where "n," "k," or both are small, the trial and error method is applied.

3.6 Molecular Diffusion Equation

The parameters of the molecular diffusion equation

$$c_x = c_s - 0.811(c_s - c_o)(e^{-Kx} + \frac{1}{9} e^{-9Kx} + \frac{1}{25} e^{-25Kx} + \ldots) \qquad (2.18)$$

are not determined under field conditions; instead, tabulated value of the coefficient of molecular diffusion "k" are used in combination with equation 2.19 to determine the values of "k" on specific problems. The values of "k" shown in the respective tables correspond to the diffusion of single substances in water, under controlled laboratory conditions.

3.7 Theis' Equation

Several methods have been developed to determine the formation constants "S" and "T" contained in equations

$$h_o - h = \frac{Q}{4\Pi T}\left(-0.5772 - \ln u + u - \frac{u^2}{2.2!} + \frac{u^3}{3.3!} - \frac{u^4}{4.4!} + \cdots\right) \quad (2.22)$$

$$u = \frac{r^2 S}{4Tx} \quad (2.23)$$

Overlay Method

The mathematical relationships involved in this method are obtained as follows:

Calling W(u) the series written in parenthesis, and making $Q/4\Pi T = C_1$, equation 2.22 becomes

$$h_o - h = C_1 W(u) \quad (3.17)$$

Making $S/4T = C_2$ in equation 2.23, yields

$$u = C_2 \frac{r^2}{x}$$

Taking natural logarithms on equations 3.17 and 3.18, adding and rearranging yields

$$\ln u - \ln W(u) = \ln C_1 C_2 + \ln \frac{r^2}{x} - \ln (h-h_o) \quad (3.19)$$

consequently, the plottings of u vs W(u) and r^2/s vs $(h-h_o)$ have exactly the same shape, and for every point on the curve u vs W(u), there is a corresponding point in the r^2/x vs $(h-h_o)$ curve.

To solve a particular problem, a curve is drawn on log-log paper, the abscissas corresponding to values of r^2/x and the ordinates to values of $(h-h_o)$, obtained from field measurements. Then a "typical curve" drawn on transparent paper and log-log scales, showing "u" in the abscissas and W(u) in the ordinates is superimposed to the "problem graph," trying to match as many points in both graphs as possible. A matching point is selected and the corresponding values of r^2/x, $(h - h_0)$, u and W(u) are read out in the respective coordinate axes; these values are used in equations 2.22 and 2.23 to determine "S" and "T".

Approximate Method

Jacob developed a quick method to evaluate "S" and "T" when the value of "u" is small; neglecting the terms beyond ln u in equation 2.22, the following equation is obtained

$$h_0 - h = \frac{Q}{4\pi T} \ln \frac{1.708S}{4T} + \frac{Q}{4\pi T} \ln \frac{r^2}{x} \tag{3.20}$$

which is the equation of a straight line when plotting $(h_0 - h)$ vs ln r^2/x. The value of "T" is determined from the slope of the line, after which "S" is determined from the intercept. Equation 3.20 can be used to estimate the value of "T" when observation wells are not available. If a well is pumped until a substantial drawdown is obtained, the levels of recovery can be measured after pumping is stopped. Calling "h", and "h_i" the levels of water in the well, at times "x_1" and "x_i" respectively, applying equation 3.20 to both conditions and substracting yields:

$$h_i - h_1 = \frac{Q}{4\pi T} \ln \frac{x_1}{x_i} \tag{3.21}$$

Plotting h_i on an arithmetic scale against x_i on a logarithmic scale, a straight line is obtained from which slope the value of "T" is obtained.

3.8 Rainfall Equation

The parameters "c", "d", and "n" of the rainfall equation

$$i = \frac{cT^m}{(x + d)^n} \tag{2.24}$$

are usually estimated by anyone of two graphical methods, the first one involves trial and error in the assumption of a value for the parameter "d", and the second considers an approximation for the values of di/dx.

Graphical Method

Since equation 2.24 may be written in its logarithmic form as

$$\ln i = \ln c + m \ln T + n \ln(x + d) \tag{3.22}$$

a family of straight lines, each line corresponding to a constant value of "T", can be obtained by plotting ln i vs ln(x + d); in order to make this plotting possible, several values of "d" are tried until a straight line is obtained for a selected value of "T". The common slope of this family of lines gives the value of the parameter "n". The determination of the value of "m" presents no problem, since it is the common slope of a family of straight lines obtained by plotting ln i vs ln T, holding "x" constant during the plotting of each line.

Approximate Method

The rate of change of rainfall intensity with respect to time is given by the equation

$$\frac{di}{dx} = -in(x + d)^{-1} \tag{3.23}$$

Taking logarithms on both sides of this equation yields

$$\ln(-\frac{di}{dx}) = \ln i + \ln(n) + \ln(x + d)^{-1} \tag{3.24}$$

Taking logarithms on equation 2.24 and rearranging yields

$$\ln(x + d)^{-1} = \frac{\ln i}{n} - \frac{\ln cT^{m}}{n} \tag{3.25}$$

so that, finally we obtain

$$\ln\left(-\frac{di}{dx}\right) = \ln(n) - \frac{1}{n}\ln cT^{m} + \left(1 + \frac{1}{n}\right)\ln i \qquad (3.26)$$

which fits a straight line when "T" is constant and ln(-di/dx) is plotted against ln i. The parameter "n" is determined from the slope of the line, and "c" from its intercept. Obviously, the values of (di/dx) have to be determined by direct measurements from a direct plotting of equation 2.24; however, the values of (di/dx) at i_{k+1} can be approximated using the relation

$$\frac{di}{dx} = \frac{i_{k+2} - i_k}{x_{k+2} - x_k} \qquad (3.27)$$

where the subscripts denote pairs of values of "i" taken from a series of intensities recorded at uniform intervals of time.

CHAPTER IV

METHOD OF DIFFERENCES

4.1 General Description

It can easily be seen that the differential forms of the transcendental equations considered in the previous two chapters present their respective parameters in a more explicit form than the transcendental equations. For instance, in the case of the first order reaction equation

$$y = L(1 - e^{-kx}) \tag{2.3}$$

its differential form is already nontranscendental and takes the form of a straight line

$$\frac{dy}{dx} = kL - ky \tag{2.2}$$

from which the values of the parameters "k" and "L" could be obtained if the values of (dy/dx) were known for each value of "y." Unforunately, this is not the case and, as has already been explained in Chapter III, the values of (dy/dx) have to be measured from a plot of y vs x on arithmetic scales, or approximated by the slope of a chord subtending two neighboring points of the point of interest. These two methods are unsatisfactory because, in the graphical method the curves y vs x are fitted by eye through an almost always small amount of spaced data which have implicit random variations on its true values, and because the accuracy of a geometrical measurement is always influenced by the instruments used, the ability of the instrument reader, and the precision of the graph scales. When the slope of the curve is approximated by the slope of a chord, the random variations and error on the data are not taken into account, and the approximation is valid only if the length of the chord approaches zero.

To avoid the inconveniences pointed out above, but trying to conserve the explicit way in which the parameters of a given transcendental equation appear in its corresponding derivatives, it seems natural to work, instead, with the difference form of the equation.

It is known from elementary calculus that for any function $y = f(x)$, to every increment Δx given to the independent variable, corresponds an increment Δy in the dependent variable

$$\Delta y = f(x + \Delta x) - f(x) \qquad (4.1)$$

where Δy expresses the difference in the values of $f(x)$ at x and $x + \Delta x$, and Δx is also called the "difference interval." It should be observed here that the values assumed by x are only restricted by the domain of the function and not by order of magnitude, and that $f(x)$ may be any kind of function, continuous or discrete.

To illustrate how the method of differences works in determining parameters, the simple case of the geometric equation is taken as an example

$$y = ae^{bx} \qquad (1.3)$$

Giving an increment Δx to x, equation 1.3 becomes

$$y + \Delta y = ae^{b(x + \Delta x)} = ae^{bx}\, e^{b\Delta x}$$

from which

$$\Delta y = (e^{b\Delta x} - 1)\, y \qquad (4.2)$$

or, making $y + \Delta y = y_{x + \Delta x}$

$$y_{x+\Delta x} = e^{b\Delta x}\, y \qquad (4.3)$$

Both equations, 4.2 and 4.3, result in straight lines when Δy vs y or $y_{x+\Delta x}$ vs y are plotted using arithmetic scales, if the value of Δx is maintained constant, i.e., if the data are equally spaced in time. The value of "b" is obtained from the slope of the line.

Obviously, in the previous example not much is gained over the traditional solution that consists in taking the logarithmic form of equation 1.3

$$\ln y = \ln a + bx \qquad (1.4)$$

and obtaining the values of "a" and "b" from a plot of ln y vs x; however, the functional form "ln y" has been removed and some amount of computation reduced.

Thus, the application of the method of differences is more advantageous when simple transformations of the type of equation 1.4 are not possible, as is the case of the transcendental equations considered in this thesis.

Also, it is interesting to notice that equation 4.3 can be readily obtained by substituting the values $(x+\Delta x,\ y_{x+\Delta x})$ in the original equation 1.3 to obtain

$$y_{x+\Delta x} = ae^{b(x+\Delta x)}$$

which divided by equation 1.3, after rearrangement, yields

$$y_{x+\Delta x} = e^{b\Delta x}\, y_x \qquad (4.3)$$

which is a recurrence equation equivalent to the difference equation 4.2.

In the remaining of this chapter, sections 4.2 to 4.8, this method will be applied to each one of the equations listed in Table 2.1, in trying to obtain simpler expressions that will allow the determination of its respective parameters in a simplified way.

4.2 First Order Reaction Equation

B.O.D. Equation

The first order reaction equation 2.3 can be rewritten to be

$$L - y = Le^{-kx} \tag{4.4}$$

Substitution of $(x+\Delta x,\ y_{x+\Delta x})$ in the previous equation yields

$$L - y_{x+\Delta x} = Le^{-k(x+\Delta x)}$$

Dividing this equation by equation 4.4 gives as a result

$$\frac{L - y_{x+\Delta x}}{L - y} = e^{-k\Delta x} \tag{4.5}$$

from which

$$y_{x+\Delta x} = L(1 - e^{-k\Delta x}) + e^{-k\Delta x}\, y \tag{4.6}$$

or, since $y_{x+\Delta x} = y + \Delta y$

$$\Delta y = L(1 - e^{-k\Delta x}) - (1 - e^{-k\Delta x})y \tag{4.7}$$

or,

$$y = L - \frac{1}{1 - e^{-k\Delta x}}\,\Delta y \tag{4.8}$$

Equations 4.6, 4.7 and 4.8 are all straight line expressions when Δx is taken as a constant; equation 4.6 may be considered superior to the other two equations, since it involves one less step in computation.

If the graphical method is used to find the parameters, arithmetic scales are used in all cases; however, the least squares method is obviously recommended.

Rate of Absorption Equation

When equation 4.6 is applied to equation

$$c_x - c_0 = (c_s - c_0)(1 - e^{-k_g x}) \tag{2.6}$$

it is obtained that

$$c_{x+\Delta x} = c_s(1 - e^{-k\Delta x}) + e^{-k\Delta x}\, c_x \tag{4.9}$$

Obviously, similar expressions to equations 4.7 and 4.8 are found, either directly taken differences from equation 2.6, or making $c_x - c_0 = y$ and $c_s - c_0 = L$ in equations 4.7 and 4.8.

From equation 4.7:

$$\Delta(c_x - c_0) = (c_s - c_0)(1-e^{-k\Delta x} - (1-e^{-k\Delta x})(c_x - c_0)$$

Since $\Delta c_0 = 0$

$$\Delta c_x = c_s(1-e^{-k\Delta x} - (1-e^{-k\Delta x})c_x \tag{4.10}$$

and from equation 4.8, since $\Delta c_s = 0$

$$c_x = c_s - \frac{1}{1 - e^{-k\Delta x}}\, \Delta c_x \tag{4.11}$$

Observe that the value of "c_0" does not play any role in equations 4.9 through 4.11, which means this is not a true parameter, and it simply corresponds to a concentration at anytime taken as zero or base value.

Rate of Stabilization of New Reservoirs

Equation 2.8 is rewritten to yield

$$\frac{y-L}{y_1-L} = e^{-k(x-1)} \tag{2.8}$$

which applied to point $(x+\Delta x,\ y+\Delta y)$ becomes

$$\frac{y_{x+\Delta x} - L}{y_1 - L} = e^{-k(x+\Delta x-1)} \tag{4.12}$$

Dividing equation 4.12 by equation 2.8

$$\frac{y_{x+\Delta x} - L}{y - L} = e^{-k\Delta x}$$

from which

$$y_{x+\Delta x} = L(1 - e^{-k\Delta x}) + e^{-k\Delta x}\, y \qquad (4.6)$$

which is obviously the same solution as that obtained for the BOD equation, since "y_1" is not a true parameter, introduced artificially to suit the functional relationships used to find the parameters "k" and "L" by the traditional methods.

4.3 Second Order Reaction Equation

Autocatalytic Equation

The parameters of the autocatalytic equation

$$x = \frac{1}{k_1 + k_2 L} \ln \frac{L(k_1 + k_2 y)}{k_1\,(L - y)} \qquad (2.10)$$

can easily be brought to an explicit form.

Applying equation 2.10 to any pair of observations ($x+\Delta x$, $y_{x+\Delta x}$), it is obtained:

$$x + \Delta x = \frac{1}{k_1 + k_2 L} \ln \frac{L(k_1 + k_2 y_{x+\Delta x})}{k_1(L - y_{x+\Delta x})} \qquad (4.13)$$

Subtracting equation 2.10 from equation 4.13, and carrying out operations yields

$$e^{\Delta x(k_1+k_2L)} = \frac{k_1L - k_1y + k_2Ly_{x+\Delta x} - k_2y\,y_{x+\Delta x}}{k_1L + k_2Ly - k_1y_{x+\Delta x} - k_2y\,y_{x+\Delta x}}\,.$$

Taking Δx constant, making

$$e^{\Delta x(k_1+k_2L)} = a \qquad (4.14)$$

and rearranging, yields

$$(ak_2L+k_1)y + (-ak_1-k_2L)y_{x+\Delta x} + (k_2-ak_2)yy_{x+\Delta x} + (ak_1L-k_1L) = 0 \quad (4.15)$$

which corresponds to the multivariate linear model 1.11.

