AUTOMATIC ESTIMATION OF HYDRAULIC PARAMETERS IN UNCONFINED AQUIFERS

by

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ABSTRACT

A computer program developed for the automatic estimation of hydraulic parameters of an unconfined aquifer is presented. The program is based on Neuman's (1974) analytical solution for flow to a partially penetrating well in an unconfined aquifer. The parameters of this solution are estimated by a nonlinear least squares procedure.

The program was tested on data generated synthetically, and on data from two pumping tests performed in Ohio and Colorado. The estimated hydraulic parameters led to a good reproduction of observed aquifer behavior.

CHAPTER 1

INTRODUCTION

One of the most common and useful techniques of determining hydraulic parameters of aquifers is the pumping test. Currently, the methods used in the analysis of pumping test data are mostly graphical and usually require curve matching.

Computer-based least square fitting techniques have lately been developed for the analysis of pumping test data in confined aquifers, e.g., Saleem (1970), Berg (1971) and Tsang et al. (1977). Based on Neuman's analytical solution for the characterization of flow to a partially penetrating well in an unconfined aquifer, a computer program was developed which enable automatic estimation of the hydraulic parameters of an unconfined aquifer using pumping test data.

Considering the aquifer parameters as decision variables, an objective function is defined as the weighted sum of squared differences between observed drawdowns and those given by the analytical solution. The values of the decision variables which minimize the objective function are assumed to be the best estimates of the aquifer parameters.

The minimization procedure used in this program is based on the subroutine found in the program library of the

University of Arizona, which minimizes non-linear functions of several variables subject to linear constraints, originally developed at the Watson Research Center. The subroutine uses a gradient "feasible direction method", proposed by Zoutendijk (1960) and requires calculating the derivatives of the objective function with respect to each decision variable.

The program was tested with synthetical generated data, and with data from two pumping tests performed in Ohio and Colorado.

The estimated hydraulic parameters led to a good reproduction of observed aquifer behavior by the analytical solution.

The method developed herein enables one to analyse pumping test data corresponding to situations in which graphical matching procedures are not easily applied, such as a partially penetrating well, or several wells pumping simultaneously at different rates. The method also makes it possible to analyse data from several observation wells, which can be partially or fully penetrating. However, the estimated parameters are not guaranteed to represent true values, and the estimation procedure is not entirely automatic. This is because the objective function is not convex and the minimization subroutine may converge to a local minimum, instead of the desired global minimum.

The theoretical development of the problem is presented in Chapter 2. Chapter 3 describes the minimization procedure. The analyses of estimation and residual errors are presented in Chapter 4. Application of this program to synthetic, and real, data is described in Chapter 5. Chapter 6 includes conclusions and recommendations.

The detailed development of the evaluation of the derivations of the objective function is given in Appendix 1. A user's guide for the program is presented in Appendix 2.

CHAPTER 2

THEORETICAL DEVELOPMENT

A partially penetrating well is assumed to be pumping at a constant discharge rate from an unconfined aquifer of infinite lateral extent, resting on an impermeable horizontal layer, as represented schematically in Figure 1. The draw-

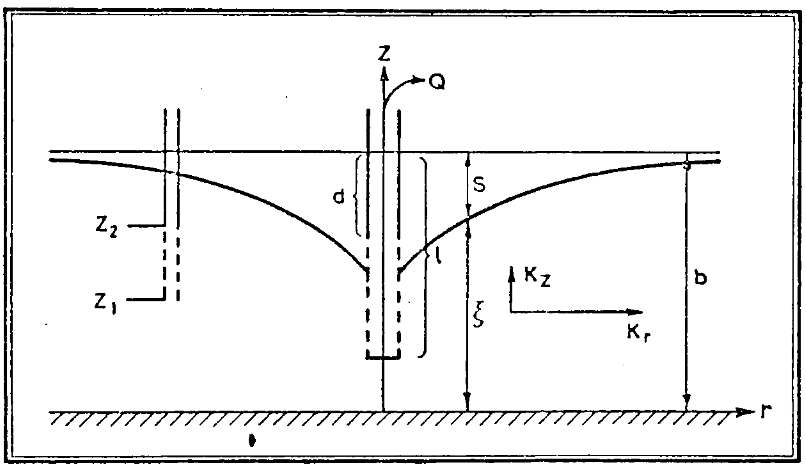

Figure 1. Schematic diagram of unconfined aquifer.

downs of the piezometric surface are assumed to be recorded at the observation well represented in this figure.

Plotting drawdon versus time on logarithmic paper, an inflected curve is obtained consisting of a steep segment at early times, a flat segment at intermediate times and, again, a steeper segment at later times (Neuman, 1975). The phenomenon associated with such a behavior is characteristic of unconfined aquifers and has been traditionally referred to in the groundwater literature as "delayed yield". In 1954, a model capable of reproducing these three segments of the time-drawdown curve was proposed by Boulton (1954b, 1963).

In this first model, the amount of water released from storage per unit horizontal area of the aquifer due to a unit average drawdown occuring at time τ was considered to be the sum of two components: S, a volume of water instantaneously released at time τ and S_y, a volume of water the release of which was delayed in time according to the formula $\alpha S_y[-\alpha(t - \tau)]$, where t is time $(t \geq \tau)$ and α is a characteristic constant of the aquifer (Neuman, 1972, 1973, 1974, 1975). This model was implemented later by Boulton (1970) and Boulton and Pontin (1971) in order to account for anisotropy and the effect of vertical flow components in the aquifer.

Boulton's model was used originally by Boulton (1963) and later by Prickett (1965) to describe a graphical procedure for determining the transmissivity T, the storage coefficients S and S_y, and the so called "delayed index", $1/\alpha$, of an unconfined aquifer, from pumping test data. Also based on Boulton's analytical model, Berkaloff (1963) presented a graphical procedure to analise pumping test data and evaluate T, S, S_y and α, following a procedure similar to that proposed by Cooper and Jacob (1946), and Jacob (1950). The method is based on the plotting of drawdowns versus time on semilogarithmic paper. Here some of the early data tend to fall on a straight line, and the late data tend to fall on another straight line parallel to the first one, while intermediate data tend to fall on a horizontal line. Thus, the methodology proposed by Cooper and Jacob (1946) and Jacob (1950) can be used to evaluat T, S, and S_y. Berkaloff (1963) also pointed out a method to determine the value of α.

Dagan (1967a, b) presented a method of determining the hydraulic parameters of an incompressible anisotropic unconfined aquifer which could be applied to pumping test data under partially penetrating conditions. As Neuman (1972, 1973, 1974, 1975) concluded later, this method is limited in its application to relatively large distances from the pumping well and to sufficiently large values of time, at which the effect of elastic storage is very small.

Recently Neuman (1972, 1973, 1974) and Streltsova (1972a, b, 1973), simultaneously and independently, presented an alternative thory based only on well defined physical parameters of the aquifer. Unlike Boulton theory the new approaches do not involve such semiepirical quantities as the delay index $1/\alpha$. Furthermore, the new model presented by Neuman takes into account aquifer anisotropy and, as such, it enables one to investigate the effects of partially penetrating wells on the drawdown when delayed gravity response is important (Neuman, 1974). Considering the unconfined aquifer as a compressible system and phreatic surface as a moving material boundary, and disregarding both air-entry effects and unsaturated flow, Neuman (1972, 1973,

the delayed gravity response characteristic of unconfined aquifers. Both authors showed that this behavior was possible while treating the specific storage and the specific yield as constants, unlike Boulton's theory which considered exponential variation of the specific yield with time. The difference between the models presented by Streltsova and Neuman is that the former requires several simplifying assumptions which the latter does not need (Neuman, 1979).

Later, Streltsova (1974) and Boulton and Streltsova (1975) adopted the approach originally proposed by Neuman (1972, 1973, 1974) and obtained a general solution for the case where the water table is located in an aquitard overlying a pumped aquifer. Their solution reduces to that of Neuman (1974) in the particular case where there is no aquitard (Neuman, 1979).

According to Neuman (1974), the drawdown s^* recorded in an observation well that is perforated between the elevations z_1 and z_2 (Figure 1) is expressed in terms of six dimensionless parameters σ, β, z_D, l_D, d_D, and ts or ty, as

$$s^* = \frac{Q}{4\pi T}\int_0^\infty 4yJ_0(y\beta^{1/2})\,[U_0(y) + \sum_{n=1}^{\infty} U_n(y)]dy \tag{2.1}$$

where

$$U_0(y) = \frac{\{1-\exp|-ts\beta(y^2-\gamma_0^2)|\}|\sinh(\gamma_0 Z_{2D}) - \sinh(\gamma_0 Z_{1D})}{\left|y^2 + (1+\sigma)\gamma_0^2 - \frac{(y^2-\gamma_0^2)^2}{\sigma}\right|\cosh(\gamma_0)}$$
$$\frac{\{\sinh|\gamma_0(1-d_D)| - \sinh|\gamma_0(1-l_D)|\}}{(Z_{2D}-Z_{1D})\gamma_0\cdot(l_D-d_D)\sinh(\gamma_0)} \tag{2.2}$$

$$U_n(y) = \frac{\{1-\exp|-ts\beta(y^2+\gamma_n^2)|\}|\sin(\gamma_n Z_{2D})-\sin(\gamma_n Z_{1D})|}{\left|y^2-(1+\sigma)\gamma_n^2 - \frac{(y^2+\gamma_n^2)^2}{\sigma}\right|\cos(\gamma_n)\cdot(Z_{2D}-Z_{1D})\gamma_n}$$
$$\frac{\{\sin|\gamma_n(1-d_D)|-\sin|\gamma_n(1-l_D)|\}}{(l_D-d_D)\sin(\gamma_n)} \tag{2.3}$$

and the terms γ_0 and γ_n are the roots of the equations

$$\sigma\gamma_0\sinh(\gamma_0) - (y^2 - \gamma_0^2)\cosh(\gamma_0) = 0 \quad \text{for} \quad \gamma_0^2 < y^2 \tag{2.4}$$

$$\sigma\gamma_n \sin(\gamma_n) + (y^2 + \gamma_n^2)\cos(\gamma_n) = 0 \quad \text{for} \tag{2.5}$$

$$(2n - 1)(\pi/2) < \gamma_n < n\pi, \quad \text{and} \quad n > 1. \tag{2.6}$$

Here

$$\sigma = \frac{S}{S_y}$$

$$K_D = \frac{K_z}{K_h}$$

$$t_s = \frac{t}{S \cdot r^2}$$

$$t_y = \frac{t}{S_y \cdot r^2}$$

$$\beta = \frac{K_D r^2}{b^2}$$

$$b_r = \frac{b}{r}$$

$$z_D = \frac{z}{b}$$

$$z_{1D} = \frac{z_1}{b}$$

$$z_{2D} = \frac{z_2}{b}$$

$$l_D = \frac{l}{b}$$

$$d_D = \frac{d}{b}$$

with

S - storage coefficient

S_y - specific yield

K_z - vertical hydraulic conductivity

K_h - horizontal hydraulic conductivity

b - aquifer thickness

r - distance from observation well to pumping well

T - transmissivity

t - time since pumping started

K_D - ratio between vertical and horizontal hydraulic conductivities

t_s - dimensionless time with respect to storage coefficient

t_y - dimensionless time with respect to specific yield

l - vertical distance from initial water table to bottom of perforations in pumping well

d - vertical distance from initial water table to top of perforations in pumping well.

The definition of the optimization problem requires the selection of the parameters to be estimated. It was considered that four parameters should be taken as decision variables for the optimization problem, the others being evaluated from these four. The four parameters considered are σ, tss, krr and b, where

$$tss = \frac{T}{S \cdot r^2}$$

$$krr = K_D \cdot r^2 .$$

As r, z, z_1, d and l are known from the design of the puping test, and t is the time corresponding to each observation, all the remaining six dimensions parameters can be evaluated from the above four decision variables.

In order to evaluate T, S, S_Y, β, and b, from estimates of the decision variables found by the minimization procedure it will be necessary to have an "a priori" reliable estimate for S or S_Y. This is a limitation of the automatic procedure that can, however, be overcome, in most of pratical cases, as long as prior hydrogeological information enable the estimation of one of the two hydraulic parameters.

The objective function $F(\sigma,tss,krr,b)$ to be minimized is defined as follows:

$$F(\sigma,tss,ker,b) = \sum_{j=1}^{m} \sum_{i=1}^{n} \omega_{ij}\{s_{ij}(\sigma,tss,krr,b) - h_{ij}\}^2 \qquad (2.7)$$

where s_{ij} is the estimated dimensionless drawdown at time i, in the observation well j, h_{ij} is the corresponding observed drawdown, and ω_{ij} is the weight assigned to this particular observed data.

Evaluation of derivates of the objective function with respect to each of the four decision variables is given in Appendix 1. These derivates are required by the minimization subroutine adopted herein. These four derivates are:

-Derivate with respect to σ

$$\frac{\partial F}{\partial \sigma}(\sigma,tss,krr,b)$$

$$= \sum_{j=1}^{m} \sum_{i=1}^{n} 2w_{ij}\{s_{ij}(\sigma,tss,krr,b) - h_{ij}\}\frac{\partial s_{ij}}{\partial \sigma}(\sigma,tss,krr,b) \qquad (2.8)$$

with

$$\frac{\partial s_{ij}}{\partial \sigma}(\sigma,tss,krr,b)$$

$$= \int_0^\infty 4yJ_0(y\beta^{1/2})\{\frac{\partial U_0(y)}{\partial \sigma} + \sum_{n=1}^{\infty} \frac{\partial U_n(y)}{\partial \sigma}\}dy. \qquad (2.9)$$

-Derivate with respect to tss

$$\frac{\partial F}{\partial tss}(\sigma,tss,krr,b)$$

$$= \sum_{j=1}^{m} \sum_{i=1}^{n} 2w_{ij}\{s_{ij}(\sigma,tss,krr,b) - h_{ij}\}\frac{\partial s_{ij}}{\partial tss}(\sigma,tss,krr,b) \tag{2.10}$$

with

$$\frac{\partial s_{ij}}{tss}(\sigma,tss,krr,b)$$

$$= \int_0^\infty 4yJ_0(y\beta^{1/2})\{\frac{U_0(y)}{\partial tss} + \sum_{n=1}^{\infty} \frac{\partial U_n(y)}{\partial tss}\}dy. \tag{2.11}$$

-Derivate with respect to krr

$$\frac{\partial F}{\partial krr}(\sigma,tss,krr,b)$$

$$= \sum_{j=1}^{m} \sum_{i=1}^{n} 2w_{ij}\{s_{ij}(\sigma,tss,krr,b) - h_{ij}\}\frac{\partial s_{ij}}{\partial krr}(\sigma,tss,krr,b) \tag{2.12}$$

with

$$\frac{\partial s_{ij}}{\partial krr}(\sigma,tss,krr,b) = \int_0^\infty \{4yJ_0(y\beta^{1/2})[\frac{U_0(y)}{\partial krr} + \sum_{n=1}^{\infty} \frac{\partial U_n(y)}{\partial krr}] - \frac{2y^2}{b^2}\beta^{-1/2}J_1(y\beta^{1/2})[U_0(y) + \sum_{n=1}^{\infty} U_n(y)]\}dy. \tag{2.13}$$

-Derivate with respect to b

$$\frac{\partial F}{\partial b} = \sum_{j=1}^{m} \sum_{i=1}^{n} 2w_{ij}\{s_{ij}(\sigma,tss,krr,b) - h_{ij}\}\frac{\partial s_{ij}}{\partial b}(\sigma,tss,krr,b) \tag{2.14}$$

with

$$\begin{aligned}\frac{\partial s_{ij}}{\partial b} = \int_0^{\infty}\{ & 4yJ_0(y\beta^{1/2})[\frac{\partial U_0(y)}{\partial b} + \sum_{n=1}^{\infty}\frac{\partial U_n(y)}{\partial b}] \\ & - [2y^2 J_1(y\beta^{1/2})\beta^{-1/2}\frac{\partial \beta}{\partial b}][U_0(y) + \sum_{n=1}^{\infty} U_n(y)]\}dy.\end{aligned} \tag{2.15}$$

Following this presentation, the minimization method chosen for solving the problem will be presented.