The parameters of equation 4.15 are obtained solving the corresponding set of equations 1.12, after which a new set of four simultaneous equations on "k_1," "k_2," "L," and "a" results. Their solution yields the desired results.

4.4 Logistic Equation

The parameters of the logistic equation

$$y = \frac{L}{me^{ax} + 1} \quad (2.12)$$

could be found from equation 4.15; however, it is simpler to proceed as follows.

First, giving increments to the variables in equation 2.12 we find

$$y_{x+\Delta x} = \frac{L}{me^{ax}\,e^{a\Delta x} + 1} \quad (4.16)$$

From equation 2.12

$$me^{ax} = \frac{L - y}{y} \quad (4.17)$$

Substituting equation 4.17 in equation 4.16 and rearranging yields

$$\frac{y}{y_{x+\Delta x}} = e^{a\Delta x} + \frac{1 - e^{a\Delta x}}{L}\, y \quad (4.18)$$

which is a straight line when "$y/y_{x+\Delta x}$" is plotted against "y" in arithmetic scales.

4.5 Rate of Purification Equation

Biological Treatment Units

In order to obtain an explicit form for the rate of purification equation 2.15, we first rewrite the equation to read

$$z^{-n} = (1 + nkx)y_0^{-n} \tag{4.19}$$

where

$$z = y_0 - y \tag{4.20}$$

Giving an increment to "z" in equation 4.19, an increment Δz corresponds to Δx, therefore

$$(z + \Delta z)^{-n} = (1 + nkx_{z+\Delta z})y_0^{-n} \tag{4.21}$$

Dividing equation 4.21 by equation 4.19 yields

$$\left(\frac{z + \Delta z}{z}\right)^{-n} = \frac{1 + nkx_{z+\Delta z}}{1 + nkx} \tag{4.22}$$

Now, if Δz is taken so that

$$\Delta z = az \tag{4.23}$$

where "a" is an arbitrary constant, equation 4.22 becomes after rearrangement of terms

$$x_{z(a+1)} = \frac{(a+1)^{-n} - 1}{nk} + (a+1)^{-n}\, x_z \tag{4.24}$$

or, if preferred

$$\Delta x = \frac{(1+a)^{-n} - 1}{nk} + [(1+a)^{-n} - 1]\, x \tag{4.25}$$

Observe that to apply equation 4.24 or equation 4.25 it is necessary to reorder the data. If equation 4.24 is solved graphically and "a" is chosen to be equal to one, the following set of data would be plotted: (x_1,x_2), (x_2,x_4), (x_3,x_6), ..., (x_i,x_{2i}) ...

Bacterial Selfpurification

The bacterial selfpurification form of equation 2.15

$$\frac{N}{N_0} = (1 + nkx)^{-1/n} \tag{2.16}$$

is solved much in the same way as equation 2.15 to yield

$$x_{N(1+a)} = \frac{(1+a)^{-n} - 1}{nk} + (1+a)^{-n}\, x \tag{4.26}$$

4.6 Molecular Diffusion Equation

To obtain an explicit form of the molecular diffusion equation 2.18, it is rewritten as

$$\frac{c_x - c_s}{-0.811(c_s - c_0)} = \left(e^{-Kx} + \frac{1}{9}\, e^{-9Kx} + \frac{1}{25}\, e^{-25Kx} + \ldots\right) \tag{4.27}$$

where the values of the parameters "K" and "c_s" are to be determined. Making

$$y = \frac{c_x - c_s}{-0.811(c_s - c_0)} \tag{4.28}$$

and applying equation 4.27 successively to a set of values (x, y_x), $(9x, y_{x.9})$, $(25x, y_{x.25})$ ..., we obtain the following arrangement

$$y_x = e^{-Kx} + \frac{1}{9}\, e^{-9Kx} + \frac{1}{25}\, e^{-25Kx} + \ldots$$

$$\frac{1}{9}\, y_{x.9} = \frac{1}{9}\, e^{-9Kx} + \frac{1}{9}\,\frac{1}{9}\, e^{-9(9)Kx} + \frac{1}{9}\,\frac{1}{25}\, e^{-9(25)Kx} + \ldots$$

$$\frac{1}{25}\, y_{x.25} = \frac{1}{25}\, e^{-25Kx} + \frac{1}{9}\,\frac{1}{25}\, e^{-25(9)Kx} + \frac{1}{25}\,\frac{1}{25}\, e^{-25(25)Kx} + \ldots$$

$$\vdots$$

where the terms after the first row and second column of the arrangement are very small as compared with the rest of the terms. Therefore, adding we obtain:

$$y_x + \frac{1}{9} y_{x.9} + \frac{1}{25} y_{x.25} + \ldots = 2y_x - e^{-Kx} + \ldots$$

from which

$$e^{-Kx} = y_x - (\frac{1}{9} y_{x.9} + \frac{1}{25} y_{x.25} + \ldots) \qquad (4.29)$$

Substituting equation 4.28 in equation 4.29 and rearranging yields

$$e^{-Kx} = \frac{c_x - \frac{1}{9}c_{x.9} - \frac{1}{25}c_{x.25} \ldots}{-0.811(c_s - c_0)} + \frac{c_s(-1 + \frac{1}{9} + \frac{1}{25} + \ldots)}{-0.811(c_s - c_0)} \qquad (4.30)$$

Making

$$z_x = c_x - \frac{1}{9} c_{x.9} - \frac{1}{25} c_{x.25} - \ldots \qquad (4.31)$$

$$A = -0.811(c_s - c_0) \qquad (4.32)$$

Since

$$(-1 + \frac{1}{9} + \frac{1}{25} + \ldots) = \frac{\Pi^2}{8} - 2 = -0.766 \qquad (4.33)$$

the following equation is obtained

$$e^{-Kx} = \frac{1}{A} z_x - \frac{0.766}{A} c_s \qquad (4.34)$$

Giving an increment x to "x" results in

$$e^{-Kx} e^{K\Delta x} = \frac{1}{A} z_{x+\Delta x} - \frac{0.766}{A} c_s \qquad (4.35)$$

Finally, substitution of equation 4.34 in equation 4.35 yields

$$z_{x+\Delta x} = 0.766(e^{-K\Delta x} - 1)c_s + e^{-K\Delta x} z_x \qquad (4.36)$$

which is the equation of a straight line when Δx is taken as a constant.

The value of "K" could be obtained from equation 4.29 when the values of "c_0" and "c_s" are known, which may generally be the case under field conditions, where the value of "c_0," at time or distance "x_0" taken as an arbitrary base, is known.

The parameters "K" and "c_s" can be obtained from equation 4.36

either graphically or analytically. In either case, a set of values $(z_x, z_{x+\Delta x})$ has first to be obtained. For instance, if Δx is chosen to be equal to 1, the set of values becomes

$$c_x - \sum_{n=1} \frac{1}{(2n+1)^2} c_{x(2n+1)^2} ; c_{x+1} - \sum_{n=1} \frac{1}{(2n+1)^2} c_{(x+1)(2n+1)^2} \tag{4.37}$$

where $c_{x(2n+1)^2}$ means the $x(2n+1)^2$ th term taking the c_x term as a basis.

Observe that "c_0" is not a true parameter, and that the constant "0.766" in equation 4.36 can be changed to take into account the number of terms of equation 4.29 considered in the desired solution.

4.7 Theis Equation

To find an equation that would show the parameters "T" an "S" from equations 2.22 and 2.23, in an explicit form, let

$$a = \frac{Q}{4\Pi T} \tag{4.38}$$

$$c = \frac{r^2 S}{T} \tag{4.39}$$

so that equation 2.23 becomes

$$u = \frac{c}{x} \tag{4.40}$$

and equation 2.22 may be rewritten as

$$h_0 - h = a\left(-0.5772 - \ln\frac{c}{x} + \frac{c}{x} - \frac{c^2}{2.2!\,x^2} + \ldots\right) \tag{4.41}$$

Giving increments to "x" and "h" we obtain

$$h_0 - h - \Delta h =$$

$$a\left(-0.5772 - \ln\frac{c}{x+\Delta x} + \frac{c}{x+\Delta x} - \frac{c^2}{2.2!\,(x+\Delta x)^2} + \ldots\right) \tag{4.42}$$

Subtracting equation 4.41 from equation 4.42 yields

$$\Delta h = a(\ln\frac{x+\Delta x}{x} + \frac{c}{x+\Delta x} - \frac{c}{x} - \frac{c^2}{2.2!\,(x+\Delta x)^2} + \frac{c^2}{2.2!\,x^2} + \ldots)$$

so that, making $\Delta x = x$, we obtain

$$\Delta h = a \ln 2 - \frac{ca}{2}\frac{1}{x} + \frac{3c^2a}{2.2!4}\frac{1}{x^2} + \ldots \qquad (4.43)$$

which is a multivariate linear form from which the values of "a" and "c" can be obtained through the application of equation 1.12. When "u" is small only the first three terms of theis' equation may be considered, to yield

$$\Delta y = 0.69\ a - \frac{ac}{2}\frac{1}{x} \qquad (4.44)$$

which is the equation of a straight line when plotting y vs 1/x using arithmetic scales. Once "a" and "c" are determined, "T" and "S" are readily obtained from equations 4.38 and 4.39 respectively.

Notice that before applying equations 4.43 or 4.44, the data have to be rearranged in accordance to the time series x, 2x, 4x, ..., $2^n x$, where n = 0, 1, 2, ...

4.8 Rainfall Equation

To determine the values of the parameters "m" "d" and "n" of the rainfall equation

$$i = \frac{cT^m}{(x+d)^n} \qquad (2.24)$$

first, consider "T" as a constant and let "x" and "i" vary, then, giving increments, it can be written

$$i + \Delta i = \frac{cT^m}{(x + \Delta x + d)^n} \qquad (4.45)$$

Dividing equation 4.45 by equation 2.24

$$\left(\frac{i+\Delta i}{i}\right)^{1/n} = \frac{x + d}{(x+\Delta x)+d}$$

making

$$\Delta i = ki$$

where "k" is an arbitrary constant, we obtain

$$(1+k)^{1/n} = \frac{x + d}{(x+\Delta x)+d}$$

from which

$$x_{i(1+k)} = d\,[(1+k)^{-1/n} - 1] + (1+k)^{-1/n}\, x_i \qquad (4.46)$$

or:

$$\Delta x = d\,[(1+k)^{-1/n} - 1] + [(1+k)^{-1/n} - 1]\; x \qquad (4.47)$$

Equations 4.46 and 4.47 are linear expressions from anyone of which the parameters "d" and "n" can be easily obtained; however, equation 4.46 involves one step less of computations. In any case, the data are selected so that $\Delta i = ki$; for instance, when k is chosen to be equal to one, the data correspond to the i-series i, 2i, 4i, ..., $2^n i$, where n = 0, 1, 2, ...

To determine the value of parameter "m," "x" is held constant, so that equation 2.24 can be written

$$i = KcT^m \qquad (4.48)$$

where

$$K = (x + d)^{-n} = \text{constant} \qquad (4.49)$$

Giving increments to "i" and "T" yields

$$i + \Delta i = Kc(T + \Delta T)^m$$

Taking

$$\Delta T = kT,\ k = \text{constant} \qquad (4.50)$$

$$i + \Delta i = KcT^m(1+k)^m \quad (4.51)$$

so that, considering equation 4.48

$$i_{(1+k)T} = (1 + k)^m \, i_T \quad (4.52)$$

which is the equation of a straight line from which the value of "m" can be easily found. Observe that "c" in equation 2.24 is not a true parameter but a scale factor, whose value depends on the units in which the variables "i" and "T" are expressed. Also, notice that equation 4.48 is non-transcendental, and therefore the value of "m" can be found using the logarithmic form 3.22.

CHAPTER V

EXAMPLES OF APPLICATION OF THE METHOD OF DIFFERENCES

5.1 Data Sources and Efficiency Criterion

The problems considered in this chapter are taken from the bibliography shown at the end of this thesis, the purpose being to compare the results obtained when the traditional methods of solution are applied with those obtained from the application of the method of differences. To compare results, the variance corresponding to each method, as applied to a particular problem, will be computed using the formula

$$V = \Sigma(y - y')^2 \tag{5.1}$$

where "V" is the variance or sum of squared errors between the observed data "y" and the corresponding computed values "y'". Obviously, the method showing the smallest variance among the methods considered to solve a particular problem should be regarded as the most efficient method in each specific case.

5.2 Procedure of Parameters Estimation

To solve each one of the problems appearing in sections 5.3 to 5.9 of this chapter, the corresponding linear forms presented in Chapter IV will be used, the data will be manipulated to conform to such forms, and then its parameters will be computed, from which the parameters of the model ruling the problem will be determined.

To compute parameters of the resulting straight line forms, the methods of least squares, averages, graphical, etc., will be used, as described in Chapter I of this thesis, on accordance to the nature of the problem, and the accuracy of the data.

All the numerical computations are performed using a Hewlet-Packard Model HP 35 calculator. In section 5.3, following, the procedure of application of the method of differences is explained in detail, to avoid repetition of the same concepts in the rest of the problems presented in sections 5.4 through 5.9.

5.3 First Order Reaction Equation

BOD Equation

Given the BOD determinations shown in column 2 of Table 5.1, find the magnitudes of parameters "k" and "L" in equation 2.3.

TABLE 5.1

SOLUTION OF THE BOD EQUATION

Data Columns		Computation Columns		
Time, Day (1); x	BOD, mg/l (2); $y=X$	(3); $y_{x+\Delta x}=Y$	(4); XY	(5); X^2
0	0	82	0	0
1	82	112	9184	6724
2	112	153	17136	12544
3	153	163	24939	23409
4	163	176	28688	26569
5	176	-	-	-
Σ	510	686	79947	69246

Analytical Solution: Least Squares Method

Equation 4.6 shows that the slope of the linear form of the BOD equation is

$$P = e^{-k\Delta x} \tag{5.2}$$

and its intercept is

$$I = L(1 - P) \tag{5.3}$$

To obtain the values of "I" and "P," we apply the least squares equations 1.13. Column 3 shows the values of $y_{x+\Delta x}$, obtained canceling the first term in column 2, writing the second term of column 1 in the first row of column two, and so on. Observe that columns 2 and 3 are labeled $y = X$, $y_{x+\Delta x} = Y$ to conserve the notations used in each of equations 4.6 and 1.13.

Columns 4 and 5 show the necessary computations to apply equations 1.13, from which we obtain

$$P = \frac{5(79947) - (510)(686)}{5(69246) - (510)^2} = 0.579$$

$$I = \frac{686}{5} - \frac{510}{5}(0.579) = 78.136$$

From equation 5.2, since $\Delta x = 1$

$$0.579 = e^{-k}; \ -k = \ln 0.579$$

$$k = 0.543 \text{ days}^{-1}$$

From equation 5.3

$$78.1 = L(1 - 0.579)$$

$$L = 185.632 \text{ ppm}$$

Efficiencies

To compare the results obtained using the method of differences (k = 0.543, L = 185.632) with the results appearing in page 33-14, vol 2 of reference 1 (k = 0.523, L = 188) these pairs of values are substituted in equation 2.3 to obtain computed values of the BOD corresponding to the method of differences and the method of moments, respectively. Afterwards, formula 5.1 is applied to obtain the respective variances. Table 5.2, below, shows the steps necessary to this object.

TABLE 5.2

EFFICIENCIES OF THE METHOD OF DIFFERENCES AND THE METHOD OF MOMENTS: BOD EQUATION

Data		Method of Differences			Method of Moments		
(1),x Observed	(2),y	(3),y' Computed	(4),(y-y') Error	(5),$(y-y')^2$ Sqd. Error	(6),y' Computed	(7),(y-y') Error	(8),$(y-y')^2$ Sqd. Error
0	0	0	0	0	0	0	0
1	82	78	14	196	77	15	225
2	112	123	-11	121	122	-10	100
3	153	149	4	16	149	4	16
4	163	164	-1	1	165	-2	4
5	176	174	2	4	174	2	4
Variance		-	-	338	-	-	349

Clearly, being the variance for the method of differences smaller than that obtained for the method of moments, proves the method of differences to be superior in the solution of this particular problem.

Analytical Solution: Method of Averages

To apply the quick method of solution described in section 1.3 to equation 4.6, we consider the groups of paired values (0,82), (82,112), (112,153), and (153,163), (163,176), which add up to (194,347) and (316,339) respectively. Substitution of these two pairs in equations 1.14 yields

$$347 = 3I + P(194)$$

$$339 = 2I + P(316)$$

from which

$$P = 0.577,\ I = 81.494$$

so that, from equation 5.2

$$0.577 = e^{-k};\ -k = \ln 0.577 = -0.550$$

$$k = 0.550\ \text{day}^{-1}$$

and, from equation 5.3

$$81.494 = L(1 - 0.577);\ L = 192.657\ \text{ppm}$$

Graphical Solution

To solve the problem we plot in arithmetic scale the values of "y" in the abscissas and the values of "$y_{x+\Delta x}$" in the ordinates, passing a line through the averages (102.0,137.2). Figure 5.1 shows the slope of the line to be P = 0.571 and the intercept I = 79.

Applying equation 5.2 we obtain

$$k = -\ln 0.571;\ k = 0.560\ \text{day}^{-1}$$

and, from equation 5.3

$$L = 79/(1 - 0.571);\ L = 184.149\ \text{ppm}$$

Summary of Results

Comparison of the results obtained by the different methods used to solve this problem appears below, the numbers rounded off to the third figure.

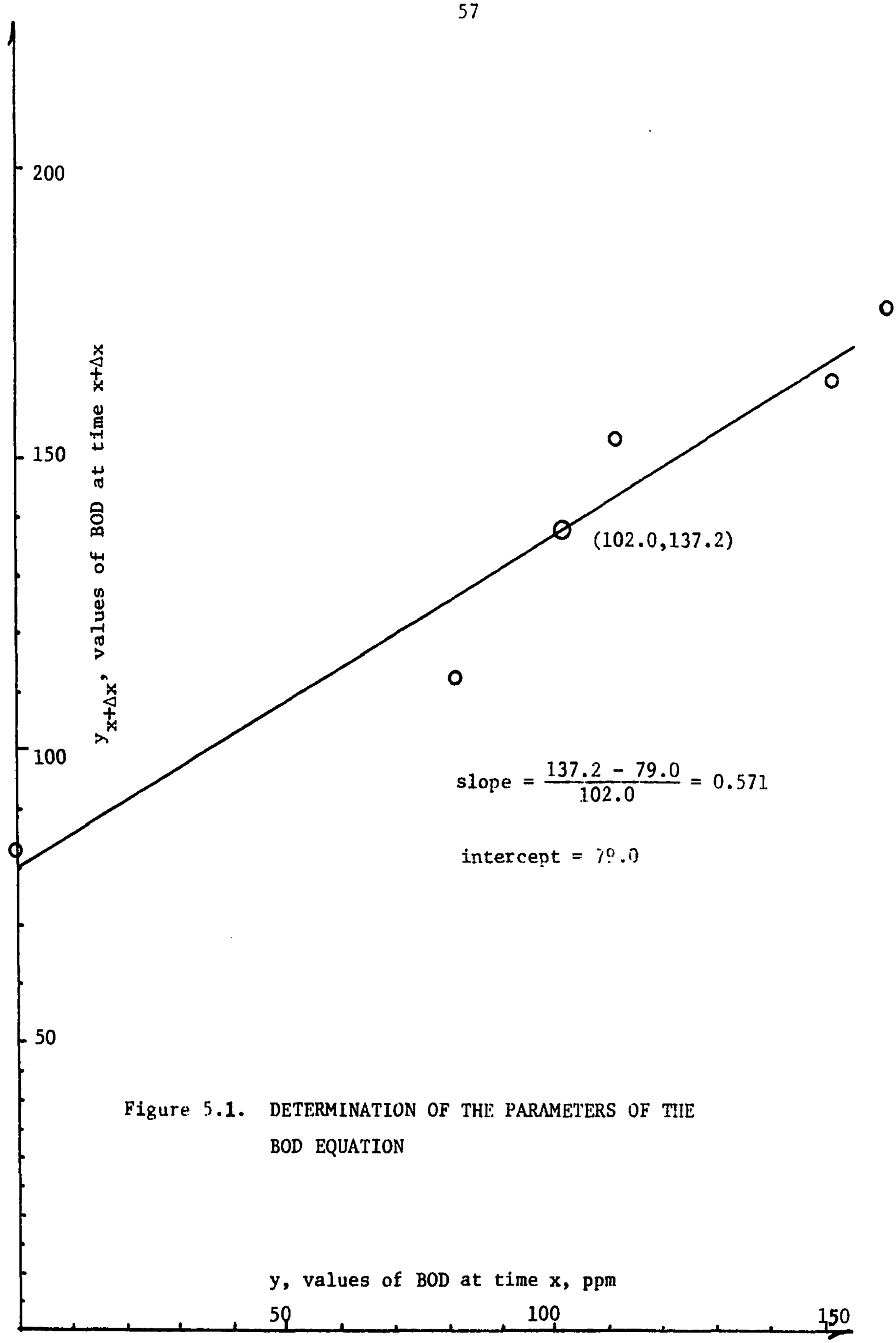


Figure 5.1. DETERMINATION OF THE PARAMETERS OF THE BOD EQUATION

Method	k, day^{-1}	L,ppm
Differences	-	-
Graphical	0.560	184
Averages	0.550	193
Least Squares	0.543	186
Moments	0.523	188

Stabilization of New Reservoirs

During fifteen years after filling, the color of the water in a large reservoir, that flooded extensive swamps that were not stripped, was measured. Use the data given in columns 1 and 2 of Table 5.3 to determine the values of the parameters "k" and "L" in equation 2.8.

TABLE 5.3

SOLUTION OF THE STABILIZATION OF NEW RESERVOIRS EQUATION

Data Columns		Computation Columns		
Time, years (1), x	Color, ppm (2), y	Plotting time (3),x	(4),y_x	(5),$y_{x+\Delta x}$
1	130	1	130	95
2	108	3	95	76
4	80	5	76	64
6	62	7	64	58
8	66	9	58	53
10	69	11	53	49
12	51	13	49	46
14	48	15	46	
15	52			
Summations			525	441
Averages			75	63

Graphical Method

With the data in columns 1 and 2, Table 5.3, figure 5.2A is drawn; this is done with the purpose of simplifying the drawing of figure 5.2B, since the original data (plotted using circles in both figures) show irregularities not corresponding to a smooth curve. Choosing $\Delta x = 2$, the plotting values of "y_x," at time "x," are read directly from the data curve, and entered in columns 3 and 4. Column 5 of Table 5.3 is obtained by shifting the values in column 4 one row up.

Passing a straight line through the points $(y_x, y_{x+\Delta x})$, Figure 5.2B, and measuring the slope and intercept we obtain

$$P = 0.585; \; I = 19 \text{ ppm}$$

so that, applying equations 5.2 and 5.3 we obtain

$$-2k = \ln 0.585; \; k = 0.268 \text{ year}^{-1}$$

$$L = \frac{1}{1 - 0.585}; \; L = 45.783 \text{ ppm}$$

Efficiency

To compare the variances of the results obtained when applying the graphical method of differences ($k = 0.268$ year^{-1}, $L = 45.783$ ppm) with those given in page 237 of reference 2, ($k = 0.156$ year, $L = 32$ ppm), both sets of parameters are used to recompute the original data applying equation 2.8. Notice that the variance resulting from the use of the method of differences is smaller than that corresponding to the application of the traditional trial and error method.

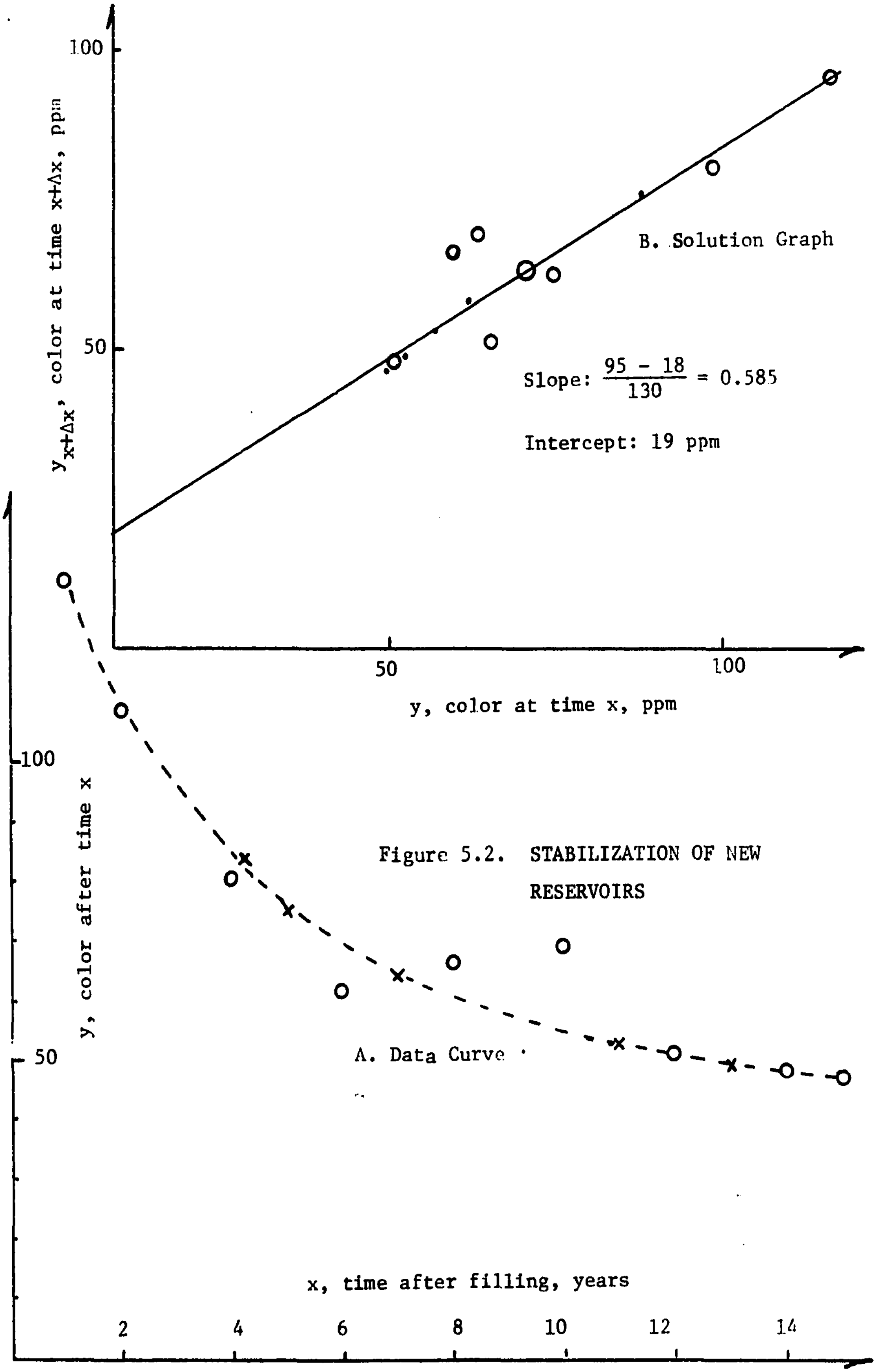


Figure 5.2. STABILIZATION OF NEW RESERVOIRS

TABLE 5.4

EFFICIENCIES OF THE METHOD OF DIFFERENCES AND THE TRIAL AND ERROR METHOD IN THE SOLUTION OF THE STABILIZATION OF NEW RESERVOIRS EQUATION

Data		Method of Differences			Trial and Error Method		
x,time (1)	y,color (2)	y' (3) comp.	(y-y') (4) error	$(y-y')^2$ (5) error sqd	y' (6) comp.	(y-y') (7) error	$(y-y')^2$ error sqd
1	130	130.0	0	0	130.0	0	0
2	108	110.2	-2.2	4.84	115.8	-7.7	59.29
4	80	83.5	-3.5	12.25	93.4	-13.4	179.56
6	62	67.8	-5.8	33.64	76.9	-14.9	222.01
8	66	58.6	+7.4	54.76	64.9	+1.1	1.21
10	69	53.3	+15.7	246.49	56.1	+12.9	166.41
12	51	50.2	-0.8	0.64	49.6	+1.4	1.96
14	48	48.4	-0.4	0.16	44.9	+3.1	9.61
15	52	47.8	+4.2	17.64	43.0	+9.0	81.00
Variances				370.42			721.05

5.4 Second Order Reaction Equation

Autocatalytic Equation

Gas production data from anaerobic decomposition of sludge from a sewage treatment plant, given as percentages of the saturation value "L," are shown in columns 1 and 2 of the table below. Estimate the values of the constants "k_1" and "k_2" of the autocatalytic equation 2.10.