CHAPTER 3

MINIMIZATION METHOD

The objective function to be minimized is a nonlinear function of the decision variables. This reduces the number of alternative minimization methods that can be chosen. Four methods were considered. Steepest descent, Newton's method, Fletcher Powell and the Zoutendijk method. Whereas the first three are unconstrained descent methods, the last one is a constrained descent method. As such, it has been adopted for this thesis.

In a descent method such as steepest descent or the method of Newton a direction of movement is determined at each point, accordingly to the specific algorithm used. A minimum of the objective function is searched for along this direction. In the constrained descent method, also called "feasible direction" method, the direction of movement at each point is determined by the constraints imposed on the variables.

The iterative algorithm of the steepest descent method is as follows:

$$\underline{x}_{K+1} = \underline{x}_K - \alpha_K \underline{g}_K \qquad (3.1)$$

where

$$\underline{g}_K = \nabla f(\underline{X}_K)^T \tag{3.2}$$

and α_K is chosen to minimize $f(\underline{X}_{K+1})$. The direction of movement at each step is defined by the negative gradient of the objective function, $f(\underline{X}_K)$.

The iterative algorithm of the Newton method is

$$\underline{X}_{K+1} = \underline{X}_K - \{F(\underline{X}_K)\}^{-1}\underline{g}_K \tag{3.3}$$

where

$$\{F(\underline{X}_K)\}^{-1} = \nabla^2 f(\underline{X}_K). \tag{3.4}$$

The direction of movement is defined by the product of the negative gradient of the objective function and the inverse of the Hessian $F(\underline{X}_K)$ of the objective function. This method appears to be more attractive than the steepest descent because it converges quadratically whereas the latter converges linearly. Newton's method may, however, result in severe reduction of the convergence rate at points remote from the global minimum. Furthermore, evaluation of the Hessian at each point is often a very slow and tedious process.

To overcome the limitations of Newton's method, algorithms have been developed (Luenberger, 1971) that can be considered to lie between the steepest descent and Newton's method. Instead of dealing with the inverse of the Hessian, an approximation of the true inverse matrix is used. These algorithms, currently known as "Quasi-Newton" methods, are considered to be the most sophisticated methods used for solving unconstrained problems. Among these the Fletcher Powel method was originally selected to solve the minimization problem of our study. The iterative procedure, which has the advantage of requiring only the evaluation of first order derivatives of the objective function with respect to each of the decision variables (the hydraulic parameters of the aquifer), is defined as

$$\underline{X}_{K+1} = \underline{X}_K - \alpha_K \underline{\underline{S}}_K \nabla f(\underline{X}_K). \tag{3.5}$$

It can be seen that if $\underline{\underline{S}}_K$ is taken as the inverse of the Hessian of $F(\underline{X}_K)$, the algorithm of Newton's method is obtained and, if $\underline{\underline{S}}_K$ is the identity matrix, the algorithm of the steepest descent method is obtained.

The matrix $\underline{\underline{S}}_K$ is selected in such a way that it can be considered a close approximation of the inverse of the Hessian. In the Fletcher Powell method, the directions generated at each point are always directions of descent, as the matrix $\underline{\underline{S}}_K$ is positive definite throughout the process. At the solution, $\underline{\underline{S}}_K$ will converge to the inverse Hessian.

The minimization subroutine MINI, developed by the New York Courant Institute and available at the University of Arizona Computer Library was chosen and adopted to the computer program developed in this thesis. After several computer runs using synthetic data, it was found that the values of the decision variables were very often not physically feasible. To overcome this limitation, a feasible direction method of minimization was selected. Such methods enable the user to impose linear constraints upon the variables, including upper and lower bounds.

The feasible direction method selected was due to Zoutendijk and a subroutine available at the University of Arizona Computer Center Library was adopted to the program. This subroutine was developed by Watson Reasearch Center and is called MGFN.

The Zoutendijk method is a feasible direction method which belongs to the group of "primal" methods. A primal method is one in which the optimal solution is searched for throughout the feasible region (defined by the constraint equations), and in which the objective function is taken as originally defined, with no simplifying assumptions. At each step in the process, the value of the variables is feasible, and the objective function constantly decreases as the minimization procedure is carried out.

Luenberger (1965) states that primal methods present three significant advantages when applied to nonlinear programming problems, and so, they are recommended for almost all such problems. The advantages are as follows:

1. As each point generated in the search procedure is feasible, the final point will be feasible and, in cases where the process is terminated before the solution is reached, it might also be a near optimal solution to the original problem.

2. When a convergent sequence is generated, the limit point of that sequence must be, at least, a local constrained minimum.

3. As most of the primal methods do not rely on special problem structure, such as convexity, they are applicable to general nonlinear programming problems.

Considering the objective function

$$F(\underline{X}) = F[X(1),X(2),X(3),X(4)]$$

an initial feasible solution, which in this minimization subroutine can be computed, or provided by the user, will be the vector

$$\underline{X}^0 = X^0(1), \quad X^0(2), \quad X^0(3), \quad X^0(4). \tag{3.6}$$

A direction feasible vector $\underline{d}^0$ is then chosen as the solution to the following linear problem: minimize a new objective function $G(\underline{x})$

$$G(\underline{x}) = \nabla F(\underline{X}^0)\cdot\underline{d} \tag{3.7}$$

subject to

$$a_i'\underline{d} \leq 0 \qquad i \in I \tag{3.8}$$

where a_i' are the coefficients of a matrix corresponding to the linear constraints system of equations, (in this case a system of linear inequality constraints of the form $a_i'x \leq b_i$, with $i = 1, N$), and with

$$\sum_{i=1}^{N} |d_i| = 1 \tag{3.9}$$

being N the number of linear inequality equations, defining the upper and lower bounds of the constraint system.

The vector $\underline{d}^0$ is a feasible direction at $\underline{X}^0$ if there is an $\bar{\alpha} > 0$ such that $\underline{X}^0 + \alpha\underline{d}^0$ is feasible for all α

$$0 \leq \alpha \leq \bar{\alpha}. \qquad (3.10)$$

According to equation (3.7) the feasible direction $\underline{d}$ is chosen so that it lines up as close as possible with the negative gradient of $F(\underline{X})$. Then, a constraint line search is developed and a new point $\underline{X}^1$ will be given by

$$\underline{X}^1 = \underline{X}^0 + \alpha^0 \underline{d}^0 \qquad (3.11)$$

where the vector α^0 is the one that minimizes the objective function $F(X)$, constrained by the condition that the new point, $\underline{X}^1$, and the line segment joining $\underline{X}^0$ and $\underline{X}^1$, be feasible. Thus the method consists of a sequence of steps, where each step includes selecting a feasible direction and a constrained line search.

At any new point $\underline{X}^K$, a feasible direction $\underline{d}^K$ is chosen, solving the linear programming sub-problem referred to in equation (3.7), and a constraint line search is developed to find the new $\underline{X}^{K+1}$. This procedure is repeated successively until the values of the objective function between two successive points reach the tolerance limit given as input to the minimization subroutine, or until the feasible direction is identically zero.

CHAPTER 4

ERROR ANALYSIS

The true values of s (drawdown) cannot be exactly measured due to the observation errors associated with the measurement procedure. If $\underline{s}$ is the measured drawdown vector corresponding to a particular pumping test, the true drawdown vector can be related to $\underline{s}$ by

$$\underline{s}^* = \underline{s} + \underline{\varepsilon} \tag{4.1}$$

where $\underline{\varepsilon}$ represents measurement errors. These errors may be introduced by various sources such as deficient instruments, misreading, or lack of accuracy in the reading of drawdowns by the observer in charge of the measurements.

Pure Error

If it was physically possible to perform several measurements of the drawdown at each specific instant of time it would be possible to estimate the statistic properties of the measurement errors from the representative sample obtained for each drawdown at each time. Let us consider, for example, a pumping test during which the drawdown is measured fifty times. Let us assume that, instead of one measurement, twenty measurements are taken at each time. For the first time, j - 1, a sample of twenty drawdowns k are obtained at point i, s_{i1}^{k}. Assuming that this can be taken as a representative sample, the mean of the measured values can be estimated as the true drawdown s_{i1} at time 1. The mean and variance of the measurement error at well i, any time t_j, would be given by

$$\bar{s}_{ij} = \frac{1}{19}\sum_{K=1}^{20} s_{ij}^{k} \tag{4.2}$$

$$\sigma(\varepsilon_{ij}) = \frac{1}{19}\sum_{K=1}^{20} (s_{i,j}^{k} - \bar{s}_{i,j}^{k})^2 \quad j = 1, \ldots, 50 \tag{4.3}$$

where the superscript k represents sample number.

Still in this case, the covariance between each set of two measurement errors at well i, (corresponding to times t_j and t_1), would be given by

$$\text{cov}(\varepsilon_{ij}, \varepsilon_{i1}) = \frac{1}{19}\sum_{K=1}^{20} (s_{i,j}^{k} - \bar{s}_{i,j}^{k})(s_{i,1}^{k} - \bar{s}_{i,1}^{k}) \tag{4.4}$$

$$j, 1 = 1, \ldots, 50 \qquad j \neq 1.$$

In practice, it is generally impossible to obtain repeated measurements at each instant of time. Thus, it is difficult to obtain information concerning the structure of the covariance matrix of the measurement errors. One must therefore make assumptions concerning the structure of the errors, and check these assumptions later by examining the residuals between the observed drawdowns and those estimated by the least square procedure.

It will be assumed that the measurement errors have zero mean, identical variances σ^2, and are mutually uncorrelated. The correlation matrix is thus taken to be $\underline{\underline{V}}_s = \underline{\underline{I}}$, and the generalized nonlinear regression approach calls for the minimization of an ordinary least-square criterion. Considering a vector $\underline{X}$ representing X(1), X(2), X(3), and X(4) decision variables, the minimization of the least square criterion can be expressed as the minimization of $J_s(\hat{\underline{X}})$, where

$$J_s(\hat{\underline{X}}) = |s^* - s(\hat{\underline{X}})|^T |s^* - s(\hat{\underline{X}})| \qquad (4.5)$$

with $s(\hat{\underline{X}})$ being the estimated drawdown from Neuman's (1972, 1973, 1974) analytical model, referred to in Equation 2.1.

Here the vector $\hat{\underline{X}}$, which minimizes the objective function, $J_s(\underline{X})$, is the estimate of $\underline{X}$. According to Draper and Smith (1966), if the model is correct, the estimate will be the minimum variance unbiased estimate.

From the estimated drawdowns obtained through the minimization procedure, the analysis of the residuals between these and the observed drawdowns will enable the confirmation of the validity of the assumptions made regarding the statistical properties (mean and covariance) of $\underline{\varepsilon}$.

Indeed, if the model is correct, and the minimum found is the global minimum of the objective function, one should expect that the residuals are only due to the differences between the "true" drawdowns, and the "measured" drawdowns. Any difference between these values (the residuals) would be the result of measurement error. It can then be expected that the evaluation of the mean and the covariance matrix of the residuals will show zero mean and off diabonal terms of this matrix equal to zero.

If the instruments, as well as the observer, do not tend to introduce a systematic measurement error, the mean of this error will be zero. However, the assumption of equal variance may not hold in all cases. In fact, the measurement errors of drawdowns recorded during the early period of pumping will often be different from those recorded at later times. As drawdowns at early times are much smaller than at later times, the former may be read by the observer with less accuracy than the latter. On the other hand, at early times the drawdowns are increasing faster than at later times. Regardless of these arguments, and in the absence of any better solution for the estimation of the variances of the errors, one may be able to accept "a priori" the simplifying assumption of the equal variances of the errors.

Based on the same type of consideration regarding the absence of any systematic measurement error introduced by the instruments, or the observer, and that, if any error is made in a measurement, it will not have any direct effect in the reading of the next measurement, one may consider that the correlation coefficients between each two pairs of data values will be zero in a "a priori" assumption.

Estimation Error

The mean and variance of the estimation error of the parameters obtained through the minimization of the objective function $J_s(\underline{X})$ are also important to judge the accuracy of this automatic method of analysing pumping test data. The estimation error of the parameters is the difference between the true value of the parameters and the corresponding estimate found,

$$\underline{e}_x = \hat{\underline{X}} - X. \qquad (4.6)$$

The moments of the errors $\underline{e}_x$ can be obtained by an approximate procedure, following a linearized error analysis in which the drawdown $s(\underline{X})$ is approximated by the linear part of its Taylor series expansion about $\hat{\underline{X}}$

$$s(\underline{X}) = s(\hat{\underline{X}}) + Z(X - \hat{X}) \qquad (4.7)$$

where $\underline{\underline{Z}}$ is the NxI Jacobian matrix, N being the number of data points used for the estimation of the parameters, and I the number of X variables. The terms of the matrix $\underline{\underline{Z}}$, z_{ni}, are defined as:

$$z_{ni} = \left.\frac{\partial s}{\partial X_i}\right|_{X_i=\hat{X}_i} . \tag{4.8}$$

The first and second order moments of the estimated parameters can be evaluated, assuming that the variance of the data σ_s^2 is known, Seber (1977)

$$E(\underline{e}_x) = 0 \tag{4.9}$$

$$\underline{\underline{V}}(\underline{e}_x) = \sigma_s^2(\underline{\underline{Z}}^T\underline{\underline{V}}_s^{-1}\underline{\underline{Z}})^{-1} \tag{4.10}$$

where $\underline{\underline{V}}(\underline{e}_x)$ is the covariance matrix of $\underline{e}_x$ and σ_s^2 and $\underline{\underline{V}}_s$ are the variance and correlation matrix of the true data respectively.

The estimate s_s^2 of the error variance σ_s^2 can be obtained, Draper and Smith (1966), by

$$s_s^2 = \frac{J}{N-4} \tag{4.11}$$

where

N is the number of observations

4 is the number of parameters being estimated

N - 4 is the number of degrees of freedom

J is the value of the objective function at the minimum found.

CHAPTER 5

APPLICATIONS

Introduction

The computer program was first tested with synthetic data, generated according to Equation 2.1. Several computer runs were performed, and the results which were closest to the true solution were selected for an error analysis, as mentioned in Chapter 4. Artificial noise was superimposed on the synthetic data, and the resulting effects on the estimation errors were evaluated.

Sets of synthetic data were generated, and the range of the values, physically permissible, for each of the four hydraulic parameters of the aquifer, was explored using the computer method developed.

Two real cases of pumping test performed in unconfined aquifers were also considered, and the results obtained appear to illustrate the practical usefullness of the proposed method.

Synthetic Data Test

Based on Equation 2.1 a pumping test was simulated assuming the following aquifer parameters:

$$X(1) = 0.0901$$
$$X(2) = 10.00$$
$$X(3) = 1.00$$
$$X(4) = 10.00.$$

Using twenty generated data points, shown in the second column of Table 1, the computer program developed for the estimation of the hydraulic parameters of the aquifer was tested, starting from several different initial solutions for the values of the hydraulic parameters.

The results closest to the real solution correspond to the initial solution:

$$X(1) = 0.0902$$
$$X(2) = 4.00$$
$$X(3) = 1.00$$
$$X(4) = 6.00.$$

For this set of values the objective function FX is equal to

$$FX = 53.17.$$

The estimated values, and the value of the objective function, corresponding to the optimum found are:

Table 1. Synthetic Data Application of the Automatic Method (20 Data Points).

Dimensionless Time	Dimensionless Drawdown (Generated)	Estimated Draw-down for the Minimum Found	Differences (Generated-Estimated)
0.030	0.461	0.254	+0.207
0.060	1.055	0.7004	+0.3546
0.090	1.463	1.05261	+0.410
0.30	2.61	2.1765	+0.433
0.60	3.07	2.689	+0.380
0.90	3.256	2.932	+0.324
4.00	3.704	3.552	+0.152
7.00	3.882	3.814	+0.068
9.00	3.979	3.960	+0.019
15.62	4.255	4.355	-0.10
30.62	4.76	4.997	-0.237
50.62	5.268	5.572	-0.304
90.62	5.962	6.284	-0.322
156.22	6.661	6.927	-0.266
306.2	7.508	7.699	-0.191
906.2	8.748	8.862	-0.114
2062.0	9.625	9.704	-0.079
20620.0	12.00	12.407	-0.407
50620.0	13.612	13.988	-0.376
206200.0	15.06	14.699	+0.361

X(1) = 0.0902

X(2) = 6.91

X(3) = 1.00

X(4) = 9.34

FX = 1.63.

Columns 2, 3 and 4, of Table 1 present the values of the dimensionless drawdowns obtained for the exact solution, for the optimum solution, and the corresponding differences between the true and estimated solution.

Using forty-eight generated data points from the same "synthetic" aquifer one obtains the results within the the columns of Table 2. The computer program was tested with the same initial guess,

X(1) = 0.0902

X(2) = 4.00

X(3) = 1.00

X(4) = 6.00.

The value of the objective function corresponding to the new data set is:

FX = 122.96.

Table 2. Synthetic Data Application of the Automatic Method (48 Data Points).

Dimensionless Time	Dimensionless Drawdown (Generated	Estimated Drawdown for the Minimum Found	Differences (Generated-Estimated
0.030	0.50	0.29	0.21
0.035	0.616	0.376	0.24
0.038	0.682	0.426	0.256
0.042	0.766	0.493	0.273
0.045	0.826	0.541	0.285
0.050	0.922	0.619	0.303
0.055	1.011	0.693	0.318
0.060	1.095	0.764	0.332
0.065	1.174	0.831	0.343
0.070	1.248	0.896	0.352
0.080	1.383	1.02	0.363
0.090	1.503	1.127	0.376
0.100	1.610	1.226	0.384
0.120	1.797	1.402	0.395
0.140	1.953	1.55	0.403
0.160	2.086	1.68	0.406
0.180	2.200	1.793	0.407
0.200	2.300	1.893	0.401
0.250	2.499	2.0997	0.3993
0.300	2.650	2.260	0.390
0.350	2.769	2.390	0.379

Table 2 -- (Continued)

Dimensionless Time	Dimensionless Drawdown (Generated)	Estimated Drawdown for the Minimum Found	Differences (Generated-Estimated)
0.400	2.864	2.494	0.370
0.450	2.942	2.583	0.359
0.500	3.007	2.658	0.349
0.600	3.110	2.776	0.334
0.700	3.187	2.866	0.321
0.800	3.247	2.948	0.299
0.900	3.296	3.010	0.286
1.500	3.468	3.230	0.238
6.00	3.864	3.820	0.044
15.00	4.269	4.420	-0.151
30.00	4.780	5.096	-0.316
60.00	5.499	5.910	-0.411
90.00	5.992	6.410	-0.418
150.00	6.647	7.016	-0.369
300.00	7.522	7.880	-0.358
600.00	8.332	8.560	-0.228
900.00	8.778	8.990	-0.212
1500.0	9.326	9.520	-0.194
3000.0	10.046	10.160	-0.114
6000.0	10.663	10.770	-0.107
9000.0	11.018	11.240	-0.222

Table 2 -- (Continued)

Dimensionless Time	Dimensionless Drasdown (Generated	Estimated Draw-down for the Minimum Found	Differences (Generated-Estimated
15000.0	11.586	12.020	-0.434
30000.0	12.676	13.300	-0.624
60000.0	13.955	14.340	-0.385
90000.0	14.569	14.640	-0.071
150000.0	15.007	14.750	0.257
600000.0	15.138	14.760	0.378

The optimum found through the minimization process is the following:

$$X(1) = 0.0902$$

$$X(2) = 7.42$$

$$X(3) = 1.00$$

$$X(4) = 9.42.$$

The value of the objective function corresponding to this minimum is:

$$FX = 5.24.$$

Columns 2, 3, and 4, of Table 2, present the value of the dimensionless drawdown obtained for the exact solution, for the optimum solution, and the differences between the true and estimated solution. In Figure 2 the curves of the dimensionless drawdown corresponding to the true, and estimated solutions are plotted.

The estimates correspond to a local minimum of the objective function. The estimate of X(4) is close to the true value of this variable (aquifer thickness), whereas the estimate of X(2) (accounting for aquifer transmissivity) is less accurate. The estimates of X(1) and X(3) were the same given as initial solution, and their values are the exact ones.

In order to get a picture of the shape of the objective function around its global minimum, as well as around the local minimum found, several computer runs were performed. In these runs, each of the decision variables was varied within a range centered about its true value, or the estimated optimum value, while keeping the other decision variables constant.

The results are given in Tables 3-18. These tables illustrate the shape of the objective function in each of the planes defined by the conditions which were considered.

As one can see, the function appears to be highly irregular, thus explaining why the minimization process leads to local minima rather than the global minimum for some of the initial solutions considered.

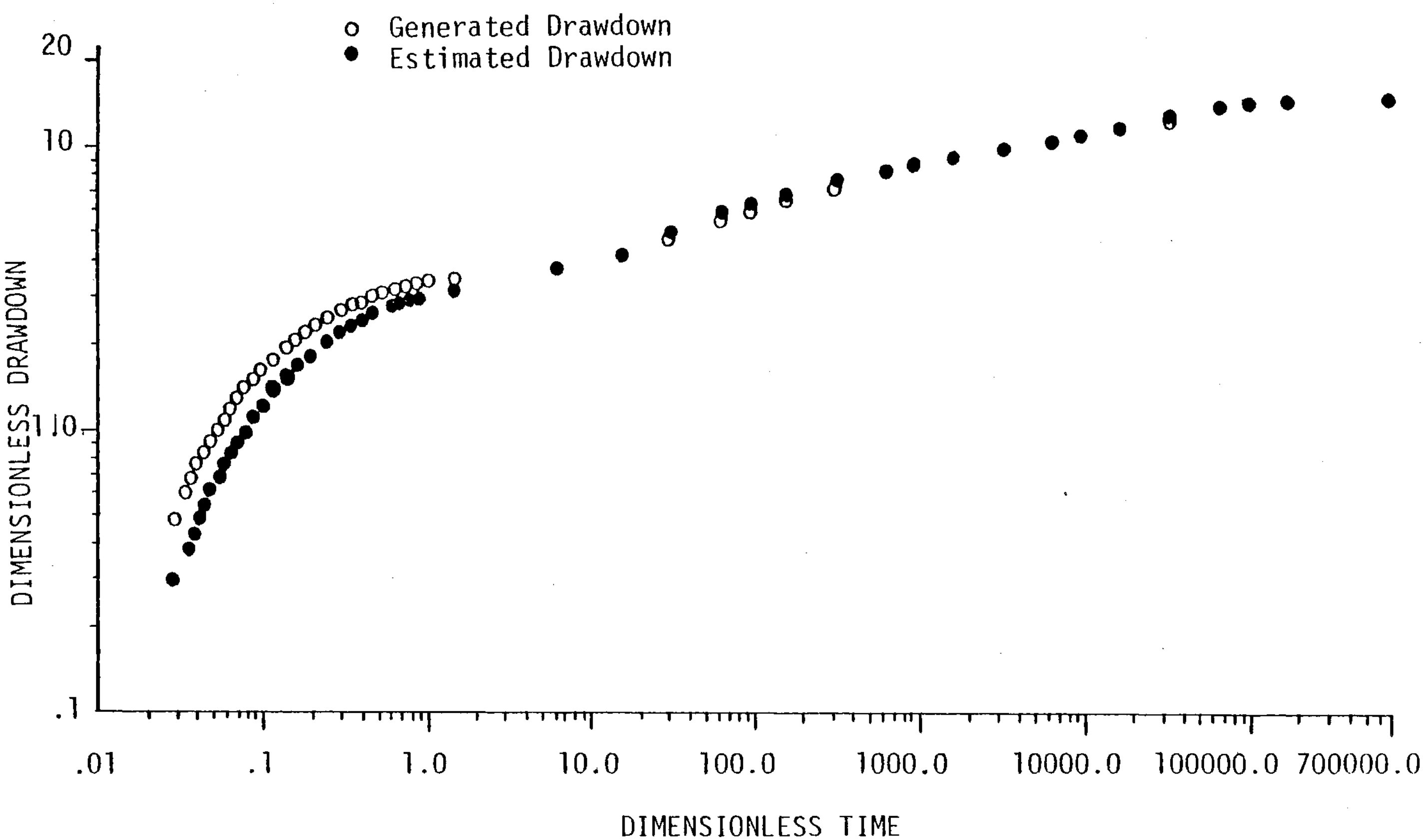

Figure 2. Synthetic data application of the automatic method (48 data points).

a)

Table 3. Relationship Between FX and X(1) for the Following Values of X(2), X(3) and X(4).

X(1)	X(2)	X(3)	X(4)	FX
0.00902	0.10	1.00	10.00	544.7
0.0302	0.10	1.00	10.00	447.2
0.0602	0.10	1.00	10.00	388.6
0.0902	0.10	1.00	10.00	354.5
0.1220	0.10	1.00	10.00	329.5
0.3300	0.10	1.00	10.00	251.7
0.6600	0.10	1.00	10.00	213.1
0.9900	0.10	1.00	10.00	197.9

b)

Table 4. Relationship Between FX and (x1) for the Following Values of X(2), X(3) and X(4).

X(1)	X(2)	X(3)	X(4)	FX
0.00902	1.00	1.00	10.00	215.6
0.0302	1.00	1.00	10.00	146.7
0.0602	1.00	1.00	10.00	109.0
0.0902	1.00	1.00	10.00	89.0
0.1220	1.00	1.00	10.00	75.3
0.3300	1.00	1.00	10.00	39.9
0.6600	1.00	1.00	10.00	25.1
0.9900	1.00	1.00	10.00	20.2

c)

Table 5. Relationship Between FX and X(1) for the Following Values of X(2), X(3) and X(4).

X(1)	X(2)	X(3)	X(4)	FX
0.00902	10.00	1.00	10.00	65.8
0.03020	10.00	1.00	10.00	16.7
0.06020	10.00	1.00	10.00	2.23
0.0902	10.00	1.00	10.00	0.000001
0.1220	10.00	1.00	10.00	1.15
0.3300	10.00	1.00	10.00	17.7
0.6600	10.00	1.00	10.00	36.5
0.9900	10.00	1.00	10.00	48.5

d)

Table 6. Relationship Between FX and X(2) for the Following Values of X(1), X(3) and X(4).

X(1)	X(2)	X(3)	X(4)	FX
0.0902	0.01	1.00	10.00	490.5
0.0902	0.05	1.00	10.00	319.7
0.0902	0.10	1.00	10.00	269.9
0.0902	0.50	1.00	10.00	136.5
0.0902	1.00	1.00	10.00	89.0
0.0902	5.00	1.00	10.00	8.37
0.0902	10.00	1.00	10.00	0.000001
0.0902	50.00	1.00	10.00	44.8
0.0902	100.0	1.00	10.00	91.8
0.0902	500.0	1.00	10.00	260.5
0.0902	1000.0	1.00	10.00	357.2

e)

Table 7. Relationship Between FX and X(2) for the Following Values of X(1), X(3) and X(4).

X(1)	X(2)	X(3)	X(4)	FX
0.0902	0.01	10.00	10.00	662.2
0.0902	0.05	10.00	10.00	508.9
0.0902	0.10	10.00	10.00	455.4
0.0902	0.50	10.00	10.00	288.0
0.0902	1.00	10.00	10.00	217.7
0.0902	5.00	10.00	10.00	77.0
0.0902	10.00	10.00	10.00	38.0
0.0902	50.00	10.00	10.00	9.4
0.0902	100.00	10.00	10.00	19.7
0.0902	500.00	10.00	10.00	106.0
0.0902	1000.00	10.00	10.00	169.3

f)

Table 8. Relationship Between FX and X(2) for the Following Values of X(1), X(3) and X(4).

X(1)	X(2)	X(3)	X(4)	FX
0.302	0.01	10.00	20.00	401.1
0.302	0.05	10.00	20.00	229.2
0.302	0.10	10.00	20.00	168.6
0.302	0.50	10.00	20.00	54.5
0.302	1.00	10.00	20.00	27.8
0.302	5.00	10.00	20.00	46.2
0.302	10.00	10.00	20.00	88.9
0.302	50.00	10.00	20.00	258.7
0.302	100.00	10.00	20.00	366.8
0.302	500.00	10.00	20.00	690.5
0.302	1000.00	10.00	20.00	836.2

g)

Table 9. Relationship Between FX and X(3) for the Following Values of X(1), X(2) and X(4).