TABLE 5.5

COMPUTATIONS FOR THE SOLUTION OF THE AUTOCATALYTIC EQUATION: ALGEBRAIC METHOD

Data Columns		Computation Columns	
x, time (1), days	y, gas prod. (2), % of "L"	$y_{x+\Delta x}$ (3)	$y \cdot y_{x+\Delta x}$ (4)
0	0	29	0
20	29	86	2494
40	86		

Algebraic Method

From equation 4.15, rearranging terms we obtain:

$$k_2 = \frac{a(L - y_{x+\Delta x}) + (y - L)}{a(y\, y_{x+\Delta x} - Ly) + (Ly_{x+\Delta x} - y\, y_{x+\Delta x})}\, k_1 \tag{5.4}$$

At point $(0, y_{x+\Delta x}, 0)$ this equation becomes

$$k_2 = \frac{a(L - y_{0+\Delta x}) - L}{L\, y_{0+\Delta x}}\, k_1; \tag{5.5}$$

Solution of the simultaneous equations 5.4 and 5.5, allows "a" to be determined.

Combination of equation 5.5 with equation 4.14 to eliminate "k_2" yields.

$$k_1 = \frac{y_{0+\Delta x} \ln a}{x(a-1)(L-y_{0+\Delta x})} \tag{5.6}$$

Once "a" and "k_1" have been determined, "k_2" may be found substituting these values in 5.5 or in equation 4.14, to obtain

$$k_2 = \frac{\ln a - k_1 \Delta x}{\Delta x\, L} \tag{5.7}$$

Applying equations 5.4 and 5.5 to the data in Table 5.5, we obtain the two simultaneous equations

$$k_2 = \frac{71a - 100}{2900} k_1; \; k_2 = \frac{14a - 71}{-406a + 6106} k_1$$

Dividing side by side and rearranging yields

$$a^2 - 15.039a + 14.039 = 0$$

which has roots 1 and 14.039. Since "ln a" has to be positive:

$$a = 14.039$$

Applying equation 5.6, we obtain

$$k_1 = \frac{29 \ln 14.039}{(20)(13.039)(100-29)}$$

$$k_1 = 0.004137$$

and from equation 5.7

$$k_2 = \frac{\ln 14.039 - 0.004137(20)}{20(100)}$$

$$k_2 = 0.0012$$

Efficiency

To compare the results from the application of the method of differences with the results given in page 36-31 of reference 1, corresponding to the assumption that the data follow a logistic curve (and therefore $k_1 = 0$), we apply the parameters found with the method of differences to the autocatalytic equation 2.10. The results from the logistic approximation are read graphically from Figure 36-12, reference 1, because there is an obvious mistake in the algebraic results reported in such reference. Notice that the variance from the method of differences is smaller than the variance for the logistic approximation.

TABLE 5.6

EFFICIENCIES OF THE METHODS OF DIFFERENCES AND LOGISTIC APPROXIMATION IN THE SOLUTION OF THE AUTOCATALYTIC EQUATION

Data		Method of Differences			Logistic Approximation		
(1),y	(2),x	(3),x'	(4),(x'-x)	(5),$(x'-x)^2$	(5),x'[1]	(6),(x'-x)	(7),$(x'-x)^2$
Observed		Comp.	Error	Error Sqd.	Comp.	Error	Error Sqd.
5	6	7	1	1	10	5	25
29	20	20	0	0	19	-1	1
68	30	32	2	4	29	-1	1
86	40	40	0	0	39	-1	1
Variances		-	-	5	-	-	28

[1] Results read graphically. Page 36-30, reference 1.

5.5 Logistic Equation

Rounded values of the population of Miami, Florida, are given in the first two columns of Table 5.7 below. Estimate the values of the parameters of the logistic equation 2.12.

TABLE 5.7

COMPUTATIONS FOR THE SOLUTION OF THE LOGISTIC EQUATION

Data Columns			Computation Columns		
	(1), x time, years	(2), y = X pop., tho's.	(3), $y/y_{x+\Delta x}$ $= Y$	(4), XY	(5), X^2
	1920	30.0	0.270	8.108	900.0
	1930	111.0	0.645	71.634	12321.0
	1940	172.0	0.691	118.811	29584.0
	1950	249.0	0.853	212.332	62001.0
	1960	292.0	-	-	-
Σ	7740	562.0	2.459	410.885	104806.0

Analytical Method: Least Squares

Column 3 figures are obtained dividing each data in column 2 by the following term in the column (e.g., 30/111 = 0.270). The terms of columns 4 and 5 are obtained as indicated in the respective headings.

From equation 4.1 we find that the intercept of the differences straight line is

$$I = e^{a\Delta x} \tag{5.8}$$

and its slope

$$P = \frac{1 - I}{L} \tag{5.9}$$

Applying equations 1.13, we find

$$P = \frac{4(410.885) - (562)(2.459)}{4(104806) - (562)^2} = 2.5302 \times 10^{-3}$$

$$I = \frac{2.459}{4} - 2.5302(\frac{562}{4}) = 0.25926$$

So that, from equation 5.8, since $\Delta x = 10$

$$a = \frac{\ln 0.25926}{10}; \; a = -0.135 \text{ year}^{-1}$$

and, from equation 5.9

$$L = \frac{1 - 0.2596}{2.5302 \times 10^{-3}}; \; L = 292.625 \; 10^3 \text{ inhab.}$$

The value of "m" is estimated considering that the averages of "x" and "y" satisfy equation 4.17, to have

$$m = \frac{nL - \Sigma y}{\Sigma y} e^{-\frac{a}{n}\Sigma x} \tag{5.10}$$

Then:

$$m = \frac{4(292.625) - 562}{562} e^{0.135(7740)/4}$$

$$m = 1.083 \; e^{0.135(1935)}$$

Efficiencies

Table 5.8 gives the computations necessary to obtain the variances of the results obtained from the application of the method of differences ($a = -0.135$ year^{-1}, $L = 292.625 \; 10^3$ inhabitants), and the results shown in page 5.9 of reference 1 ($a = -0.122$, $L = 313.000 \; 10^3$ inhabitants).

TABLE 5.8

EFFICIENCIES FOR THE METHOD OF DIFFERENCES AND THE METHOD OF VERHULST IN THE SOLUTION OF THE LOGISTIC EQUATION

Data		Method of Differences			Method of Verhulst		
(1),x Observed	(2),y Observed	(3),y' Comp.	(4),(y-y') Error	(5),$(y-y')^2$ Error Sqd.	(6),y' Comp.	(7),(y-y') Error	(8),$(y-y')^2$ Error Sqd.
20	30.0	32	-2	4	30	0	0
30	111.0	94	17	289	83	28	784
40	172.0	189	-17	289	172	0	0
50	249.0	256	-7	49	252	-3	9
60	292.0	282	10	100	292	0	0
Variance		-	-	731	-	-	793

Observe that the results obtained by the traditional method are misleading, since in this problem there are only four data points. The three points chosen as a basis to compute "L" have to agree with the observed data; however, the method of differences proves to be superior, since its variance is the smallest.

Analytical Method: Averages

Dividing the data in columns 2 and 3, Table 5.7, in two groups, adding and applying equations 1.14, we obtain

$$0.915 = 2I + 141P$$

$$1.544 = 2I + 421P$$

which solved simultaneously, yield

$$P = 2.246 \times 10^{-3}$$

$$I = 0.299157$$

Substitution in equations 5.8 and 5.9 yields

$$a = \frac{\ln 0.299}{10}; \; a = -0.1207 \text{ year}^{-1}$$

$$L = \frac{1 - 0.299}{2.246 \times 10^{-3}}; \; L = 312.110 \; 10^{3} \text{ inhab.}$$

Observe that although this solution agrees with the results from the traditional method, it is obviously less accurate than the solution obtained using the least squares method.

From equation 5.10

$$m = \frac{4(312.110) - 562}{562} e^{0.1207(1935)}$$

$$m = 1.221 \; e^{0.1207(1935)}$$

Graphical Method

Figure 5.3 is a graph obtained from plotting the values of $y/y_{x+\Delta x}$ against "y," using arithmetic scales. Direct measurements of the intercept and slope of the line crossing the averages yield

$$P = 2.133 \times 10^{-3}$$

$$I = 0.290$$

Applying equations 5.8 and 5.9 gives:

$$a = \frac{\ln 0.290}{10}; \; a = -0.124 \text{ year}^{-1}$$

$$L = \frac{1 - 0.290}{2.133 \times 10^{-3}}; \; L = 332.864 \; 10^{3} \text{ inhab}$$

and, from equation 5.10

$$m = \frac{4(332.864) - 562}{562} e^{0.124(1935)}$$

$$m = 1.369 \; e^{0.124(1935)}$$

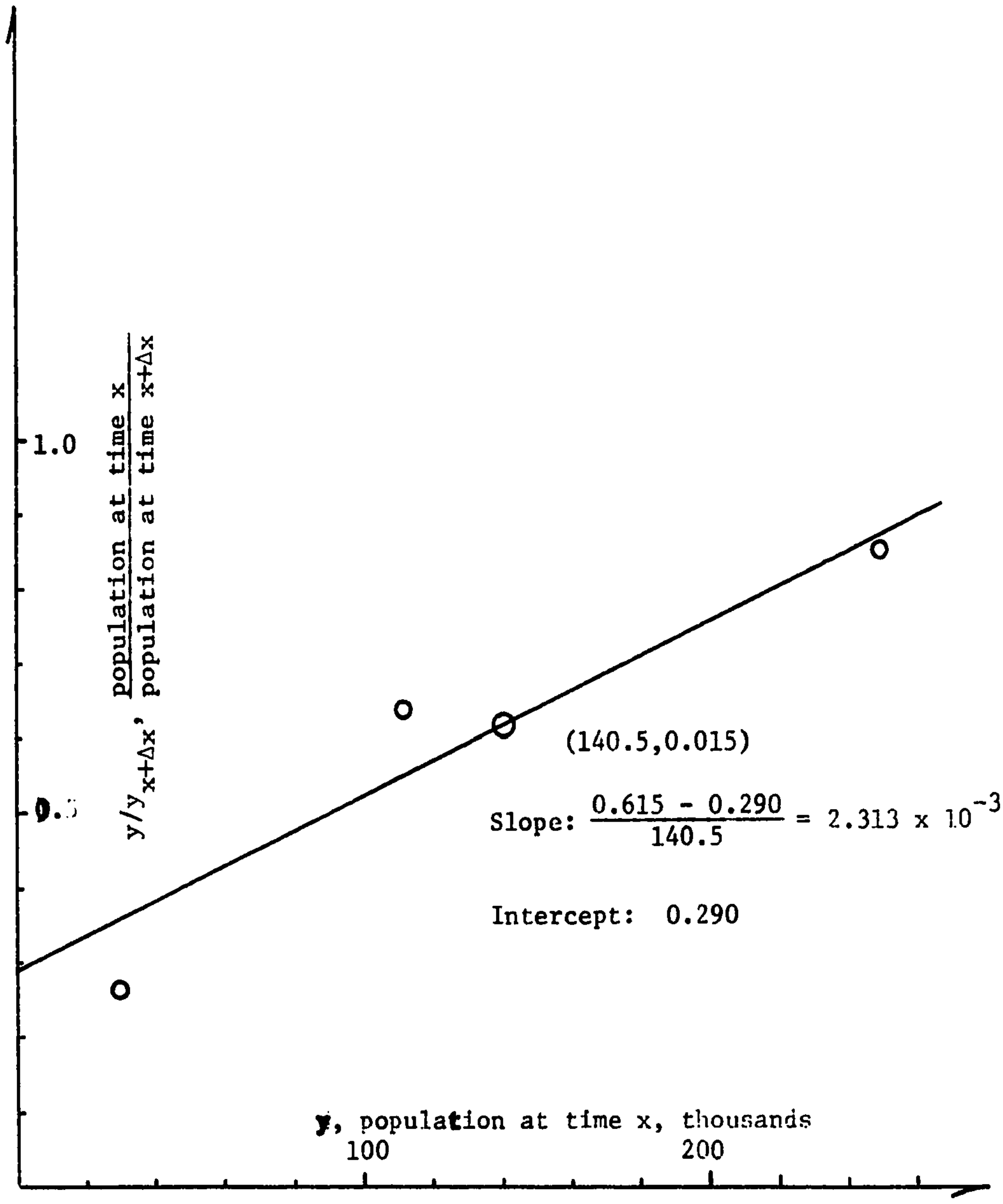


Figure 5.3. DETERMINATION OF THE PARAMETERS OF THE LOGISTIC EQUATION

Summary of Results

Method of Differences	a, year^{-1}	L, 10^3 inh.
Graphical	-0.124	332.864
Analytical Averages	-0.127	312.110
Analytical Least Squares	-0.135	292.625
Method of Verhulst	-0.122	313.000

5.6 Rate of Purification Equation

The observed BOD removal for a trickling filter operated at a rate of 4.5 mgd was as follows

Depth, x (ft)	0	2	4	6	10
BOD remaining, z (ppm)	85	39	19	10	8

Find the values of the parameters "k" and "n" in equation 2.15.

To solve this problem, the linear form 4.24 is used.

From equation 4.23, choosing a = -0.4, we obtain

$$z_{(1+a)x} = z_x(1+a); \; z_{0.6x} = 0.6z_x$$

Taking z_0 = 85 ppm as base value, the sequence of z_x values appearing in column 1 of the following table is obtained (51 = 85 x 0.6, 30.6 = 51 x 0.6, ...)

(1), z_x	(2), x_z	(3), $x_{0.6z}$
85.0	0.0	1.2
51.0	1.2	2.7
30.6	2.7	4.1
18.4	4.1	5.8
11.0	5.8	
Σ	8.0	13.8

To determine the time values at which the BOD remaining is z_x, Figure 5.4A has been drawn plotting the data pairs x,z. Notice that the last data (10,8) has been corrected to be (10,4). The values of x_z are found by interpolating directly in the curve, and are entered in column 2 of the table above. The values in column 3 are the values in column 2 transfered one row up.