X(1)	X(2)	X(3)	X(4)	FX
0.0902	1.00	0.001	10.00	131.6
0.0902	1.00	0.005	10.00	76.7
0.0902	1.00	0.01	10.00	54.3
0.0902	1.00	0.05	10.00	23.4
0.0902	1.00	0.10	10.00	22.8
0.0902	1.00	0.50	10.00	58.5
0.0902	1.00	1.00	10.00	89.0
0.0902	1.00	5.00	10.00	182.5
0.0902	1.00	10.00	10.00	217.7
0.0902	1.00	50.00	10.00	275.8
0.0902	1.00	100.00	10.00	285.6
0.0902	1.00	500.00	10.00	288.8

h)

Table 10. Relationship Between FX and X(3) for the Following Values of X(1), X(2) and X(4).

X(1)	X(2)	X(3)	X(4)	FX
0.0902	10.00	0.001	10.00	525.9
0.0902	10.00	0.005	10.00	350.6
0.0902	10.00	0.010	10.00	268.9
0.0902	10.00	0.05	10.00	116.3
0.0902	10.00	0.10	10.00	66.9
0.0902	10.00	0.50	10.00	5.30
0.0902	10.00	1.00	10.00	0.000001
0.0902	10.00	5.00	10.00	22.5
0.0902	10.00	10.00	10.00	38.0
0.0902	10.00	50.00	10.00	68.9
0.0902	10.00	100.00	10.00	74.8

i)

Table 11. Relationship Between FX and X(3) for the Following Values of X(1), X(2) and X(4).

X(1)	X(2)	X(3)	X(4)	FX
0.0902	50.00	0.001	10.00	926.5
0.0902	50.00	0.004	10.00	661.9
0.0902	50.00	0.010	10.00	528.2
0.0902	50.00	0.05	10.00	287.3
0.0902	50.00	0.10	10.00	206.7
0.0902	50.00	0.50	10.00	77.3
0.0902	50.00	1.00	10.00	44.8
0.0902	50.00	5.00	10.00	10.4
0.0902	50.00	10.00	10.00	9.4
0.0902	50.00	50.00	10.00	15.6
0.0902	50.00	100.00	10.00	17.5
0.0902	50.00	500.00	10.00	18.3
0.0902	50.00	1000.00	10.00	17.9

j)

Table 12. Relationship Between FX and X(3) for the Following Values of X(1), X(2) and X(4).

X(1)	X(2)	X(3)	X(4)	FX
0.0902	100.00	0.001	10.00	1176.0
0.0902	100.00	0.005	10.00	823.6
0.0902	100.00	0.010	10.00	669.5
0.0902	100.00	0.05	10.00	396.5
0.0902	100.00	0.10	10.00	301.9
0.0902	100.00	0.50	10.00	138.3
0.0902	100.00	1.00	10.00	91.8
0.0902	100.00	5.00	10.00	28.9
0.0902	100.00	10.00	10.00	18.7
0.0902	100.00	50.00	10.00	14.5
0.0902	100.00	100.00	10.00	14.6

k)

Table 13. Relationship Between FX and X(3) for the Following Values of X(1), X(2) and X(4).

X(1)	X(2)	X(3)	X(4)	FX
0.0902	100.00	0.001	20.00	7888.1
0.0902	100.00	0.005	20.00	5871.6
0.0902	100.00	0.010	20.00	5080.3
0.0902	100.00	0.05	20.00	3454.9
0.0902	100.00	0.10	20.00	2821.5
0.0902	100.00	0.50	20.00	1520.9
0.0902	100.00	1.00	20.00	1099.2
0.0902	100.00	5.00	20.00	393.9
0.0902	100.00	10.00	20.00	213.1
0.0902	100.00	50.00	20.00	37.8
0.0902	100.00	100.00	20.00	20.5
0.0902	100.00	500.00	20.00	15.1
0.0902	100.00	1000.00	20.00	14.9

ℓ)

Table 14. Relationship Between FX and X(3) for the Following Values of X(1), X(2) and X(4).

X(1)	X(2)	X(3)	X(4)	FX
0.302	1.00	0.001	20.00	10986.6
0.302	1.00	0.005	20.00	1917.8
0.302	1.00	0.010	20.00	1699.2
0.302	1.00	0.050	20.00	1121.3
0.302	1.00	0.10	20.00	860.6
0.302	1.00	0.50	20.00	341.3
0.302	1.00	1.00	20.00	195.6
0.302	1.00	5.00	20.00	32.3
0.302	1.00	10.00	20.00	27.8
0.302	1.00	50.00	20.00	100.1
0.302	1.00	100.00	20.00	136.1
0.302	1.00	500.00	20.00	178.6
0.302	1.00	1000.00	20.00	180.2

m)

Table 15. Relationship Between FX and X(3) for the Following Values of X(1), X(2) and X(4).

X(1)	X(2)	X(3)	X(4)	FX
0.302	0.10	0.001	15.00	344.7
0.302	0.10	0.005	15.00	221.7
0.302	0.10	0.010	15.00	179.7
0.302	0.10	0.050	15.00	92.5
0.302	0.10	0.10	15.00	61.8
0.302	0.10	0.50	15.00	50.2
0.302	0.10	1.00	15.00	74.9
0.302	0.10	5.00	15.00	192.1
0.302	0.10	10.00	15.00	258.4
0.302	0.10	50.00	15.00	376.9
0.302	0.10	100.00	15.00	408.1
0.302	0.10	500.00	15.00	421.9
0.302	0.10	1000.00	15.00	421.8

n)

Talbe 16. Relationship Between FX and X(4) for the Following Values of X(1), X(2) and X(3).

X(1)	X(2)	X(3)	X(4)	FX
0.09020	1.00	1.00	5.00	238.6
0.09020	1.00	1.00	6.00	227.0
0.09020	1.00	1.00	7.00	190.5
0.09020	1.00	1.00	8.00	154.2
0.09020	1.00	1.00	10.00	89.0
0.09020	1.00	1.00	20.00	94.4
0.09020	1.00	1.00	50.00	3965.1
0.09020	1.00	1.00	100.00	19346.4

o)

Table 17. Relationship Between FX and X(4) for the Following Values of X(1), X(2) and X(3).

X(1)	X(2)	X(3)	X(4)	FX
0.302	2.00	100.00	5.00	117.5
0.302	2.00	100.00	6.00	117.5
0.302	2.00	100.00	7.00	117.7
0.302	2.00	100.00	8.00	117.4
0.302	2.00	100.00	10.00	115.7
0.302	2.00	100.00	20.00	81.0
0.302	2.00	100.00	50.00	52.4
0.302	2.00	100.00	100.00	766.2
0.302	2.00	100.00	300.00	11615.7

p)

Table 18. Relationship Between FX and X(4) for the Following Values of X(1), X(2) and X(3).

X(1)	X(2)	X(3)	X(4)	FX
0.0902	10.00	1.00	5.00	56.4
0.0902	10.00	1.00	10.00	0.000001
0.0902	10.00	1.00	20.00	425.1
0.0902	10.00	1.00	50.00	30115.8
0.0902	10.00	1.00	100.00	78527.7

The residuals in Table 1 were analized using the methodology of Chapter 4. A careful look at the residuals in column 4 of Table 1 will reveal that the residuals are not randomly distributed about zero (their supposed mean). On the other hand, they show a systematic deviation.

The first and second moments of the residuals $\underline{r}$ defined by the differences between the "true" and the "estimated" drawdowns, were as follows, according to Equations 4.2 and 4.3

$$E(\underline{r}) = 0.0157$$

$$V(\underline{r}) = 0.0854.$$

As it was considered to be useful to get a picture of the correlation structure of the residuals, two, three and four sets of the residuals were considered, corresponding to the lag of one, two, three, and the following statistical parameters $\underline{\underline{V}}(\underline{r})$ and $\underline{\underline{R}}(\underline{r})$ were obtained, respectively, the variance and the correlation matrix of the residuals r, according to Equations 4.3 and 4.4.

For two sets of residuals $\underline{r}_a$ and $\underline{r}_b$, corresponding to a lag of 1

$$\underline{r}_a = (r_1, \ldots, r_{19})$$
$$\underline{r}_b = (r_2, \ldots, r_{20})$$
$$V(\underline{r}_a) = 0.0832$$
$$V(\underline{r}_b) = 0.0880$$
$$\text{cov}(\underline{r}_a, \underline{r}_b) = 0.0641$$

$$\underline{\underline{V}}(r) = \begin{bmatrix} 0.0832 & 0.0641 \\ 0.0641 & 0.0880 \end{bmatrix}$$

$$\underline{\underline{R}}(r) = \begin{bmatrix} 1.0000 & 0.7489 \\ 0.7489 & 1.0000 \end{bmatrix}.$$

For three sets of residuals, corresponding to lags of one and two,

$$\underline{r}_a = (r_1, \ldots, r_{18})$$
$$\underline{r}_b = (r_2, \ldots, r_{19})$$
$$\underline{r}_c = (r_3, \ldots, r_{20})$$

$$\underline{\underline{V}}(r) = \begin{bmatrix} 0.0794 & 0.0761 & 0.0491 \\ 0.0761 & 0.0854 & 0.0633 \\ 0.0491 & 0.0633 & 0.0856 \end{bmatrix}$$

$$\underline{\underline{R}}(\underline{r}) = \begin{bmatrix} 1.0000 & 0.9242 & 0.5948 \\ 0.9242 & 1.0000 & 0.7406 \\ 0.5848 & 0.7082 & 1.0000 \end{bmatrix}$$

For four sets of residuals, corresponding to lags of one, two, and three,

$$\underline{r}_a = (r_1, \ldots, r_{17})$$
$$\underline{r}_b = (r_2, \ldots, r_{18})$$
$$\underline{r}_c = (r_3, \ldots, r_{19})$$
$$\underline{r}_4 = (r_4, \ldots, r_{20})$$

$$\underline{\underline{V}}(r) = \begin{bmatrix} 0.0724 & 0.0707 & 0.0627 & 0.0468 \\ 0.0707 & 0.0820 & 0.0763 & 0.0468 \\ 0.0627 & 0.0763 & 0.0817 & 0.0569 \\ 0.0468 & 0.0468 & 0.0569 & 0.0791 \end{bmatrix}$$

$$\underline{\underline{R}}(r) = \begin{bmatrix} 1.0000 & 0.9169 & 0.8149 & 0.6190 \\ 0.9169 & 1.0000 & 0.9314 & 0.5815 \\ 0.8149 & 0.9314 & 1.0000 & 0.7082 \\ 0.6190 & 0.5815 & 0.7082 & 1.0000 \end{bmatrix}.$$

As it is illustrated, even for a lag of 4, the autocorrelation matrix shows a high degree of correlation between the residuals. This means that two possible situations may be happening: The model may not be corrected, or, the estimates may not be the "real" ones, which is tantamount to say that the global minimum was not reached. This seems to be the case of this example.

One can conclude that although the automatic estimation method enables one to simulate aquifer behavior quite well, the simulation results are nevertheless likely to be over or underestimated in a systematic way, as seen in Tables 1 and 2 and Figure 1.

In order to evaluate the accuracy of the automatic estimation method, "white Gaussian noise" with mean zero and variance of one foot was superimposed on the "true values". The covariance matrix of the estimated variables $\underline{e}_x$ was computed, assuming that the covariance matrix of the data, $\underline{\underline{V}}_s$, is the identity matrix.

The terms of the Z matrix at the optimum are indicated in Table 19

$$\hat{X}(1) = 0.0902$$
$$\hat{X}(2) = 7.00$$
$$\hat{X}(3) = 1.00$$
$$\hat{X}(4) = 9.007.$$

Table 20 gives the new drawdowns, corresponding to the superposition of the synthetic drawdowns and random noise.

Table 19. Matrix $\underline{\underline{Z}}$ for $\underline{\underline{V}}_s = \underline{\underline{I}}$.

0.00247	0.06324	-0.20155	0.16261
0.00713	0.10841	-0.23659	0.26712
0.01401	0.12542	-0.28132	0.35049
0.10196	0.11912	-0.57951	0.63978
0.28089	0.08909	-0.84082	0.79186
0.48741	0.07152	-0.98193	0.85423
2.73175	0.06163	-1.12844	0.83557
4.56777	0.07770	-1.06457	0.73812
5.59253	0.08809	-1.01675	0.67732
8.09429	0.11655	-0.87239	0.50668
10.86884	0.15131	-0.68192	0.27771
12.10966	0.16731	-0.59385	0.13291
12.43384	0.17154	-0.57862	0.03330
11.98947	0.16585	-0.62433	-0.00814
11.2222	0.15599	-.069619	-0.02316
10.73951	0.15007	-0.73900	-0.03097
9.61764	0.13441	-0.84904	-0.01122
18.81784	0.26381	0.42239	-0.21492
14.12467	0.19792	-0.40421	-0.11281
0.14734	0.00172	-1.77898	-0.19228

Table 20. Synthetic Data Application of the Automatic Method. (Data Superimposed with Random Noise, for $\underline{\underline{V}}_{\hat{s}} = \underline{\underline{I}}$.)

Dimensionless Time	Dimensionless Drawdown	Random Noise	Generated Drawdown	Estimated Drawdown (for the Minimum Found)	Differences (Generated-Estimated)
0.03	0.351	+0.018	0.479	0.236	+0.243
0.06	1.055	-0.26	0.795	0.658	+0.137
0.09	1.463	-0.04	1.423	0.995	+0.428
0.30	2.61	-0.194	2.416	2.089	+0.327
0.60	3.07	-0.464	2.606	2.610	-0.004
0.90	3.256	+0.15	3.406	2.841	+0.565
4.00	3.704	-0.344	3.360	3.458	-0.098
7.00	3.882	-0.406	3.476	3.728	-0.252
9.00	3.979	-0.284	3.695	3.872	-0.177
15.62	4.255	+0.41	4.665	4.264	+0.401
30.62	4.76	+0.005	4.765	4.899	-0.134
50.62	5.268	-0.43	4.838	5.465	-0.627
90.62	5.962	-0.22	5.742	6.149	-0.407
156.2	6.661	+0.35	7.011	6.798	+0.213
306.2	7.508	+0.044	7.552	7.560	-0.008
906.2	8.748	+0.155	8.903	8.715	+0.188
2062.0	9.625	-0.417	9.208	9.555	-0.347
20620.0	12.00	-0.102	11.898	12.259	-0.361
50620.0	13.612	+0.123	13.735	13.839	-0.104
206200.0	15.06	+0.033	15.093	14.546	+0.547

According to Equation 4.10, the variance of the estimation error of each of the four estimating variables was computed as follows

$$(\underline{\underline{Z}}^T \underline{\underline{V}}_s^{-1} \underline{\underline{Z}}) = \begin{bmatrix} .1576E-04 & .2224E+02 & -.7269E+02 & .1289E+02 \\ .2224E+02 & .3714E+00 & -.1342E+01 & .4988E+00 \\ -.7269E+02 & -.1342E+01 & .1318E+02 & -.5550E+01 \\ .1289E+02 & .4988E+00 & -.5550E+01 & .4139E+01 \end{bmatrix}.$$

Now, as $\underline{\underline{V}}(\underline{e}_x) = \sigma_s^2 (\underline{\underline{Z}}^T \underline{\underline{V}}_s^{-1} \underline{\underline{Z}})^{-1}$

$$\underline{\underline{V}}(\underline{e}_x) = \begin{bmatrix} .007433 & -0.4539 & 0.01852 & 0.05639 \\ -0.4539 & 32.02 & -0.6261 & -3.285 \\ 0.01852 & -0.6261 & 0.2797 & 0.3928 \\ 0.05639 & -3.285 & 0.3928 & 0.9886 \end{bmatrix}$$

$$S_{D1} = 0.0862 \qquad \sigma^2(\sigma) = 0.007433$$

$$S_{D2} = 5.667 \qquad \sigma^2(tss) = 32.02$$

$$S_{D3} = 0.5287 \qquad \sigma^2(krr) = 0.2797$$

$$S_{D4} = 0.994 \qquad \sigma^2(b) = 0.9886.$$

It is important to emphasize that the variance of the estimation error of the X(2) variable is high, in this particular case, about three times greater than its true value, which means that some differences between the "true" and the "estimated" value of $X(2)$ may be expected. On the other hand the variances of the estimation errors of $X(1)$, $X(3)$, and $X(4)$ are smaller than their corresponding true values.

The autocorrelation matrix of the estimation error is

$$\underline{\underline{R}}(e_X) = \begin{bmatrix} 1.0000 & -0.9304 & 0.4062 & 0.6578 \\ -0.9304 & 1.0000 & -0.2092 & -0.5839 \\ 0.4062 & -0.2092 & 1.0000 & 0.7470 \\ 0.6578 & -0.5839 & 0.7470 & 1.0000 \end{bmatrix}.$$

There appears to be some degree of correlation between the variables. If this could be expected "a priori" for $X(2)$ and $X(3)$, which depend somehow on common parameters, the same cannot be said about the other variables.

In this synthetic example, the estimation errors obtained through the minimization process are respectively,

$$e_{X(2)} = 10.0 - 7.0 = 3.0$$
$$e_{X(4)} = 10.0 - 9.0 = 1.0$$

$e_{X(2)}$ being significantly smaller than its corresponding standard derivation obtained through the linearized error analysis, which means that the minimization process led to a close estimate of this variable

$$\hat{s}_{X(2)} = 5.67$$
$$\hat{s}_{X(4)} = 0.99.$$

Another example was worked out with a $\underline{\underline{V}}_s$ matrix different than the identity matrix. Assuming that as before measurement errors are independent from each other, the variance of these errors was now allowed to increase with time.

The variance matrix of the data $\underline{\underline{V}}_s$, while diagonal, was then taken as

Table 21. Matrix $\underline{\underline{V}}_s$.

$$\begin{bmatrix} 0.1 \\ & 0.2 \\ & & 0.3 \\ & & & 0.4 \\ & & & & 0.5 \\ & & & & & 0.6 \\ & & & & & & 0.7 \\ & & & & & & & 0.8 \\ & & & & & & & & 0.9 \\ & & & & & & & & & 1.0 \\ & & & & & & & & & & 1.1 \\ & & & & & & & & & & & 1.2 \\ & & & & & & & & & & & & 1.3 \\ & & & & & & & & & & & & & 1.4 \\ & & & & & & & & & & & & & & 1.5 \\ & & & & & & & & & & & & & & & 1.6 \\ & & & & & & & & & & & & & & & & 1.7 \\ & & & & & & & & & & & & & & & & & 1.8 \\ & & & & & & & & & & & & & & & & & & 1.9 \\ & & & & & & & & & & & & & & & & & & & 2.0 \end{bmatrix}$$

The corresponding generated random noise (still normally distributed) is shown in Table 22, as well as the drawdowns corresponding to the superposition of this random noise on the synthetic values.

The newly generated data were then used to obtain new drawdown estimates, as shown in Table 24, together with the corresponding residuals. The latter are again highly correlated.

The sensitivity matrix $\underline{\underline{Z}}$ corresponding to the optimum found is given in Table 23.

Other results are as follows:

$$(\underline{\underline{Z}}^T V_s^{-1} \underline{\underline{Z}}) = \begin{bmatrix} .1130E+04 & .1544E+02 & -.7264E+02 & .1937E+02 \\ .1544E+02 & .4264E+00 & -.1957E+01 & .1159E+01 \\ -.7264E+02 & -.1957E+01 & .1716E+02 & -.9845E+01 \\ .1937E+02 & .1159E+01 & -.9845E+01 & .764E+01 \end{bmatrix}.$$

$$V(\underline{e}_x) = \sigma_s^2 (\underline{\underline{Z}}^T \underline{\underline{V}}_s^{-1} \underline{\underline{Z}})^{-1}$$

$$\underline{\underline{V}}(\underline{e}_x) = \begin{bmatrix} 0.003442 & -0.1285 & 0.2333 & 0.04081 \\ -0.1285 & 9.740 & -0.3607 & -1.614 \\ 0.02335 & -0.3607 & 0.4343 & 0.5550 \\ 0.04081 & -1.614 & 0.5550 & 0.9869 \end{bmatrix}$$

Table 22. Synthetic Data Application of the Automatic Method. (Data Superimposed with Random Noise for $\underline{\underline{V}}_s \neq \underline{\underline{I}}$.)

Dimen-sionless Time	Dimen-sionless Drawdown	Random Noise	Generated Drawdown	Estimated Drawdown (for the Minimum Found)	Differences (Generated-Estimated)
0.03	0.461	+0.002	0.463	0.282	+0.181
0.06	1.055	-0.052	1.003	0.746	+0.257
0.09	1.463	-0.012	1.451	1.105	+0.346
0.30	2.61	-0.078	2.532	2.213	+0.319
0.60	3.07	-0.232	2.838	2.722	+0.116
0.90	3.256	+0.090	3.346	2.949	+0.397
4.00	3.704	-0.241	3.463	3.565	-0.102
7.00	3.882	-0.325	3.557	3.841	-0.284
9.00	3.979	-0.256	3.723	3.992	-0.269
15.62	4.255	+0.41	4.665	4.900	-0.235
30.62	4.760	+0.006	4.766	5.047	-0.281
50.62	5.268	-0.516	4.752	5.628	-0.876
90.62	5,962	-0.286	5.676	6.341	-0.665
156.2	6.661	+0.49	7.15	6.980	+0.170
306.2	7.508	+0.066	7.574	7.748	-0.174
906.2	8.748	+0248	8.996	8.907	+0.089
2062.0	9.625	-0.710	8.915	9.734	-0.819
20620.0	12.00	-0.184	11.816	12.498	-0.682
50620.0	13.612	+0.233	13.845	14.052	-0.207
206200.0	15.06	+0.066	15.126	14.684	+0.442

Table 23. Matrix $\underline{\underline{Z}}$ for $\underline{\underline{V}}_s \neq \underline{\underline{I}}$.

0.00239	0.06838	-0.23197	0.16815
0.00717	0.11188	-0.28485	0.28691
0.01437	0.12544	-0.34296	0.37547
0.10562	0.11637	-0.66987	0.67596
0.29394	0.08598	-0.93962	0.82603
0.51074	0.06858	-1.08422	0.88655
2.8570	0.05993	-1.22313	0.86009
4.7654	0.07664	-1.1470	0.75041
5.82656	0.08716	-1.09542	0.68295
8.40274	0.11545	-0.9450	0.50337
11.22455	0.14931	-0.7520	0.26999
12.45032	0.16445	-0.66174	0.13173
12.70718	0.16767	-0.65283	0.03416
12.17732	0.16116	-0.70632	-0.00538
11.32087	0.15062	-0.78620	-0.01871
10.77752	0.14420	-0.83446	-0.02509
9.51267	0.12731	-0.95835	-0.00307
18.95432	0.25448	-0.37898	-0.20504
13.50342	0.18120	-0.56418	-0.09034
0.11306	0.00120	-1.88120	0.19222

$$s_{D1} \equiv 0.05867 \qquad \sigma_1^2 = 0.00342$$
$$s_{D2} \equiv 3.121 \qquad \sigma_2^2 \equiv 9.74$$
$$s_{D3} = 0.6590 \qquad \sigma_3^2 = 0.4343$$
$$s_{D4} = 0.993 \qquad \sigma_4^2 = 0.9869.$$

This solution is quite similar to that obtained earlier with $\underline{\underline{V}}_s = \underline{\underline{I}}$, indicating that the consideration of different variances for the errors associated with each drawdown measurement has no significant effect on the results obtained. It can be noted, though, that the variances of the estimation errors X(1) and X(2) are smaller than in the preceeding case, the variance of the estimation error of X(4) is nearly the same, and the variance of the estimation error of X(3) is now greater than it was before.

Two negative aspects should be noted based on the tests performed with these synthetic data. The first is that the residuals (the differences between the estimated and true data) appear to be always highly correlated, implying a systematic overestimation or underestimation of drawdowns. The second negative aspect is that, at least for the range of values of the variables tested, the objective function appears to be irregularly shaped. This may lead the minimization procedure to local minima quite different from the global one, if the initial solution is not close enough to the real solution.

Finally, it was considered useful to evaluate the influence on the results obtained through the minimization process of the values assigned as initial solutions to each of the estimated variables.

a) Considering the following values assigned to the estimated variables

$$X(1) = 0.09020$$
$$X(2) = 10.00$$
$$X(3) = 100.00$$
$$X(4) = 10.00$$

the dimensionless hydraulic parameters of the aquifer, used in the generation of new synthetic data, were the following

$$\sigma = 0.0920$$
$$\beta = 1.00$$
$$PD = 0.50$$
$$BD = 0.00$$
$$ZD = 0.00$$
$$Z_{D1} = 0.50$$
$$Z_{D2} = 1.00.$$

The objective function, for the following initial solution (the same as the previous example), took the value FX = 22.6

X(1) = 0.09020

X(2) = 4.00

X(3) = 1.00

X(4) = 6.00.

The minimization process lead to a local minimum, for which FX = 4.29, which correspond to the following estimates of the variables

X(1) = .09020

X(2) = 1.33

X(3) = 1.00

X(4) = 5.00.

Though the following variables were allowed to vary, only the X(2) and X(4) indeed changed the values from the ones assigned in the initial solution. The minimum reached is, though, quite different than the global one.

b) Considering the following values assigned to the estimation variables

X(1) = 0.02020

X(2) = 10.00

$$X(3) = 100.00$$

$$X(4) = 10.00.$$

The dimensionless hydraulic parameters of the aquifer, used in the generation of new synthetic data, were the following

$$\sigma = 0.02020$$

$$\beta = 1.00$$

$$P_D = 0.50$$

$$B_D = 0.00$$

$$Z_D = 0.00$$

$$Z_{D1} = 0.50$$

$$Z_{D2} = 1.00.$$

The objective function, for the following initial solution (the same as in the previous examples), took the value FX = 124.74

$$X(1) = 0.09020$$

$$X(2) = 4.00$$

$$X(3) = 1.00$$

$$X(4) = 6.00.$$

The minimization process lead to a local minimum, for which

FX = 6.66, which correspond to the following estimates of the variables

$$X(1) = 0.9020$$
$$X(2) = 0.124$$
$$X(3) = 1.00$$
$$X(4) = 5.00.$$

Again, only X(2) and X(4) had their values changed from the ones assigned as initial solution, and the response of the program was similar to the precedent one, again with a local minimum reached quite different than the global one.

c) Considering the following values assigned to the estimation variables

$$X(1) = 0.66$$
$$X(2) = 10.00$$
$$X(3) = 1.00$$
$$X(4) = 10.00.$$

The dimensionless hydraulic parameters of the aquifer, used in the generation of new synthetic data, were the following

$$\sigma = 0.66$$
$$\beta = 0.01$$

$$P_D = 0.50$$

$$B_D = 0.00$$

$$Z_{D1} = 0.50$$

$$Z_{D1} = 1.00.$$

The objective function, for the following initial solution (again the same as in the previous examples), took the value FX = 8.5, which correspond to the following estimates of the variables

$$X(1) = 0.09020$$

$$X(2) = 6.72$$

$$X(3) = 1.00$$

$$X(4) = 8.72.$$

Again, only X(2) and X(4) had their values changed from the ones assigned in the initial solution. This time, though, that change was, in the case of both variables, a change in the direction of the global minimum. The value of X(4) is not very different than the corresponding "real" one, and X(2) became significantly close to the corresponding "real" one.

d) Considering the following values assigned to the estimation variable

$$X(1) = 0.9020$$
$$X(2) = 10.00$$
$$X(3) = 100.00$$
$$X(4) = 10.00.$$

The dimensionless hydraulic parameters of the aquifer, used in the generation of new synthetic data, were the following

$$\sigma = 0.9020$$
$$\beta = 1.00$$
$$P_D = 0.50$$
$$B_D = 0.00$$
$$Z_D = 0.00$$
$$Z_{D1} = 0.50$$
$$Z_{D2} = 1.00.$$

The objective function, for the following initial solution (the same taken in the previous examples), took the value FX = 47.4

$$X(1) = 0.9020$$
$$X(2) = 4.00$$
$$X(3) = 1.00$$
$$X(4) = 6.00.$$

The process lead to a local minimum, for which FX = 7.3, which correspond to the following estimates of the variables

X(1) = 0.09020

X(2) = 0.701

X(3) = 1.00

X(4) = 5.00.

Again, only the variable X(2) suffered a change, leading to a local minimum quite far from the global one.

From the above examples, and other computer runs performed, it was concluded that this minimization procedure is not very sensitive to the values assumed to the X(1) and X(3) variables. As a matter of fact in none of the above examples these two variables had their values changed from the ones assigned in the initial solution. Furthermore, it seems that if X(3) is assigned a value significantly different than the "real" one, the minimization process is likely to lead to local minima far away from the global one, with X(2) and X(4) assuming values much different than their corresponding "real" ones.

Pumping Test of Fairborn, Ohio

The program developed was tested on "real" data from a pumping test reported by Lohman (1972) near Fairborn, Ohio, in October of 1954.

A well is pumped at a constant rate of 1080 gpm for fifty hours. The pumped well is eighty-five feet deep, and reportedly screened to the full depth of a glacial formation of sand and gravel. The observation well is ninety-five feet deep and penetrates seventy-five feet of the water-bearing formation. The corrected drawdowns in the observation well are given in column 1 of Table 24.

Initial values of $\underline{X}$ were based on Lohman's analysis of the data. The best result obtained corresponds to the following solution:

$$X(1) = 0.085$$

$$X(2) = 2.67$$

$$X(3) = 160.0$$

$$X(4) = 75.00$$

at which the objective function took the value of FX = 4.68. Figure 3 shows the drawdons versus time curves for the optimum results, compared to the observed ones.

In order to evaluate better the behavior of the objective function, and its dependence on the initial values assigned to each of the variables, several computer runs were performed using only twenty data observations. Again, the highly irregular shape of the objective function led to

Table 24. Ohio Data Application of the Automatic Method.