Figure 5.4B was drawn by plotting the values of $x_{0.6z}$ against the values of x_z, using arithmetic scales. Measuring the slope and intercept of this line yields

$$P = 1.0975; \; I = 1.255 \text{ ft}$$

From equation 4.24

$$n = -\frac{\ln P}{\ln (a+1)} \tag{5.11}$$

$$k = \frac{P - 1}{nI} \tag{5.12}$$

So that, substituting the values of "P" and "I" in equations 5.11 and 5.12, we obtain, respectively

$$n = -\frac{\ln 1.0975}{\ln 0.6} = \frac{0.093}{0.511} \qquad n = 0.18199$$

$$k = \frac{1.0975 - 1}{1.2555(0.18199)} \qquad k = 0.4269 \text{ ft}^{-1}$$

Efficiencies

The following table shows the errors in the values of the BOD remaining, "z_x," after application of the parameters obtained by the method of differences (n = 0.182, k = 0.427) and after the application of the parameters reported in page 730, reference 2, corresponding to the trial and error method (n = 0.5, k - 0.53). Notice that the variance is smaller for the method of differences even in the case in which the

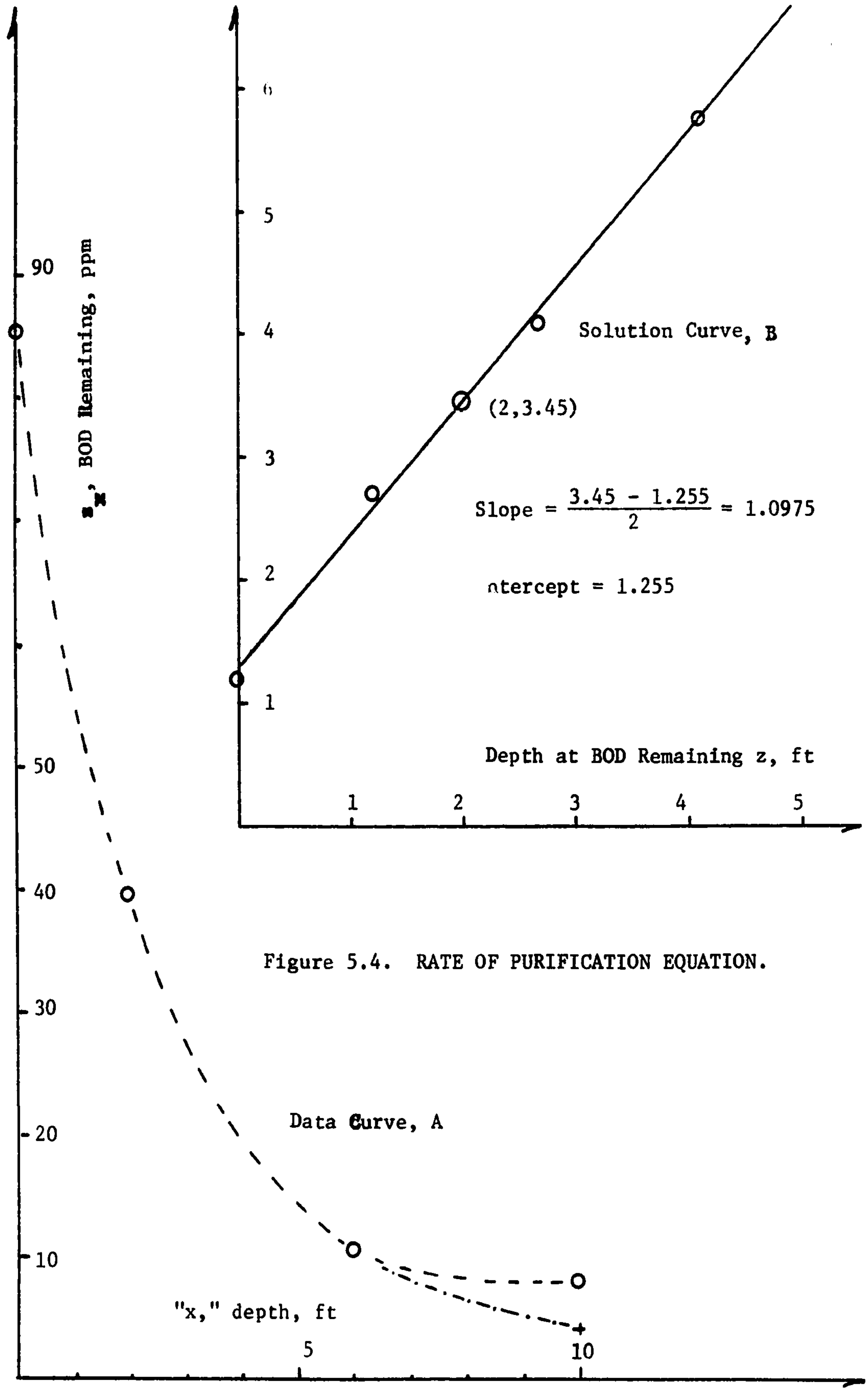


Figure 5.4. RATE OF PURIFICATION EQUATION.

last data are not corrected.

TABLE 5.9

EFFICIENCIES OF THE METHODS OF DIFFERENCES AND TRIAL AND ERROR IN THE SOLUTION OF THE RATE OF PURIFICATION EQUATION

Observed Data		Method of Differences			Trial and Error Method		
(1),x	(2),z	(3),z' Comp.	(4),(z'-z) Error	(5),$(z-z')^2$ Error Sqd.	(6),z' Comp.	(7),(z'-z) Error	(8),$(z'-z)^2$ Error Sqd.
0	85	85	0	0	85	0	0
2	39	38	-1	1	36	-3	9
4	19	19	0	0	20	1	1
6	10	10	0	0	13	3	9
10	4,(8)[1]	4	0,(-4)	0,(16)	6	2,(-2)	4,(4)
Variance				1,(17)			23,(23)

(1)Figures in parentheses correspond to datum without correction.

5.7 Molecular Diffusion Equation

Salt water containing 5850 ppm of sodium chloride lies beneath a 1 ft lens of fresh water which is essentially salt free. After contact between layers, the originally salt free layer shows at 20 days 1000 ppm of sodium chloride, and 2816 ppm after 180 days. Determine the value of the diffusion constant k.

To solve this problem we use equations 4.28 and 4.29. Since c_s = 5850 ppm, c_0 = 0 ppm, and 180 days = 9(20)days , we obtain, from equation 4.28:

$$y_{20} = \frac{1000 - 5850}{-0.811(5850)}; \; y_{20} = 1.02206$$

$$\frac{1}{9}\, y_{9x20} = \frac{2816 - 5850}{-0.811(5850)};\ \frac{1}{9}\, y_{9x20} = 0.07106$$

and from equation 4.29

$$e^{-K(20)} = y_{20} - \frac{1}{9}\, y_{9x20} = 0.951$$

$$-K = \frac{\ln 0.951}{20} = \frac{-0.050}{20}$$

$$K = 2.5 \times 10^{-3} \text{ day}^{-1}$$

Finally, applying equation 2.19

$$k = \frac{K41^2}{\Pi^2};\ k = \frac{2.5 \times 10^{-3}(4)(1)^2}{\Pi^2}\,\frac{ft^2}{day}\,\frac{30.48^2\ cm^2}{ft^2}$$

$$k = 0.94 \text{ cm}^2/\text{day}$$

which is the same value than that shown in page 23-6 of reference 1.

Notice that data for this problem have been obtained from the results of the problem shown in the reference, and that to find the value of "k," if not using the method of differences, one would have to find it by trial and error.

5.8 Theis Equation

The values of the drawdown in an observation well 200 ft apart from a well being pumped at a rate of 500 gal/min, appear in the first two columns of Table 5.10. Determine the formation constants of the aquifer.

TABLE 5.10

COMPUTATIONS FOR THE SOLUTION OF THEIS' EQUATION

Data Columns		Computation Columns			
time, min. (1), x	drawdown, ft. (2), (h_0-h), y	(3), $\frac{1}{x}$ =X	(4), Δy=Y	(5), XY	(6), X^2
1	0.66	1	0.33	0.33	1
2	0.99	0.5	0.37	0.185	0.25
4	1.36	0.25	0.39	0.0975	0.0625
8	1.75		0.39		
16	2.14		0.38		
32	2.52				
3	1.21	0.333	0.38	0.1267	0.1111
6	1.59				
	Σ	2.0833	1.47	0.7392	1.4236

Analytic Method: Least Squares

Column 4 shows the increments of the data listed in Column 3 (0.99 - 0.66 = 0.33). Observe that after x = 4 min., the increments in the drawdown tend to decrease; this is impossible because Δy is an increasing function of "x" (equation 4.43). Obviously, after x = 8, the data do not show the precision required to yield any useful information to determine parameters using the method of differences; therefore, all the data after x = 8 min. are disregarded.

Applying equations 1.13, we obtain

$$P = \frac{4(0.7392) - 2.0833(1.47)}{4(1.4236) - (2.0833)^2}; \; P = -0.780 \text{ ft-min}$$

$$I = \frac{1.47}{4} + (0.0780)\frac{2.0833}{4};\ I = 0.40812 \text{ ft}$$

Combining equations 4.44, 4.38 and 4.39 yields

$$T = 0.055\ \frac{Q}{I} \tag{5.13}$$

$$S = -5.544\ \frac{PT}{Ir^2} \tag{5.14}$$

so that

$$T = 0.055\ \frac{500}{0.40812}\ \frac{\text{gal.}}{\text{min. ft.}}\ \frac{24(60)\text{min.}}{\text{day}}$$

$$T = 97030.285\ \frac{\text{gal}}{\text{ft-day}}$$

$$S = 5.544\ \frac{97030.285(0.078)}{(0.40812)(200)^2}\ \frac{\text{ft-min}}{\text{ft-ft}^2}\ \frac{\text{ft-day}}{\text{gal}}\ \frac{\text{ft}^3}{7.48\ \text{gal}}\ \frac{\text{day}}{24(60)\text{min}}$$

$$S = 2.3862 \times 10^{-4}$$

Efficiencies

To compare the results obtained using the method of differences ($T = 97{,}030.285$ gal/ft-day, $S = 2.3862 \times 10^{-4}$), with the results from the application of the method of Theis appearing in page 92 of reference 3 ($T = 103000$ gal/ft-day, $S = 1.98 \times 10^{-4}$), both pairs of parameters were used in formula 2.22. The values of the parentheses in this formula were computed by interpolation in Table 4.1 of the same reference. The errors and variances corresponding to both methods appear in the following table. Observe that the method of differences shows the smallest variance.

TABLE 5.11

EFFICIENCIES FOR THE APPLICATION OF THE METHODS OF DIFFERENCES AND SUPERPOSITION OF CURVES IN THE SOLUTION OF THEIS EQUATION

Data		Method of Differences			Method of Theis		
(1), x	(2), y Observed	(3), y' Compd.	(4), y-y' Error	(5), $(y-y')^2$ Error Sqd.	(6), y' Compd.	(7), y-y' Error	(8), $(y-y')^2$ Error Sqd.
1	0.66	0.60	0.60	0.0036	0.85	-0.19	0.0361
2	0.99	0.96	0.03	0.0009	1.00	-0.01	0.0001
3	1.21	1.26	-0.05	0.0025	1.20	0.01	0.0001
4	1.36	1.30	0.06	0.0036	1.36	0.00	0.0000
8	1.75	1.70	0.05	0.0025	1.73	0.02	0.0004
16	2.14	2.12	0.02	0.0004	2.13	0.01	0.0001
32	2.51	2.50	0.01	0.0001	2.49	0.02	0.0004
64	2.91	2.91	0.00	0.0000	2.87	0.04	0.0016
Variances				0.0136			0.0388

Analytical Method: Averages

Considering equations 3.14, and the data from columns 3 and 4, Table 5.10, dividing the useful data in two groups, each containing two data, it is obtained:

$$0.70 = 2I + 1.5P$$

$$0.77 = 2I + 0.583P$$

from which

$$P = -0.0763 \text{ ft-min}$$

$$I = 0.4072 \text{ ft}$$

Applying equations 5.13 and 5.14

$$T = 0.055 \frac{500}{0.4072} \frac{\text{gal}}{\text{min ft}} \frac{60 \times 24 \text{ min}}{\text{day}}$$

$$T = 97{,}249.508 \text{ gal/day-ft}$$

$$S = +5.544 \frac{0.0763(97{,}249.508)}{0.4072(200)^2(7.48)(24)(60)} \frac{\text{ft-min}}{\text{ft}} \frac{\text{gal}}{\text{ft-day ft}^2} \frac{\text{ft}^3 \text{ day}}{\text{gal min}}$$