Time (min)	Corrected Drawdown (ft)	Estimated Drawdown (ft)	Differences (ft)
0.165	0.12	0.156	-0.036
0.25	0.195	0.236	-0.041
0.34	0.255	0.303	-0.048
0.42	0.33	0.35	-0.02
0.50	0.39	0.39	+0.00
0.58	0.43	0.42	+0.01
0.66	0.49	0.45	+0.04
0.75	0.53	0.48	+0.05
0.83	0.57	0.51	+0.06
0.92	0.61	0.53	+0.08
1.00	0.64	0.55	+0.09
1.08	0.67	0.57	+0.10
1.16	0.70	0.59	+0.11
1.24	0.72	0.60	+0.12
1.33	0.74	0.62	+0.12
1.42	0.76	0.63	+0.13
1.50	0.78	0.64	+0.14
1.68	0.82	0.66	+0.16
1.85	0.84	0.69	+0.15
2.00	0.86	0.70	+0.16
2.15	0.87	0.72	+0.15
2.35	0.90	0.73	+0.17

Table 24 -- (Continued)

Time (min)	Corrected Drawdown (ft)	Estimated Drawdown (ft)	Differences (ft)
2.50	0.91	0.75	+0.16
2.65	0.92	0.76	+0.16
2.80	0.93	0.77	+0.16
3.0	0.94	0.78	+0.16
3.5	0.95	0.81	+0.14
4.0	0.97	0.83	+0.14
4.5	0.975	0.845	+0.13
5.0	0.98	0.86	+0.12
6.0	0.99	0.89	+0.10
7.0	1.00	0.91	+0.09
8.0	1.01	0.92	+0.09
9.0	1.015	0.94	+0.075
10	1.02	0.95	+0.07
12	1.03	0.97	+0.06
15	1.04	1.00	+0.04
18	1.05	1.03	+0.02
20	1.05	1.04	+0.02
25	1.08	1.08	+0.00
30	1.13	1.11	+0.02
35	1.15	1.14	+0.01
40	1.17	1.17	+0.00
50	1.18	1.22	-0.03

Table 24 -- (Continued)

Time (min)	Corrected Drawdown (ft)	Estimated Drawdown (ft)	Differences (ft)
60	1.22	1.26	-0.04
70	1.25	1.30	-0.05
80	1.28	1.34	-0.06
90	1.29	1.37	-0.08
100	1.31	1.40	-0.09
120	1.36	1.46	-0.10
150	1.45	1.53	-0.08
200	1.52	1.62	-0.10
250	1.59	1.70	-0.11
300	1.65	1.76	-0.11
365	1.70	1.82	-0.12
400	1.75	1.86	-0.11
500	1.85	1.94	-0.09
600	1.95	2.00	-0.05
700	2.01	2.06	-0.05
800	2.09	2.11	-0.02
900	2.15	2.15	+0.00
1000	2.20	2.19	+0.01
1200	2.27	2.25	+0.02
1500	2.35	2.33	+0.02
2000	2.48	2.43	+0.06
2500	2.59	2.52	+0.07

Table 24 -- (Continued)

Time (min)	Corrected Drawdown (ft)	Estimated Drawdown (ft)	Differences (ft)
3000	2.66	2.58	+0.08
3340	4.05	4.00	+0.05
3400	4.05	4.02	+0.03
3460	4.07	4.03	+0.04
3820	4.14	4.11	+0.03
4180	4.20	4.19	+0.01
4240	4.21	4.20	+0.01
4270	4.20	4.20	+0.00

successive convergences of local minima rather than the global one. Table 25 shows some of the results obtained.

Finally, and using again all the data available, a new computer run was performed, considering the following initial guess

$$X(1) = 0.04$$

$$X(2) = 8.90$$

$$X(3) = 50000.00$$

$$X(4) = 75.00$$

for which the objective function took the value FX = 663.8.

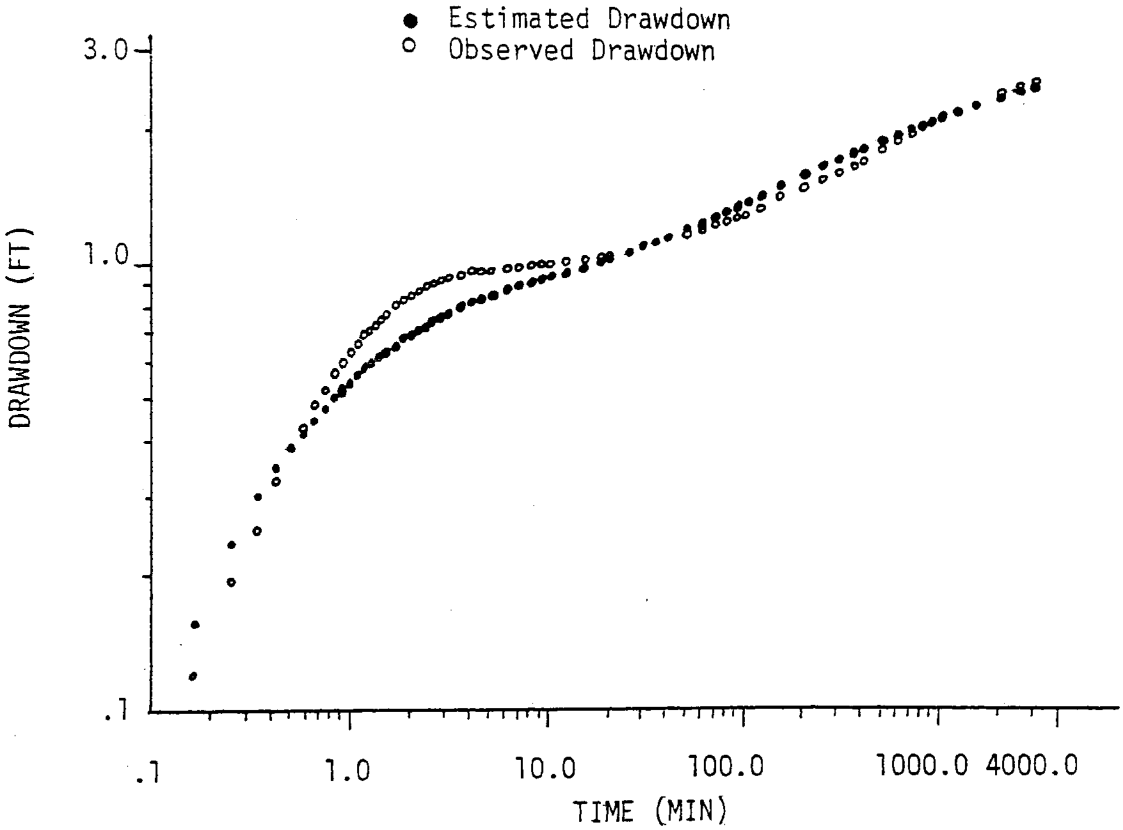

Figure 3. Automatic estimation of aquifer parameters Ohio pumping test.

Table 25. Minimum of Objective Function for Various Initial Guesses.

	Initial Guess	Minimum	Initial Guess	Minimum	Initial Guess	Minimum	Initial Guess	Minimum
X(1)	0.0902		0.29		0.0702		0.07	
X(2)	90.00		90.00		60.00		90.00	
X(3)	144.00		144.00		191.00		144.00	
X(4)	76.00		76.00		76.00		76.00	
FX	10.47		28.74		40.4		8.41	
X(1)	0.05		0.03	0.03	0.03	0.03	0.03	0.03
X(2)	90.00		99.00	89.015	89.00	87.31	88.00	89.09
X(3)	144.00		144.00	144.00	50.00	50.00	250.00	250.00
X(4)	76.00		76.00	76.00	76.00	76.00	76.00	76.00
FX	7.09		7.50	7.20	11.15	10.86	6.40	6.04
X(1)	0.03	0.03	0.03	0.03	0.03			
X(2)	89.00	89.015	89.00	89.081	89.00			
X(3)	500.00	500.00	10000.00	10000.00	50000.00			
X(4)	76.00	76.00	76.00	76.00	76.00			
FX	5.55	5.11	5.01	4.52	4.50			

The minimum found, FX = 100.5, a local minimum, corresponds to the following estimates

$$X(1) = 0.04$$
$$X(2) = 70.00$$
$$X(3) = 50000.00$$
$$X(4) = 75.00.$$

In conclusion, the best results, shown in Figure 3, corresponding to the ones presented in Lohman's analysis, are the following:

$$X(1) = 0.085$$
$$X(2) = 2.64$$
$$X(3) = 160.0$$
$$X(4) = 75.00.$$

From the test run, where X(4) was always kept constant, and equal to its true value, it can be concluded that the minimization procedure did not appear to be very sensitive to the values assigned to the X(1) variable as initial guesses; only the variable X(2) was automatically adjusted in the minimization process for an adequate range of the X(3) variable; the highly irregular shape of the objective function did not enable a convergence to the global minimum of the objective function.

Pumping Test of Iowa, Colorado

A second example concerns data from a pumping test performed in August of 1967 near Iowa, Colorado, and reported by Lohman (1972).

The data taken from Lohman's work are given in Table 26, correspond to observation well 82-66-7dda 2, which is sixty-three feet from a fully penetrating, fully screened well pumped at an average rate of 1170 gpm for seventy-one hours. The wells are located in unconfined alluvium, having an initial saturated thickness of 39.4 feet. The pumping well is 56.5 feet deep and the observation well penetrates to a depth of 25.8 feet.

From the analysis of the data developed by Lohman (1972) several initial solutions were considered, and the computer program tested, using the sixty-seven data points presented in Table 26.

The best result obtained corresponds to the following solution:

$$X(1) = 0.04$$

$$X(2) = 0.66$$

$$X(3) = 58.00$$

$$X(4) = 40.00.$$

Table 26. Colorado Data Application of the Automatic Method.

Time	Corrected Drawdown (ft)	Estimated Drawdown (ft)	Differences (ft)
1	0.28	0.31	-0.03
2	0.38	0.46	-0.08
3	0.38	0.53	-0.15
4	0.44	0.58	-0.14
5	0.48	0.62	-0.14
6	0.50	0.65	-0.15
7	0.52	0.67	-0.15
8	0.53	0.69	-0.16
9	0.56	0.71	-0.15
10	0.56	0.73	-0.13
12	0.61	0.75	-0.14
14	0.65	0.78	-0.13
16	0.67	0.80	-0.13
18	0.70	0.82	-0.12
20	0.72	0.83	-0.11
24	0.79	0.86	-0.07
28	0.82	0.89	-0.07
36	0.92	0.93	-0.01
40	0.86	0.96	+0.00
50	1.00	1.01	-0.01
60	1.15	1.06	+0.09

Table 26 -- (Continued)

Time (min)	Corrected Drawdown (ft)	Estimated Drawdown (ft)	Differences (ft)
70	1.24	1.11	+0.13
80	1.30	1.15	+0.15
90	1.38	1.20	+0.18
100	1.42	1.24	+0.18
120	1.55	1.33	+0.22
140	1.67	1.41	+0.26
160	1.74	1.49	+0.25
180	1.84	1.56	+0.28
200	1.93	1.63	+0.30
240	2.05	1.75	+0.30
280	2.12	1.87	+0.30
320	2.27	1.97	+0.30
360	2.36	2.07	+0.29
400	2.48	2.16	+0.32
460	2.55	2.28	+0.27
520	2.66	2.38	+0.28
580	2.74	2.48	+0.26
700	2.91	2.64	+0.27
820	3.02	2.78	+0.24
940	3.17	2.91	+0.26
1060	3.22	3.02	+0.20

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Table 26 -- (Continued)

Time (min)	Corrected Drawdown (ft)	Estimated Drawdown (ft)	Differences (ft)
3160	4.02	3.96	+0.06
3220	4.04	3.97	+0.07
3280	4.03	3.99	+0.04

For these values, the corresponding value of the objective was FX = 3.50.

Figure 4 shows the curves drawdown versus time correspondent to the initial solution, and to the minimum found.

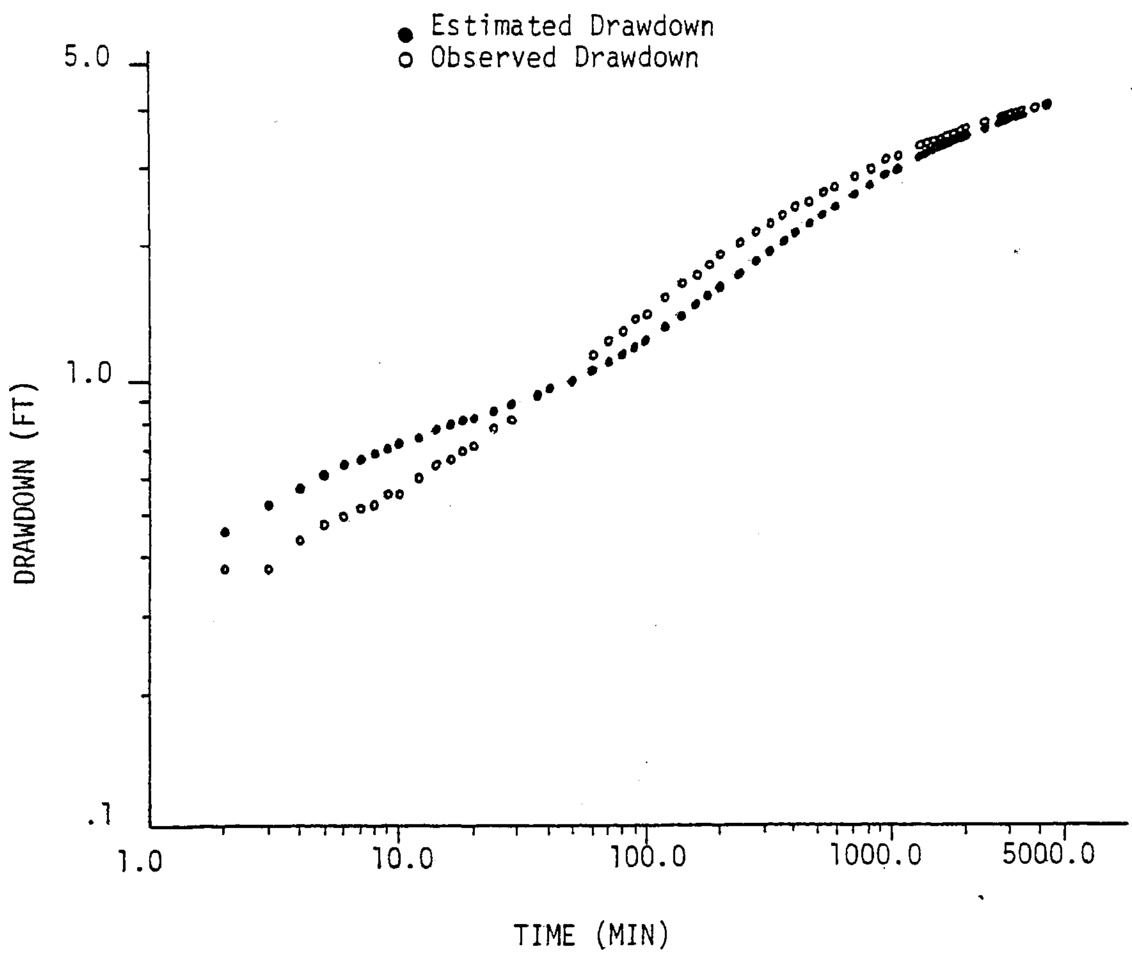

Figure 4. Automatic estimation of aquifer parameters Colorado pumping test.

CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

The method presented in this thesis enables the automatic analysis of pumping test data from unconfined aquifers. Good judgement has, however, still to be considered in using this automatic method, namely the choice of the initial solutions.

The computer program developed for the automatic estimation of the hydraulic parameters of unconfined aquifers is based on Neuman' analytical solution for drawdowns, and it uses a minimization subroutine developed for non-linear functions. This subroutine uses a gradient "feasible directions method", and it required the development of subroutines for the evaluation of the first order derivatives of the analytical drawdown, in order to each of the hydraulic parameters of the aquifer to be estimated.

The computer program was tested using synthetic data, and using data from two pumping tests performed in unconfined aquifers. It enabled a close simulation of the aquifers behavior.

As the objective function which is minimized is not convex, the minimization subroutine may converge to local minima instead of the desired global minimum.

It is then advisable to take into account the following recommendations in the use of this program:

1. consider at the beginning a reduced number of data points, instead of all the available data. A number of ten to twenty data points should be adequate to provide the user with a picture of the behavior of the minimization subroutine in its particular case, without requiring too much computer time spent in the preliminary computer runs;

2. for this reduced number of data points, and starting from the best initial solution that the available information allows, perform a computer run considering high values for the tolerence error TOLFX, and limiting the number of iterations NIBR to values of the order of six to twelve;

3. based on the analysis of the results obtained, perform a series of computer runs changing methodically the new initial solutions to new values that might be more adequate, and increasing slowly the tolerance error TOLFX and the number of iterations NIBR as the function is converging to a minimum that might be considered a global one;

4. once the minimum is found, perform several other computer runs, changing at a time the values of each of the estimated variables, in order to develop a sensitivity analysis of the results obtained;

5. finally, for the estimates found, get the value of the hydraulic parameters of the aquifer from the

expressions presented in Chapter 2. It is necessary to start by evaluating the values of S or S_y, that should not be difficult as the early or late drawdown will follow the Theys equation.

Form the analysis developed, it was concluded that the subroutine used for the minimization task is not very adequate for this type of program.

On the other hand, it is important to emphasize that, from the sensitivity analyses developed with synthetic and real data, the values assigned to the variable X(3) which corresponds to the hydraulic parameter K_D, play a significant role in the minimization process, though the value of this variable is not likely to suffer any significant change during this process. The same was verified with the variable X(1), which correpsonds to the ratio S/S_y. It is then important, in order to guarantee a successful convergency to the globel minimum of the objective function, that to X(1) and X(3) are assigned values not very different than the correspondent "true" ones.

The analysis of the results obtained also show that it would be important to consider another type of objective function, namely, one defined by the square of the differences between the natural logarithms of the estimated and the observed drawdowns. Such an objective function would tend to represent in a better way the aquifer response in the early part of the pumping test.

It is then the intention of the author to proceed with this work, trying to get a better performing computer program, and, at the same time, introducing a choice for an alternative objective function which will underestimate the weight of the late drawdown data. In this future development, a fifth decision variable, the distance from the observation well to a natural boundary of the aquifer system will be also introduced, to allow a more generalized use of this automatic method.

APPENDIX 1

EVALUATION OF THE DERIVATIVES

Derivative of F(σ,tss,krr,b) in Order to σ

$$\frac{\partial F}{\partial \sigma}(\sigma,tss,krr,b) = \sum_{i=1}^{m} 2[s_i(\sigma,tss,krr,b) - \ell_i]\frac{\partial s_i}{\partial \sigma}(\sigma,tss,krr,b)$$

$$\frac{\partial s_i}{\partial \sigma} = \int_0^{\infty} 4yJ_0(y\beta^{1/2})\left[\frac{\partial U_0(y)}{\partial \sigma} + \sum_{n=1}^{\infty}\frac{\partial U_n(y)}{\partial \sigma}\right]dy$$

$$\frac{\partial U_0(y)}{\partial \sigma} = \{[\{-\exp[-ts\beta(y^2-\gamma_0^2)]\}\cdot[2ts\beta\gamma_0\cdot\frac{\partial \gamma_0}{\partial \sigma}][\sinh(\gamma_0 Z_{2D})$$

$$- \sinh(\gamma_0 Z_{1D})]\cdot\{\sinh[\gamma_0(1-d_D)] - \sinh[\gamma_0(1-\ell_D)]\}$$

$$+ \{1 - \exp[-ts\beta(y^2-\gamma_0^2)]\}$$

$$\cdot [Z_{2D}\cosh(\gamma_0 Z_{2D})\frac{\partial \gamma_0}{\partial \sigma} - Z_{1D}\cosh(\gamma_0 Z_{1D})\frac{\partial \gamma_0}{\partial \sigma}]$$

$$\cdot \{\sinh[\gamma_0(1-d_D)] - \sinh[\gamma_0(1-\ell_D)]\}$$

$$+ \{1 - \exp[-ts\beta(y^2-\gamma_0^2)]\}\cdot[\sinh(\gamma_0 Z_{2D}) - \sinh(\gamma_0 Z_{1D})]$$

$$\cdot \{(1-d_D)\cosh[\gamma_0(1 - d_D)\cdot\frac{\partial \gamma_0}{\partial \sigma}$$

$$- (1-\ell_D)\cosh[\gamma_0(1-\ell_D)\ \frac{\partial\gamma_0}{\partial\sigma}\}]$$

$$\cdot\ \{[y^2 + (1+\sigma)\gamma_0^2 - \frac{(y^2-\gamma_0^2)^2}{\sigma}]\cosh(\gamma_0)$$

$$\cdot\ (Z_{2D}-Z_{1D})\gamma_0(\ell_D-d_D)\cdot\sinh(\gamma_0)$$

$$- [\{1-\exp[-ts\beta(y^2-\gamma_0^2)]\ [\sinh(\gamma_0 Z_{2D}) - \sinh(\gamma_0 Z_{1D})]$$

$$\cdot\ \{\sinh[\gamma_0(1-d_D)] - \sinh[\gamma_0(1-\ell_D)]$$

$$\cdot\ \{[+2\gamma_0\ \frac{\partial\gamma_0}{\partial\sigma} + \gamma_0^2 + 2\sigma\gamma_0\ \frac{\partial\gamma_0}{\partial\sigma} - 2(y^2-\gamma_0^2)\frac{(-2\gamma_0)}{\sigma}\cdot\frac{\partial\gamma_0}{\partial\sigma}$$

$$+ \frac{(y^2-\gamma_0^2)^2}{\sigma^2}]\cdot[\cosh(\gamma_0)\cdot(Z_{2D}-Z_{1D})\gamma_0\cdot(\ell_D-d_D)\cdot\sinh(\gamma_0)]$$

$$+ [y^2 + (1+\sigma)\ {}_0^2 - \frac{(y^2-\gamma_0^2)^2}{\sigma}]\cdot[\sinh(\gamma_0)\ \frac{\partial\gamma_0}{\partial\sigma}\cdot(Z_{2D}-Z_{1D})\gamma_0$$

$$\cdot\ (\ell_D-d_D)\sinh(\gamma_0) + \cosh(\gamma_0)\ (Z_{2D}-Z_{1D}0\ \frac{\partial\gamma_0}{\partial\sigma}$$

$$\cdot\ (\ell_D-d_D)\cdot\sinh(\gamma_0) + \cosh(\gamma_0)\cdot(Z_{2D}-Z_{1D})\cdot\gamma_0$$

$$\cdot\ (\ell_D-d_D)\cdot\cosh(\gamma_0)\frac{\partial\gamma_0}{\partial\sigma}]\}]\}/\{[y^2 + (1+\sigma)\gamma_0^2 - \frac{(y^2-\gamma_0^2)^2}{\sigma}]$$

$$\cdot\ \cosh(\gamma_0)\ (Z_{2D}-Z_{1D})\gamma_0\cdot(\ell_D-d_D)\cdot\sinh(\gamma_0)\}^2$$

$$\frac{\partial U_n(y)}{\partial \sigma} = \{[\{-\exp[-ts\beta(y^2+\gamma_n^2)]\}\cdot[-2ts\beta\gamma_n\frac{\partial\gamma_n}{\partial\sigma}]$$

$$\cdot\ [\sin(\gamma_n Z_{2D}) - \sin(\gamma_n Z_{1D})]\cdot\{\sin[\gamma_n(1-d_D)]$$

$$-\ \sin[\gamma_n(1-\ell_D)]\} + \{1 - \exp[-ts\beta(y^2+\gamma_n^2)]\}$$

$$\cdot\ [Z_{2D}\cos(\gamma_n Z_{2D})\frac{\partial\gamma_n}{\partial\sigma} - Z_1\ \cos(\gamma_n Z_{1D})\cdot\frac{\partial\gamma_n}{\partial\sigma}]$$

$$\cdot\ \{\sin[\gamma_n(1-d_D)] - \sin[\gamma_n(1-\quad)]\}$$

$$+\ \{1- \exp[-ts\beta(y^2+\gamma_n^2)]\}\cdot[\sin(\gamma_n Z_{2D}) - \sin(\gamma_n Z_{1D})]$$

$$\cdot\ \{(1-d_D)\cos[\gamma_n(1-d_D)]\frac{\partial\gamma_n}{\partial\sigma} - (1-\ell_D)\cos[\gamma_n(1-\ell_D)]\cdot\frac{\partial\gamma_n}{\partial\sigma}\}$$

$$\cdot\ [[y^2-(1+\sigma)\gamma_n^2 - \frac{(y^2+\gamma_n^2)^2}{\sigma}]\cdot\cos(\gamma_n)\cdot(Z_{2D}-Z_{1D})\gamma_n$$

$$\cdot\ (\ell_D-d_D)\sin(\gamma_n)] - [\{1 - \exp[-ts\beta(y^2+\gamma_n^2)]$$

$$\cdot\ [\sin(\gamma_n Z_{2D}) - \sin[\gamma_n Z_{1D})]\cdot\{\sin[\gamma_n(1-d_D)]$$

$$-\ \sin[\gamma_n(1-\ell_D)]\}\cdot\{[-2\gamma_n\frac{\partial\gamma_n}{\partial\sigma} - \gamma_n^2 - 2\sigma\gamma_n\cdot\frac{\partial\gamma_n}{\partial\sigma}$$

$$-\ 2(y^2+\gamma_n^2)\cdot\frac{2\gamma_n}{\sigma}\cdot\frac{\partial\gamma_n}{\partial\sigma} + \frac{(y^2+\gamma_n^2)^2}{\sigma^2}]$$

$$\cdot\ [\cos(\gamma_n)(Z_{2D}-Z_{1D})\gamma_n(\ell_D-d_D)\sin(\gamma_n)]$$

$$+\ [y^2 - (1+\sigma)\gamma_n^2 - \frac{(y_2+\gamma_n^2)^2}{\sigma}]\cdot[-\sin(\gamma_n)\ \frac{\partial\gamma_n}{\partial\sigma}\cdot(Z_{2D}-Z_{1D})\gamma_n$$

$$\cdot\ (\ell_D-d_D)\cdot\sin(\gamma_n) + \cos(\gamma_n)\cdot(Z_{2D}-Z_{1D})\frac{\partial\gamma_n}{\partial\sigma}\cdot(\ell_D-d_D)$$

$$\cdot\ \sin(\gamma_n) + \cos(\gamma_n)\cdot(Z_{2D}-Z_{1D})\cdot\gamma_n\cdot(\ell_D-d_D)\cdot\cos(\gamma_n)$$

$$\cdot\ \frac{\partial\gamma_n}{\partial\sigma}]\}]\}/\{[y^2 - (1+\sigma)\gamma_n^2 - \frac{(y^2+\gamma_n^2)^2}{\sigma}]\ \cos(\gamma_n)$$

$$\cdot\ (Z_{2D}-Z_{1D})\gamma_n\cdot(\ell_D-d_D)\cdot\sin(\gamma_n)\}.$$

The derivatives $\frac{\partial\gamma_0}{\partial\sigma}$ and $\frac{\partial\gamma_n}{\partial\sigma}$ are obtained from the Equations (2.4) and (2.5) respectively.

$$\frac{d}{d\sigma}[\sigma\gamma_0\sinh(\gamma_0) - (y^2 - \gamma_0^2)\cosh(\gamma_0)] = 0$$

$$\gamma_0\sinh(\gamma_0) + \sigma[\frac{\partial\gamma_0}{\partial\gamma}\sinh(\gamma_0) + \cosh(\gamma_0)\cdot\gamma_0\ \frac{\partial\gamma_0}{\partial\sigma}]$$

$$-\ \sinh(\gamma_0)\cdot(y^2 - \gamma_0^2)\ \frac{\partial\gamma_0}{\partial\gamma} + \cosh(\gamma_0)$$

$$\cdot\ (-2\gamma_0)\cdot\frac{\partial\gamma_0}{\partial\sigma}] = 0$$

$$\gamma_0\sinh(\gamma_0) + \sigma\sinh(\gamma_0)\frac{\partial\gamma_0}{\partial\sigma} + \sigma\gamma_0\cosh(\gamma_0)\frac{\partial\gamma_0}{\partial\sigma}$$

$$- \; (y^2-\gamma_0^2)\cdot \sinh(\gamma_0)\frac{\partial\gamma_0}{\partial\sigma} \; + \; 2\gamma_0 \cosh(\gamma_0)\,\frac{\partial\gamma_0}{\partial\gamma} \; = \; 0$$

$$\frac{\partial\gamma_0}{\partial\sigma} = - \frac{{}_0(\sinh(\;{}_0)}{\sigma\sinh(\gamma_0)+\sigma\gamma_0\cosh(\gamma_0)-(y^2-\gamma_0^2)\sinh(\gamma_0)+2\gamma_0\cosh(\gamma_0)}$$

$$\frac{d}{d\sigma}[\sigma\gamma_n \sin(\gamma_n) \; + \; (y^2 \; + \; \gamma_n^2)\cos(\gamma_n)] \; = \; 0$$

$$\gamma_n \sin(\gamma_n) \; + \; \sigma\sin(\gamma_n) \; \frac{\partial\gamma_n}{\partial\sigma} \; + \; \sigma\cos(\gamma_n)\gamma_n \cdot \frac{\partial\gamma_n}{\partial\sigma}$$

$$+ \; 2\gamma_n(\cos(\gamma_n) \; \frac{\partial\gamma_n}{\partial\sigma} \; - \; (y^2 \; + \; \gamma_n^2)\sin(\gamma_n)\cdot\frac{\partial\gamma_n}{\partial\sigma} \; = \; 0$$

$$\frac{\partial\gamma_n}{\partial\sigma} = - \frac{\gamma_n \sin(\gamma_n)}{\sigma\sin(\gamma_n)+\sigma\gamma_n\cos(\gamma_n)+2\gamma_n\cos(\gamma_n)-(y^2+\gamma_n^2)\sin(\gamma_n)}.$$