$$S = 2.224 \times 10^{-4}$$

Graphical Method

Figure 5.5 shows that,

$$S = 0.0795 \text{ ft-min}$$

$$I = 0.409 \text{ ft}$$

so that applying equations 5.13 and 5.14, we obtain

$$T = 0.055 \frac{500}{0.4072}(60)(24)$$

$$T = 97249.509 \frac{\text{gal}}{\text{ft-day}}$$

$$S = 5.544 \frac{0.0795(97{,}249.509)}{0.0409(200)^2(7.48)(24)(60)}$$

$$S = 2.4324 \times 10^{-4}$$

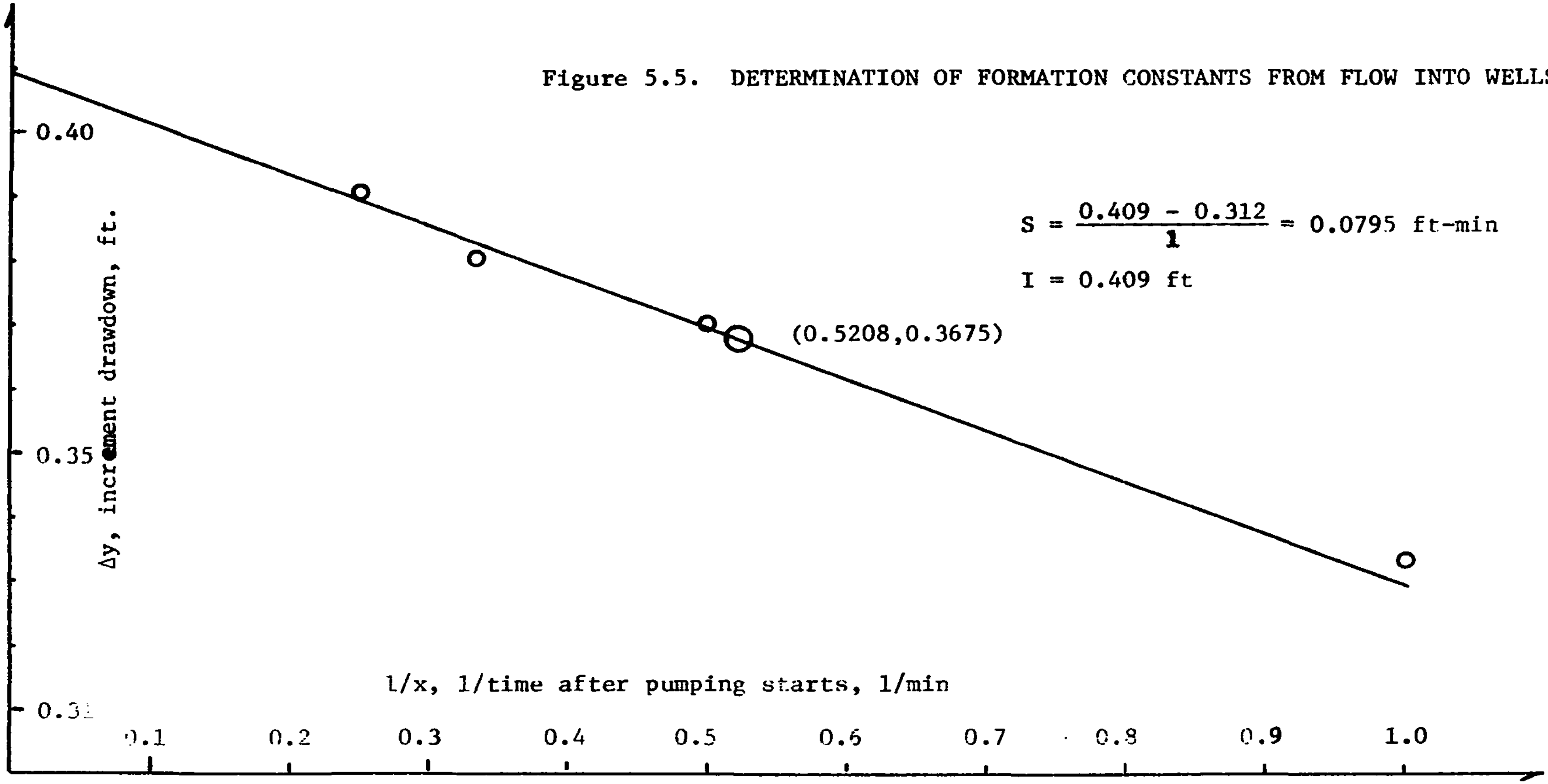
Summary of Results

Method of Differences	T,gal/day-ft	$S, 10^{-4}$
Graphical	97,248	2.4324
Analytical: Averages	97,250	2.2240
Analytical: Least Squares	97,030	2.3862
Theis Method	103,000	1.9800

5.9 Rainfall Equation

Intensity of storms data, recorded for New York City from 1869 to

Figure 5.5. DETERMINATION OF FORMATION CONSTANTS FROM FLOW INTO WELLS.



1913 are given in Figure 5.6, and also in the first two columns of Table 5.13. Determine the value of the parameters of the rainfall equation 2.24.

Graphic Solution

From equation 4.46, the linear form of the rainfall equation, we obtain:

$$P = (1 + k)^{-\frac{1}{n}}; \; n = -\frac{\ln(1 + k)}{\ln P} \tag{5.15}$$

$$I = d(P - 1); \; d = \frac{I}{P - 1} \tag{5.16}$$

Since $k = \Delta i/i$; $1 + k = i_{x+\Delta x}/i_x$, so that choosing $k = -0.2$, yields

$$\frac{i_{x+\Delta x}}{i_x} = 0.8$$

Starting with the first data of the graph intensity vs duration, Figure 5.6A, one obtains the set of "i_x" values shown in column 1 of Table 5.12A (6.50 x 0.8 = 5.20; 5.20 x 0.8 = 4.16). The "x" values in column 2 are obtained by direct reading in the same graph. Notice that this procedure yields better results than the use of arithmetic interpolation, due to the curvature of the graph.

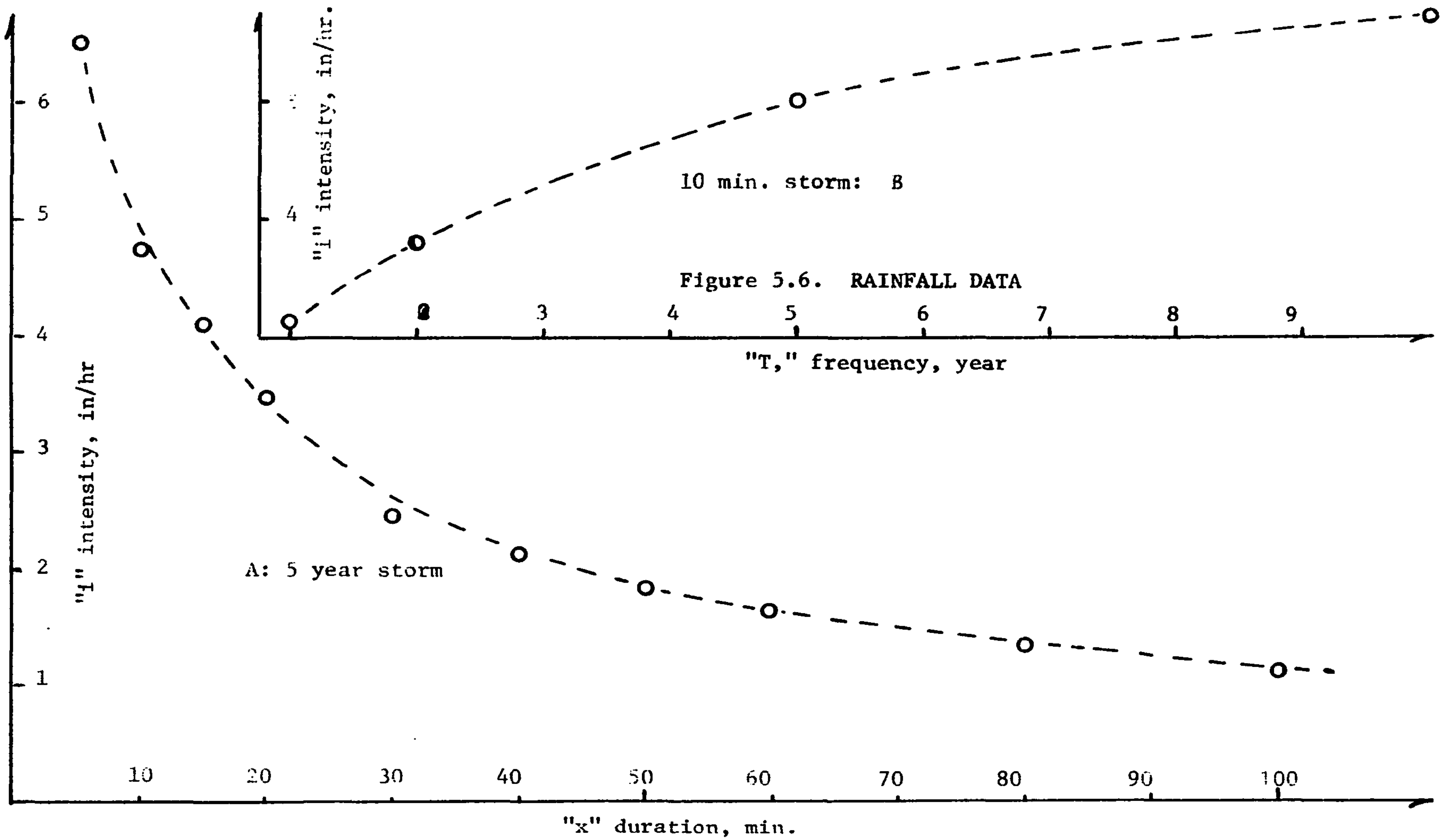


Figure 5.6. RAINFALL DATA

TABLE 5.12

COMPUTATIONS FOR THE SOLUTION OF THE RAINFALL EQUATION

A: Data to Determine "n" and "d"			B: Data to Determine "m"		
Rainfall Intensity in/hr (1), i_x	Time Elapsed min. (2), $x_i = X$	$Y = x_{i(1+k)}$ (3)	Frequency of Rainfall Year (1), T_i	Intensity of Rainfall in/hr (2), $i_T = X$	$Y = i_{T(1+k)}$ (3)
6.50	5.0	9.0	10.0	5.75	
			8.0	5.50	5.75
5.20	9.0	14.0	6.4	5.30	5.50
4.16	14.0	20.5	5.12	5.05	5.30
			4.096	4.75	5.05
3.33	20.5	28.5	3.276	4.44	4.75
2.66	28.5	39.5	2.62	4.15	4.44
			2.097	3.85	4.15
2.13	39.5	58.0	1.678	3.62	3.85
1.70	58.0	80.0	1.342	3.37	3.62
1.36	80.0	101.0	1.073	3.20	3.37
1.09	101.6				
	254.5	350.5		43.23	45.78

The values in column 3 are obtained displacing column 2 one row up. The values of Y vs X from Table 5.12A appear plotted in Figure 5.7, from which we obtain

$$P = 1.28, \; I = 2.6 \text{ min}$$

Substitution of these values in equation 5.15 and 5.16 yield, respectively

$$n = -\frac{\ln 0.8}{\ln 1.28} = \frac{0.22314}{0.24686}; \; n = 0.90392$$

$$d = \frac{2.6}{1.28 - 1} = \frac{2.6}{0.28}; \; d = 9.2857$$

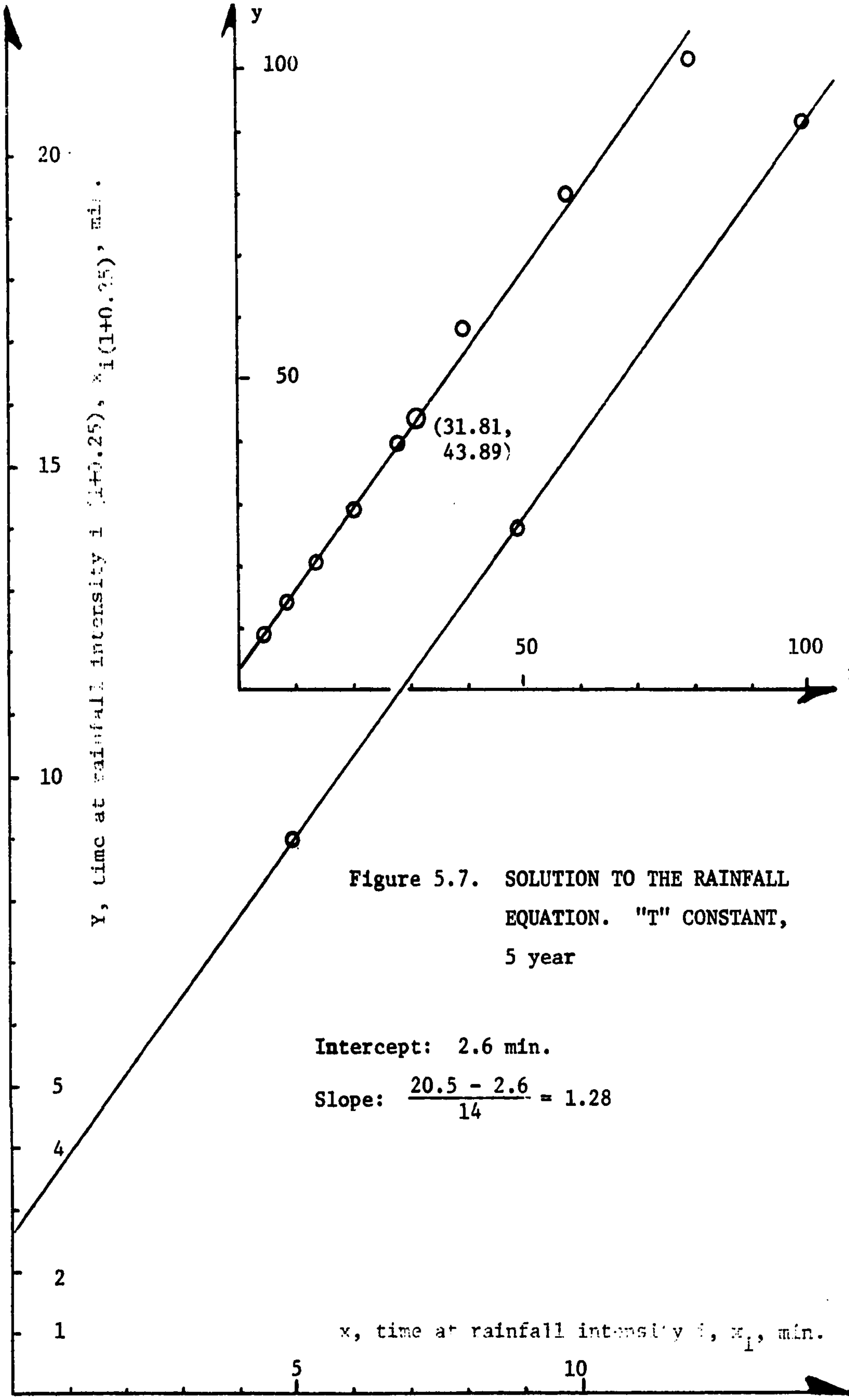


Figure 5.7. SOLUTION TO THE RAINFALL EQUATION. "T" CONSTANT, 5 year

Intercept: 2.6 min.

Slope: $\frac{20.5 - 2.6}{14} = 1.28$

To determine the value of the parameter "m," we use the linear form 4.52, where

$$P = (1 + k)^m; \; m = \frac{\ln P}{\ln (1+k)} \qquad (5.17)$$

Choosing k = 0.25,

$$\frac{i_{(1+0.25)T}}{i_T} = 1.25$$

Starting with the last data of the frequency vs. intensity graph we obtain the set of "T" values shown in column 1, Table 5.12B (10/1.25 = 8; 8/1.25 = 6.4, ...). The values in column 2 are obtained by direct reading from the same graph. Column 3 presents the same values that column 2, displaced one row down.

The values in columns 2 and 3 are plotted in Figure 5.8, from which we obtain

$$P = 1.06$$

so that substitution in equation 5.17 yields

$$m = \frac{\ln 1.06}{\ln 1.25} = \frac{0.05827}{0.22314}; \; m = 0.26113$$

Finally, the value of the scale factor "c," is computed from equation 2.24 using the base values i = 5 in/hr, T = 5 year, x = 10 min.

$$c = \frac{i(x+d)^n}{T^m} \qquad (5.18)$$

$$c = \frac{5(10+9.2857)^{0.90393}}{5^{0.26113}}; \; c = 47.666$$

Efficiencies

Table 5.13 shows the results obtained when applying the rainfall equation 2.24, considering the values of the parameters obtained by

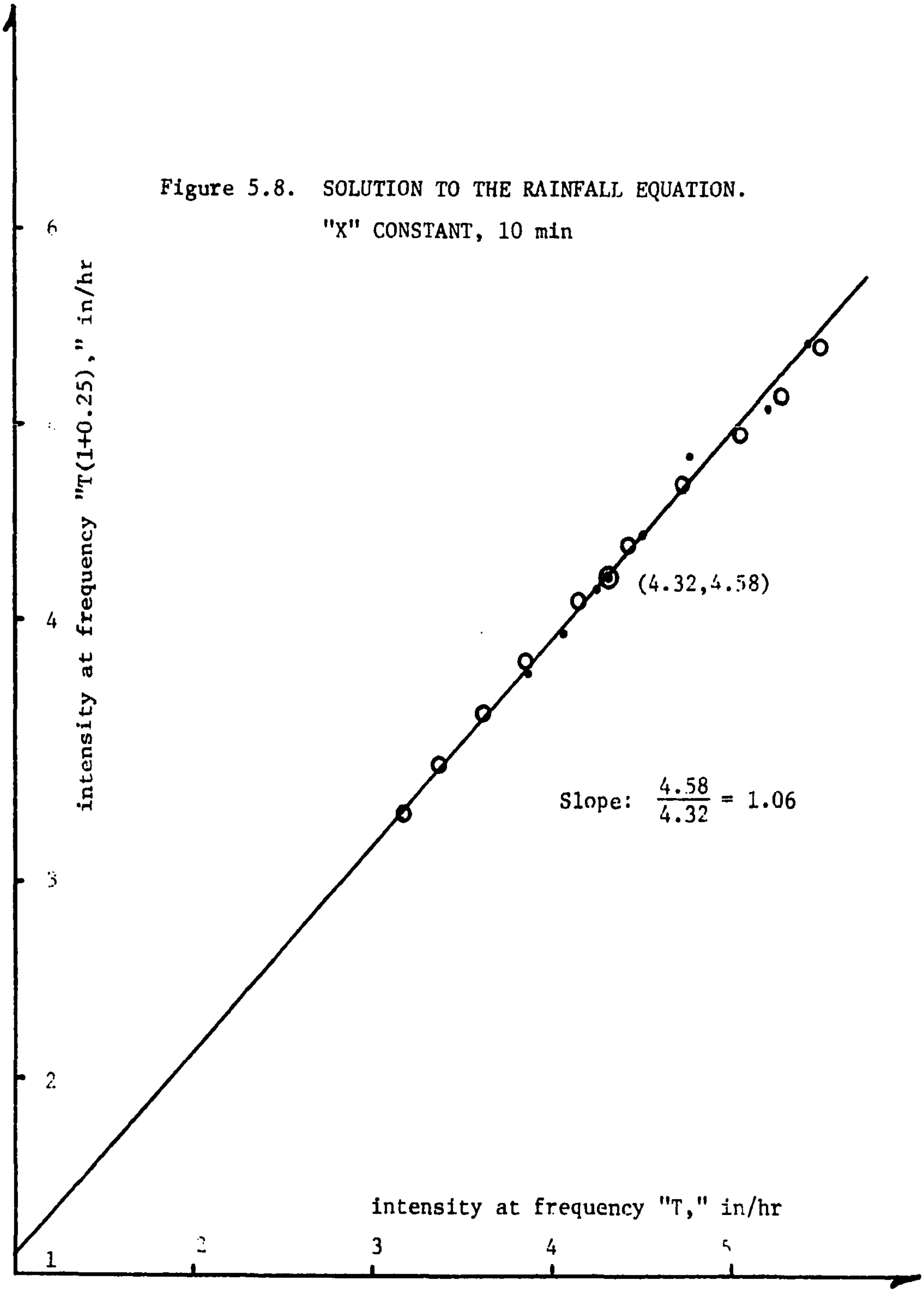


Figure 5.8. SOLUTION TO THE RAINFALL EQUATION.
"X" CONSTANT, 10 min

applying the method of differences graphically (n = 0.9039, d = 9.2857, m = 0.2611, c = 47.6666) and considering the values of the parameters obtained from the application of the traditional trial and error graphical method, pages 7-9, reference 1 (n = 0.66, d = 2, m = 0.31, c = 16). Notice that the variance of the method of difference is smaller than the variance shown by the traditional method.

Obviously, in this particular problem the application of least squares to the method of differences would be superfluous, since the data for the solution given here have been obtained graphically and the data used in the reference shown above were obtained by linear interpolation.

TABLE 5.13

EFFICIENCIES FOR THE METHODS OF DIFFERENCES AND TRIAL AND ERROR IN THE SOLUTION OF THE RAINFALL EQUATION

Data [(1)]		Method of Differences			Traditional Method		
(1), x min	(2), i=y in/hr	(3), y'	(4), y-y'	(5), $(y-y')^2$	(6), y'	(7), y-y'	(8), $(y-y')^2$
Observed		Comp.	Error	Error Sqd.	Comp.	Error	Error Sqd.
5	6.50	6.56	-0.06	0.0036	7.30	-0.20	0.6400
10	5.00[(2)]	5.00	0	0	5.11	-0.11	0.0121
15	4.14	4.06	0.08	0.0064	4.06	0.08	0.0064
20	3.50	3.43	0.07	0.0049	3.43	0.07	0.0049
30	2.46	2.63	-0.17	0.0289	2.68	-0.22	0.0484
40	2.17	2.14	0.03	0.0009	2.24	-0.07	0.0049
50	1.88	1.81	0.07	0.0049	1.94	-0.06	0.0036
60	1.66	1.57	0.09	0.0081	1.73	-0.07	0.0049
80	1.36	1.25	0.11	0.0121	1.44	-0.08	0.0064
100	1.11	1.04	-0.07	0.0049	1.24	-0.13	0.0169
Variance		-	-	0.0698	-	-	0.7485

[(1)] Appearing in reference 1, pages 7-8, corresponding to T = 5 yr.

[(2)] Corrected by graphical interpolation; real observed value is 4.75. If this value is considered, the variance in the traditional method is incremented more than the variance in the method of differences.

Summary of Results

Parameter	Method of Differences	Traditional Method
n	0.9039	0.66
d	9.2857	2.00
m	0.2611	0.31
c	47.6666	16

CHAPTER VI

DISCUSSION

6.1 Computational Advantages

The main advantages of the method of differences over the traditional methods used to estimate parameters in transcendental equations derive from the precision and simplicity of its mathematical basis, i.e., the concepts of increment and straight line, which allow for analytical, as well as graphical solutions using simple arithmetic scales.

The explicit form in which the parameters appear in the linear forms obtained in Chapter IV eliminates the necessity of guessing and the use of special graphs or tables, which make the traditional methods cumbersome, and in many cases unreliable. For instance, in solving the logistic equation to find the saturation and rate of growth parameters, a value of the saturation is first estimated from a set of equations satisfying only three points of the curve, and then a special "logistic scale" is used to plot the data, while in the case of the solution of the equation representing the stabilization of new reservoirs, pure trial and error is involved.

The linear forms obtained to solve transcendental equations allow complete freedom to select the method of solution of the particular straight line under consideration, as well as the method of computation. If high precision is desired the method of least squares may be used, if not, the method of averages may be applied, or a graphical solution obtained. If the number of data is such that the use of a computer is mandatory, any program to determine parameters of the multilinear model can be employed, since the method of differences is numerical in nature.

A definite advantage of the use of the method of differences results in the possibility of further application of the statistical theory to the estimators obtained by these means. For instance, confidence intervals could be easily obtained for the "k" value of a given sample of sewage when working on a BOD problem, or the saturation value "L" related to the growth of a certain population.

Also, it is interesting to point out that the general character of the method of differences overcomes the restrictions imposed by the traditional methods in regard to the system of physical units used in the solution of particular problems and the range of variation of the parameters involved. For instance, a "type graph" used in the determination of the formation constants of a given aquifer is drawn for definite units of the variables "u" and "W(u)," so that, if the data are given in a different system of units, the pertinent conversions have to be made previously to the solution of the problem under consideration. Also, in the case of stabilization of new reservoirs, although the model equation is the same as the BOD equation, the curves corresponding to the method of moments to solve the latter cannot be used to estimate the parameters of the stabilization equation, since the units in both problems are different and the ranges of the data and the parameters do not correspond in magnitude.

Summarizing, the computational advantages of the method of differences are the following:

--use of computers is possible

--simplicity and generality

--flexibility in selecting method to finally determine parameters in accordance to quality of data and precision desired

--possibility of further application of statistical theory to estimators of the parameters

--independence from physical units and range of parameters and data

--higher efficiency

6.2 Further advantages

The method of differences permits one, in many cases, to determine if a set of data corresponds to a preassigned model, especially in the cases involving two parameters. For instance, if a set of data pertaining to BOD determinations is plotted in accordance to the linear form 4.6, they should lay on a straight line. If this is not so, either the consumption of oxygen is not following the first order equation model, or the experimental procedures are not being carried out correctly. Since the data can be plotted from the beginning of the laboratory determinations, the method proposed provides a means to control the quality of such determinations.

A problem frequently found in engineering consists in determining how much data are necessary and over what period of time it should be collected in order to solve a particular problem. The first question depends on the precision desired for the solution and is dealt with by the statistical theory whose application is favored if the method of differences is used. The answer to the second question depends on the model itself, and on the accuracy of the systems used to obtain the data; for instance, if the method of differences is used to determine the formation constants of an aquifer, it becomes clear that the time limit to take measurements of the level of the drawdown curve corresponds to that on which the differences in between two consecutive measurements can be detected, in accordance to the precision of the system used to determine the drawdown levels. The time intervals in between measurements should not necessarily be constant, but follow instead the pattern dictated by the model itself, as indicated, in this case, in section 4.7. Obviously, data are more valuable where the curvature of a model changes faster because the percent errors in this area are smaller in between consecutive readings. The very common practice of trying to obtain data through long periods of time, besides being uneconomic, introduces error in the determination of the parameters.

Summarizing, further advantages of the method of differences are the following:

--permits one to determine if the data correspond to the model

--provides a way to control quality of laboratory results

--provides patterns to determine time sequences for the collection of data, resulting in economical savings

6.3 Level of Difficulty and Efficiency

In Chapter V of this thesis the sum of squared errors was taken as a measurement of the efficiency of the method of differences as compared with the applicable traditional methods of solution. In all the cases analyzed, the sum of squared errors is smaller for the method of differences, which constitutes an advantage from the standpoint of precision of the results. On the other hand, this fact would not be considered a real improvement if the level of difficulty in the application of the method of differences were greater than that corresponding to the traditional methods of solution.

To establish an index to measure the level of difficulty in the application of a certain method of solution to a particular problem, several factors should be considered:

--time and mathematical background required to understand and learn to use the method

--time spent and difficulties encountered in preparing special backing material as graphs and tables

--time of computation and nature of the computations involved in the actual application of the method to a particular problem

--time of drawing if the actual application is graphical.

The mathematical background required to understand the method of differences does not go beyond that which is normally thought of in a first course of analytic geometry, where the concepts of increment and equation of a straight line are first introduced. On the other hand, the traditional methods, other than the trial and error method, may require at least some knowledge of statistics, as is the case of the method of moments used to solve the first order reaction equation.

In regard to the time spent in preparing special graphs or tables to help in the solution of a particular problem, no requirements of this sort exist for the method of differences, unless the data are given in such a way that graphical or arithmetical interpolation becomes convenient. The nature of the computations involved in the method of differences is such that in most cases only the four elementary arithmetical operations are employed along the procedure of problem solution, and only in the last stage of the solution a natural, or if preferred a common, logarithm has to be taken. Obviously, this characteristic of the method of differences results in a substantial reduction in the time spent in computing operations, and diminishes the probability of incurring in errors during the process.

If the graphical solution of the straight line forms obtained by the method of differences is preferred, the time spent in plotting the straight line overcompensates for the time spent in computational operations while using analytical solutions. Evenmore, since drawing a straight line is a simple procedure, it is always helpful to gain some knowledge of the final results by solving a problem graphically, before the analytical solution is tried.

Since the first two factors listed before are difficult to evaluate, a level of difficulty index is here established based solely on the time employed in solving the problems presented in Chapter V of this thesis. A value of 4 for this index corresponds to the maximum difficulty, or more than 40 minutes employed to obtain the solution, an index value of 3 corresponds to time spent in between 20 and 30 minutes, and so on. The following table shows the levels of difficulty of the examples presented in Chapter V, in accordance with the methods employed in their solutions.

TABLE 6.1

LEVELS OF DIFFICULTY IN PROBLEMS SOLUTION WHEN USING THE METHOD OF DIFFERENCES AND THE TRADITIONAL METHODS

Equation	Method of Differences				Traditional Methods			
	Least Squares	Averages	Graphic	Direct	Trial and Error	Moments	Verhulst	Superposition
Chemical Second Order:								
Autocatalytic				2	4		4	
Logistic	3	1	1				4	
Theis	3	1	1					4
Rainfall			2		4			
Molecular diffusion				1	4			
Rate of purification			2		4			
Chemical First Order:								
BOD	3	1	1			4		
Stabilization of new reservoirs			2		4			
Average level of difficulty for method	3	1	1.5	1.5	4	4	4	4

CHAPTER VII

INTERPOLATION AND ALTERNATE METHODS

The lack of one or more observations in a sequence of data is a problem occurring frequently when the parameters of a given equation are to be determined. There are many different methods available to fulfill this problem; most of them use the difference concept to develop more or less complicated formulas resulting, in many cases, in n-degree polynomials approximating the model equation.

Obviously, the linear equations developed in Chapter IV can be used with interpolation purposes, but if it is preferred not to determine the parameters of the equation, alternate procedures can be found, so that the knowledge of said parameters becomes unnecessary to this object.

7.1 First Order Reaction Equation

To find an interpolation formula corresponding to the difference form 4.6 of the first order reaction equation 4.4, we apply equation 4.5 to a set of data (y_i, y_{i+1}), (y_j, y_{j+1}), where $i \neq j+1$, and $i,j = 1,2, \ldots,$ to obtain:

$$\frac{L - y_i}{L - y_{i+1}} = \frac{L - y_j}{L - y_{j+1}} = e^{-k\Delta x} \tag{7.1}$$

from which

$$L = \frac{y_i y_{j+1} - y_j y_{i+1}}{(y_i + y_{j+1}) - (y_j + y_{j+1})} \tag{7.2}$$

in which the numerator corresponds to the cross-products, and the denominator to the cross-sums, of the arrangement

$$\begin{matrix} y_1, & y_2, & y_3, & y_4, & y_5, & \ldots, & y_{n-1} \\ y_2, & y_3, & y_4, & y_5, & y_6, & \ldots, & y_n \end{matrix} \tag{7.3}$$

so that, if for instance, the second datum were missing, in a series of six observations taken at regular time intervals, the following relationship would be used

$$L = \frac{y_3y_5 - y_4^2}{(y_3+y_5)-(2y_4)} = \frac{y_3y_6 - y_4y_5}{(y_3+y_6)-(y_4+y_5)} = \frac{y_4y_6 - y_5^2}{(y_4+y_6)-(2y_5)}$$

$$= \frac{y_1y_3 - y_2^2}{(y_1+y_3)-(2y_2)} = \ldots$$

Collecting terms,

$$L = \frac{y_3y_5 + y_3y_6 + y_4y_6 - (y_4^2 - y_4y_5 + y_5^2)}{2(y_3 + y_6) - 2(y_4 + y_5)}$$

$$= \frac{y_1y_3 - y_2^2}{(y_1 + y_3) - (2y_2)} = \ldots \tag{7.4}$$

from which the value of the missing datum "y_2" as well as the parameter "L," if desired, can be estimated. Obviously, once this is known, "k" may be estimated from equation 7.1.

Example

Considering the data given below corresponding to a sewage sample, estimate the value of the parameter "L" in the BOD equation 2.3, and determine the magnitude of the missing datum.

Time, days	0	1	2	3	4	5
BOD, ppm	0	23	-	54	65	71

From arrangement 7.3 we obtain

$$\frac{y_2y_3 - y_1y_4}{(y_2+y_3) - (y_1+y_4)} = \frac{y_1y_5 - y_3y_3}{(y_1+y_5) - (y_3+y_3)} = L$$

so that

$$\frac{y_2(54) - (23)(65)}{(y_2+54) - (23+65)} = \frac{(23)(71)-(54)^2}{(23+71) - 2(54)} = 91.64$$

$$L = 91.64 \text{ ppm}$$

$$y_2 = 43.06 \text{ ppm}$$

7.2 Second Order Reaction Equation

Applying equation 4.17 to a set of paired data (x_i,y_i), (x_{i+1},y_{i+1}), where $i = 1,2,3, \ldots$, after division of the two resulting equations by each other, it is obtained that

$$e^{a\Delta x} = \frac{(L-y_{i+1})y_i}{(L-y_i)y_{i+1}} \tag{7.5}$$

and, similarly, for a set (x_j,y_j), (x_{j+1},y_{j+1}), $j = 1,2,3, \ldots$;

$$e^{a\Delta x} = \frac{(L-y_{j+1})y_j}{(L-y_j)y_{j+1}} \tag{7.6}$$

so that, equating equations 7.5 and 7.6 and rearranging, yields, for $j \neq i+1$

$$L = \frac{y_iy_{j+1}(y_{i+1}+y_j) - y_jy_{i+1}(y_{j+1}+y_i)}{y_iy_{j+1} - y_jy_{i+1}} \tag{7.7}$$

which is an expression whose terms may be derived from the minors of the arrangement 7.3. For instance, if the second term in a series of six observations taken at regular intervals of time were missing, we would write

$$L = \frac{y_3y_5(y_4+y_4) - y_4y_4(y_5+y_3)}{y_3y_5 - y_4y_4} = \ldots$$

$$= \frac{y_4y_6(y_5+y_6) - y_5^2(y_6+y_4)}{y_4y_6 - y_5^2} \qquad (7.8)$$

and also

$$L = \ldots = \frac{y_1y_4(y_2+y_3) - y_2y_3(y_4+y_1)}{y_1y_4 - y_2y_3} \qquad (7.9)$$

Equating equations 7.8 and 7.9, the value of the missing datum "y_2" can be obtained. If desired, the values of "L" and "a" can be estimated from equations 7.5 and 7.8, respectively.

A formula to determine "L," easier to apply than equation 7.9, is obtained directly from equation 7.5, to yield:

$$e^{a\Delta x} = \frac{(L-y_{i+1})y_i}{(L-y_i)y_{i+1}} = \frac{Ly_{n-1} - y_ny_{n-1}}{Ly_n - y_ny_{n-1}} \qquad (7.10)$$

where "n" denotes the last known datum.

Taking sums:

$$e^{a\Delta x} = \frac{L\Sigma y_i - \Sigma y_iy_{i+1}}{L\Sigma y_{i+1} - \Sigma y_iy_{i+1}} = \frac{Ly_{n-1} - y_ny_{n-1}}{Ly_n - y_ny_{n-1}} \qquad (7.11)$$

so that:

$$L = \frac{y_ny_{n-1}(\Sigma y_{i+1}-\Sigma y_i) - (y_n-y_{n-1})\Sigma y_i\Sigma y_{i+1}}{y_{n-1}\Sigma y_{i+1} - y_n\Sigma y_i} \qquad (7.12)$$

Example

Considering the data given in the first two columns of Table 7.1, in which the third datum is missing, estimate the saturation value "L" of the logistic equation 2.12, and estimate the value of the missing datum.

TABLE 7.1

INTERPOLATION: LOGISTIC EQUATION

Data Columns		Computation Columns	
Time, year (1), x	Population, thousands (2), y	(3), y_{i+1}	(4), $y_i y_{i+1}$
1910	5.5	30.0	165.0
1920	30.0	-	-
1930	-	-	-
1940	172.0	249.0	42,828.0
1950	249.0	292.0	72,708.0
1960	292.0		
Sums	426.5	571.0	115,701.0

Applying equation 7.12, we obtain

$$L = \frac{(292)(249)(571-426.5) - 115{,}701(292-249)}{249(571) - 292(426.5)}$$

$$L = 313.540 \quad 10^3 \text{ inhabitants}$$

The population in year 1930 is obtained from equation 7.11

$$\frac{313.5(426.5) - 115{,}701}{313.5(571) - 115{,}701} = \frac{313.5\, y_3 - 172\, y_3}{313.5(172) - 172\, y_3}$$

$$y_3 = 80.4 \quad 10^3 \text{ inhabitants}$$

APPENDIX

SUMMARY OF EQUATIONS AND NOMENCLATURE

Transcendental Equations and Its Linear Form

Linear Model

$$Y = I + PX$$

Least Squares

$$I = \frac{\Sigma Y}{n} - P\,\frac{\Sigma X}{n}$$

$$P = \frac{n\Sigma XY - \Sigma X \Sigma Y}{n\Sigma X^2 - (\Sigma X)^2}$$

First Order Reaction Equation

$$y = L(1 - e^{-kx})$$

Linear form:

$$y_{x+\Delta x} = L(1 - e^{-k\Delta x}) + e^{-k\Delta x}\, y_x;\ \Delta x = \text{const.}$$

Parameters:

$$k = -\ln P/\Delta x;\ L = I/(1-P)$$

Second Order Reaction Equation: Autocatalytic

$$x = \frac{1}{k_1 + k_2 L} \ln \frac{L(k_1+k_2 y)}{k_1\ (L - y)}$$

Linear form:

$$(ak_2L + k_1)y_x - (ak_1 + k_2L)y_{x+\Delta x} + (k_2 - ak_2)y_x y_{x+\Delta x}$$

$$+ (ak_1L - k_1L) = 0$$

Δx = const.

Parameters, algebraic method, "L" known:

"a": found by elimination of "k_1" and "k_2" from

$$k_2 = \frac{a(L - y_{x+\Delta x}) + (y_x - L)}{a(y_x y_{x+\Delta x} - Ly_x) + (Ly_{x+\Delta x} - y_x y_{x+\Delta x})} k_1$$

$$k_2 = \frac{a(L - y_{0+\Delta x}) - L}{Ly_{0+\Delta x}} k_1$$

"k_1": found from

$$k_1 = y_{0+\Delta x} \ln a/\Delta x \ (a-1)(L-y_{0+\Delta x})$$

"k_2": found from

$$k_2 = (\ln a - k_1\Delta x)/\Delta x \ L$$

Second Order Reaction Equation: Logistic

$$y = L(me^{ax} + L)^{-1}$$

Linear form:

$$y_x/y_{x+\Delta x} = e^{a\Delta x} + (1 - e^{a\Delta x})L^{-1} \ y_x; \ \Delta x = \text{const.}$$

Parameters:

$$a = \ln I/\Delta x$$

$$L = (1 - I)/P$$

Rate of Purification Equation

$$y/y_0 = 1 - (1 + nkx)^{-1/n}$$

Linear form:

$$x_{z(a+1)} = [(a+1)^{-n} - 1]/nk + (a+n)^{-n}\, x_z$$

$$z = y_0 - y_x;\ \Delta z = az;\ a = \text{const.}$$

Parameters:

$$n = -\ln P/\ln(a+1);\ k = (P - 1)/nI$$

Molecular Diffusion Equation

$$c_x = c_s - 0.811(c_s - c_0)(e^{-Kx} + \frac{1}{9} e^{-9Kx} + \frac{1}{25} e^{-25Kx} + \ldots)$$

$$K = \Pi^2\, k/4\ell^2;\ \ell = \text{constant}$$

Simplified linear form:

$$e^{-kx} = (z_x/A) - (0.766/A)c_s = B$$

$$x = \text{const};\ c_s = \text{const. known};\ B = \text{const.}$$

$$A = 0.811(c_s - c_0);\ c_0 = \text{const. known.}$$

$$z_x = c_x - \frac{1}{9} c_{9x} - \frac{1}{25} c_{25x} - \ldots$$

Parameters:

$$K = -\ln B/x$$

Theis' Equation

$$h_0 - h = \frac{Q}{4\Pi T} (-0.5772 - \ln u + u - \frac{u^2}{2.2!} + \frac{u^3}{3.3!} - \frac{u^4}{4.4!} + \ldots)$$

$$u = r^2 S/4Tx$$

Linear form:

$$\Delta y = 0.69a - (ac/2)\ x;\ \Delta x = x$$

$$\Delta y = \Delta(h_0 - h);\ a = Q/4\Pi T;\ c = r^2 S/4T$$

Parameters:

$$T = 0.055\ Q/I;\ S = -5.544\ PT/Ir^2$$

Rainfall Equation

$$i = cT^m/(x+d)^{-n}$$

Linear form: "T" constant:

$$x_{i(1+k)} = d[(1+k)^{-1/n} - 1] + (1+k)^{-1/n} x_i; \ \Delta i = ki$$

$$k = \text{constant}$$

Parameters:

$$n = -\ln(1+k)/\ln P; \ d = I/(P-1)$$

Linear form: "x" constant:

$$i_{(1+k)T} = (1+k)^m i_T$$

Parameters:

$$m = -\ln P/\ln (1+k)$$

Interpolation Formulas

First Order Reaction Equation

$$L = \frac{y_3y_5 - y_4^2}{(y_3+y_5)-2y_4} = \frac{y_3y_6 - y_4y_5}{(y_3+y_6)-(y_4+y_5)} = \dots = \frac{y_1y_3 - y_u^2}{(y_1+y_u)-2y_u}$$

y_u = unknown datum

Second Order Reaction Equation: Logistic

$$\frac{L\Sigma y_i - \Sigma y_i y_{i+1}}{L\Sigma y_{i+1} - \Sigma y_i y_{i+1}} = \frac{Ly_{n-1} - y_n y_{n-1}}{Ly_n - y_n y_{n-1}}$$

Let "n" stand for last known datum and determine "L," then, let "n" stand for unknown datum and use the same formula for its determination.

Other Transcendental Equations and Its Linear Forms

Normalized Standard Equation

$$y = y_0 e^{-cx^2}$$

Linear form:

$$y_{i+1}/y_i = e^{2c(\Delta x)^2}(y_{i+2}/y_{i+1});\ \Delta x = \text{const.}$$

Parameters:

$$c = \ln P/2(\Delta x)^2$$

Poisson Equation

$$y_i = e^{-m}\, m^x/x!$$

Linear form:

$$y_{i+1} = m(y_i/x_{i+1});\ \Delta x = 1$$

Parameters:

$$m = P$$

Geometric Growth

$$y = ae^{bx}$$

Linear form:

$$y_{i+1} = e^{b\Delta x}\, y_i;\ \Delta x = \text{constant}$$

Parameters:

$$b = \ln P/\Delta x$$

Parabolic Equation

$$y = c + ax^b$$

Linear form:

$$\Delta y = -c[(1+k)^b-1] + [(1+k)^b-1]\, y;\ \Delta x = kx$$

$$k = \text{constant}$$

Parameters:

$$b = \ln (P+1)/\ln (1+k);\ c = -I/P$$

Interest Equation

$$y = y_0(1+i)^x$$

Linear form:

$$y_{x+\Delta x} = (1+i)^{\Delta x} y_x; \quad \Delta x = \text{constant}$$

Parameters:

$$i = P^{1/\Delta x} - 1$$

Binomial Equation

$$b(n,x) = \frac{n!}{(n-x)!x!} p^x q^{n-x}$$

Linear form:

$$b(n,x+1)/b(n,x) = (np/q) - (p/q)x; \text{ "n" known}$$

Nomenclature

a,b,c,d, - constants or parameters

b(x,n) - binomial function of "x" and "n"

e - base of natural logarithms

h - drawdown level

i - variable in rainfall equation; used as subscript represents order of datum

k - constant or parameter

l - distance

m - parameter

n - number of data in a given set, or parameter

0 - used as subscript represents base datum

p,q - parameters

r - distance

x, y, z - variables

c_x - variable, function of "x"

A, B - constants

I - intercept of a linear form

K - parameter

L - parameter, saturation value

P - slope of a linear form

Q - rate of flow

S - storage coefficient

T - frequency, transmissibility coefficient

X, Y, Z - variables

Δ - increment

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