<u>Derivative of $F(\sigma,tss,ker,b)$ in Order to tss</u>

$$\frac{\partial F}{\partial tss}(\sigma,tss,krr,b) \; = \; \sum_{i=1}^{n} 2[s_i(\sigma,tss,krr,b) \; - \; \ell_i]\frac{\partial s_i}{\partial tss}$$

$$\frac{\partial U_0(y)}{\partial tss} \; = \; \{-\exp[-ts\beta(y^2 \; - \; \gamma_0^2)]\}[-\beta(y^2 \; - \; \gamma_0^2)t]$$

$$\cdot \; [\sinh(\gamma_0 Z_{2D}) \; - \; \sinh(\gamma_0 Z_{1D})]\cdot\{\sinh[(\gamma_0(1-d_D)]$$

$$- \; \sinh[\gamma_0(1-\ell_b)2\}/\{[y^2 \; + \; (1+\sigma)\gamma_0^2 \; - \; \frac{(y^2-\gamma_0^2)^2}{\sigma}]$$

$$\cosh(\gamma_0)\cdot(Z_{2D}-Z_{1D})\gamma_0\cdot(\ell_D-d_D)\cdot\sinh(\gamma_0)\}$$

$$\frac{\partial U_n(y)}{\partial tss} = \{-\exp[-ts\beta(y^2+\gamma_n^2)]\}[-\beta(y^2+\gamma_n^2)t]$$

$$\cdot\ [\sin(\gamma_n Z_{2D}) - \sin(\gamma_n Z_{1D})]$$

$$\cdot\ \{\sin[\gamma_n(1-d_D)] - \sin[\gamma_n(1-\ell_D)]\}/$$

$$\cdot\ \{[y^2 - (1+\sigma)\gamma_n^2 - \frac{(y^2+\gamma_n^2)^2}{\sigma}]\cos(\gamma_n)\cdot(Z_{2D}-Z_{1D})\gamma_n$$

$$\cdot\ (\ell_D-d_D)\cdot\sin(\gamma_n)\}.$$

<u>Derivatives of F(σ,tss,krr,b) in Order to krr</u>

$$\frac{\partial F}{\partial krr}(\sigma,tss,krr,b) = \sum_{i=1}^{n} 2[s_i(\sigma,tss,krr,b) - \ell_i]\frac{\partial s_i}{\partial krr}$$

$$\frac{\partial s_i}{\partial krr} = \int_0^\infty \frac{\partial[4yJ_0(y\beta^{1/2})]}{\partial(krr)}[U_0(y) + \sum_{n=1}^{\infty} U_n(y)]dy$$

$$= \int_0^\infty 4yJ_0(y\beta^{1/2})[\frac{\partial U_0(y)}{\partial krr} + \sum_{n=1}^{\infty} \frac{\partial U_n(y)}{\partial krr}]$$

$$- \frac{2y^2\beta^{-1/2}}{b^2}J_1(y\beta^{1/2})[U_0(y) + \sum_{n=1}^{\infty} U_n(y)]dy$$

$$\frac{\partial U_0(y)}{\partial krr} = \{-\exp[-ts\beta(y^2-\gamma_0^2)]\}[-ts(y^2-\gamma_0^2)/b^2]$$

$$\cdot\ [\sinh(\gamma_0 Z_{2D}) - \sinh(\gamma_0 Z_{1D})]$$

$$\cdot\ \{\sinh[\gamma_0(1-d_D)] - \sinh[\gamma_0(1-\ell_D)]\}/$$

$$\cdot \{[y^2+(1+\sigma)\gamma_0^2 - \frac{(y^2-\gamma_0^2)^2}{\sigma}]$$

$$\cdot \cosh(\gamma_0)\cdot(Z_{2D} - Z_{1D})\gamma_0\cdot(\ell_D-d_D)\cdot\sinh(\gamma_0)\}$$

$$\frac{\partial U_n(y)}{\partial krr} = \{-\exp[-ts\beta(y^2+\gamma_n^2)]\}[-ts(y^2+\gamma_n^2)/b^2]$$

$$\cdot [\sin(\gamma_n Z_{1D}) - \sin(\gamma_n Z_{2D})]$$

$$\cdot \{\sin[\gamma_n(1-d_D)] - \sin[\gamma_n(1-\ell_D)]\}/$$

$$\cdot \{[y^2-(1+\sigma)\gamma_n^2 - \frac{(y^2+\gamma_n^2)^2}{\sigma}]$$

$$\cdot \cos(\gamma_n)\cdot(Z_{2D}-Z_{1D})\gamma_n\cdot(\ell_D-d_D)\cdot\sin(\gamma_n)\}.$$

Derivatives of $F(\sigma,tss,krr,b)$ in Order to b

$$\frac{\partial F(\sigma,tss,krr,b)}{\partial b} = \sum_{i=1}^{n} 2[s_i(\sigma,tss,krr,b) - \ell_i]\frac{\partial s_i}{\partial b}$$

$$\frac{\partial s_i}{\partial b} = \int 4yJ_0(y\beta^{1/2})[\frac{\partial U_0(y)}{\partial b} + \sum_{n=1}^{\infty} \frac{\partial U_n(y)}{\partial b}]$$

$$- 2y^2J_1(y\beta^{1/2})\cdot\beta^{-1/2}\cdot\frac{\partial\beta}{\partial b}[U_0(y) + \sum_{n=1}^{\infty} U_n(y)]dy$$

$$\frac{\partial U_0(y)}{\partial b} = \{1 - \exp[-ts\beta(y^2-\gamma_0^2)]\}/$$

$$\cdot \{[y^2+(1+\sigma)\gamma_0^2 - \frac{(y^2-\gamma_0^2)^2}{\sigma}]\cosh(\gamma_0)\cdot\sinh(\gamma_0)\}$$

$$\cdot \{[\gamma_0 \cosh(\gamma_0 Z_{2D}) \frac{\partial Z_{2D}}{\partial b} - \gamma_0 \cosh(\gamma_0 Z_{1D}) \cdot \frac{\partial Z_{1D}}{\partial b}]$$

$$\cdot \{\sinh[\gamma_0 (1-d_D)] - \sinh[\gamma_0 (1-\ell_D)]$$

$$\cdot \frac{1}{(Z_{2D}-Z_{1D})\gamma_0} \frac{1}{(\ell_D - d_D)} + [\sinh(\gamma_0 Z_{2D}) - \sinh(\gamma_0 Z_{1D})]$$

$$\cdot \{\cosh[\gamma_0 (1-d_D)] \cdot (-\gamma_0 \frac{\partial d_D}{\partial b}) - \cosh[\gamma_0 (1-\ell_D)] \cdot (-\gamma_0 \frac{\partial \ell_D}{\partial b})\}$$

$$\cdot \frac{1}{(Z_{2D}-Z_{1D})\gamma_0} \frac{1}{(\ell_D - d_D)} + [\sinh(\gamma_0 Z_{2D}) - \sinh(\gamma_0 Z_{1D})]$$

$$\cdot \{\sinh[\gamma_0 (1-d_D)] - \sinh[\gamma_0 (1-\ell_D)\}$$

$$\cdot [- \frac{(\frac{\partial Z_{2D}}{\partial b} - \frac{\partial Z_{1D}}{\partial b})}{\gamma_0 (Z_{2D}-Z_{1D})^2}] \cdot \frac{1}{(\ell_D - d_D)}$$

$$+ [\sinh(\gamma_0 Z_{2D}) - \sinh(\gamma_0 Z_{1D})]$$

$$\cdot \{\sinh[\gamma_0 (1-d_D)] - \sinh[\gamma_0 (1-\ell_D)][- \frac{\frac{\partial \ell_D}{\partial b} - \frac{\partial d_D}{\partial b}}{(\ell_D - d_D)^2}]$$

$$+ \{-\exp[-ts\beta(y^2-\gamma_0^2)][-ts(y^2-\gamma_0^2)] \cdot \frac{\partial \beta}{\partial b}$$

$$\cdot [\sinh(\gamma_0 Z_{2D}) - \sinh(\gamma_0 Z_{1D})]$$

$$\cdot \{\sinh[\gamma_0 (1-d_D 0] - \sinh[\gamma_0 (1-\ell_D]\}$$

$$\cdot \frac{1}{(Z_{2D}-Z_{1D})\gamma_0} \frac{1}{\ell_D - d_D} / \{[y^2 + (1+\sigma)\gamma_0^2 - \frac{(y^2-\gamma_0^2)^2}{\sigma}]$$

$$\cdot \cosh(\gamma_0) \cdot \sinh(\gamma_0)$$

$$\frac{\partial U_n(y)}{\partial b} = \{(-\exp[-ts\beta(y^2 + \gamma_n^2)]\}/$$

$$\cdot \{[y^2 - (1+\sigma)\gamma_n^2 - \frac{(y^2+\gamma_n^2)^2}{\sigma}] \cdot \cos(\gamma_n) \cdot \sin(\gamma_n)$$

$$\cdot \{[\gamma_n \cos(\gamma_n Z_{2D}) \cdot \frac{\partial Z_{2D}}{\partial b} - \gamma_n \cos(\gamma_n Z_{1D}) \cdot \frac{\partial Z_{1D}}{\partial b}]$$

$$\cdot \{\sin[\gamma_n(1-d_D) - \sin[\gamma_n(1-\ell_D)]\}$$

$$\cdot \frac{1}{(Z_{2D}-Z_{1D})\gamma_n} \frac{1}{(\ell_D - d_D)} + \sin(\gamma_n Z_{2D}) - \sin(\gamma_n Z_{1D})]$$

$$\cdot \{\cos[\gamma_n(1-d_D)] \cdot (-\gamma_n \frac{\partial d_D}{\partial b}) - \cos[\gamma_n(1-\ell_D)](-\gamma_n \frac{\partial \ell_D}{\partial b})$$

$$\cdot \frac{1}{(Z_{2D}-Z_{1D})\gamma_n} \frac{1}{(\ell_D - d_D)} + [\sin(\gamma_n Z_{2D}) - \sin(\gamma_n Z_{1D})]$$

$$\cdot \{\sin[\gamma_n(1-d_D)] - \sin[\gamma_n(1-\ell_D)]\} \cdot [- \frac{(\frac{\partial Z_{2D}}{\partial b} - \frac{\partial Z_{1D}}{\partial b})}{\gamma_n (Z_{1D}-Z_{2D})^2}]$$

$$\cdot \frac{1}{(\ell_D - d_D)} + [\sin(\gamma_n Z_{2D}) - \sin(\gamma_n Z_{1D})]$$

$$\cdot \{\sin[\gamma_n(1-d_D)] - \sin[\gamma_n(1-\ell_D)]\}$$

$$\cdot \frac{1}{(Z_{2D}-Z_{1D})\gamma_n} \cdot \left[\frac{\left(\frac{\partial \ell_D}{\partial b} - \frac{\partial d_D}{\partial b}\right)}{(\ell_D - d_D)^2}\right]\}$$

$$+ \{\exp[-ts\beta(y^2 + \gamma_n^2)] \cdot [ts(y^2 + \gamma_n^2)] \cdot \frac{\partial \beta}{\partial b}\}$$

$$\cdot [\sin(\gamma_n Z_{2D}) - \sin(\gamma_n Z_{1D})]$$

$$\cdot \{\sin[\gamma_n(1-d_D)] - \sin[\gamma_n(1-\ell_D]\}$$

$$\cdot \frac{1}{(Z_{2D}-Z_{1D})\gamma_n} \frac{1}{(\ell_D - d_D)} /$$

$$\cdot \{[y^2 - (1+\sigma)\gamma_n^2 - \frac{(y^2+\gamma_n^2)^2}{\sigma}]\cos(\gamma_n)\sin(\gamma_n)\}$$

where

$$\frac{\partial \beta}{\partial b} = - \frac{2k_D r^2}{b3}$$

$$\frac{\partial Z_{2D}}{\partial b} = - \frac{Z_2}{b^2}; \quad \frac{\partial Z_{1D}}{\partial b} = - \frac{Z_1}{b^2}; \quad \frac{\partial d_D}{\partial b} = - \frac{d}{b^2}; \quad - \frac{\partial \ell_D}{\partial b} = - \frac{\ell}{b^2}.$$

APPENDIX 2

SYNTHETIC MANUAL OF UTILIZATION OF THE PROGRAM

Introduction - Brief Description of Computer Program

The algorithm consists of a main program called ESTPBR (estimation of parameters) which performs the reading of the input values and calls the subroutine MGFN which performs the minimization process. Along with this subroutine, and as it was mentioned before, another subroutine, BVSUB is called by MGFN for the computation of the feasible direction.

The minimization subroutine requires the existence of two more subroutines; one for the evaluation of the value of the objective function, (the subroutine COMFN); the other for the evaluation of its derivatives in order to each of the parameters (the subroutine PDSUB).

The subroutine COMFN calls the subroutine D(s) for the evaluation of the drawdown at each point, according to Neuman's analytical solution for the response of an unconfined aquifer when a pumping test is performed. This subroutine corresponds to the solution presented by Neuman (1972) in the Water Resources-Research, Vol. 10, 1974.

The subroutine PDSUB calls for four subroutines, DDSY, DDTS, DDBB, and DDLD, developed for this method, which give the value of the derivative of the function s(σ, tss, krr, b) in order to each of the parameters, respectively.

For the evaluation of Neuman's analytical solution for the drawdown, and its derivative in order to each of the four parameters, three more subroutines are called. The subroutine BESO which computs the Bessel function $J_0(x)$, the subroutine DBESJ which computes the Bessel function $J_1(x)$, and the routine function GAUSS, for the integration of the analytical expression by the Gaussian Quadrature method.

<u>Input Statement</u>

1. ZD - Ratio between vertical distance from the bottom of the aquifer to the observation point, in the observation well, and the initial saturated aquifer thickness. Leave blank if the average drawdown from ZD1 to ZD2 is pretended. This value will be taken as an initial guess.

   ZD1 - Ratio between vertical distance from the bottom of the aquifer to the bottom of the perforations in the observation well, and the initial aquifer thickness. Leave blank if the drawdown at a point is pretended. This value will be taken as an initial guess.

ZD2 - Ratio between vertical distance from the bottom of the aquifer to the top of the perforations in the observation well, and the initial saturated aquifer thickness. Leave blank if the drawdown at a point is pretended. This value will be taken as an initial guess.

2. N - Number of variables that will be considered in the minimization process (four parameters plus eight dummy variables corresponding to the two linear restrictions imposed on each of the four variables, that define the upper and lower bounds of the range of the values each can assume).

N1 - Control variable. If to N1 is assigned any value different than 1, the parameter SIGMA is assumed to be known "a priori", and in the process of minimization it will be taken as a constant.

N2 - Control variable. If to N2 is assigned any value different than 1, the parameter tss is assumed to be known "a priori", and in the process of minimization it will be taken as a constant.

N3 - Control variable. If to N3 is assigned any value different than 1, the parameter Krr is assumed to be known "a priori", and in the process of minimization it will be taken as a constant.

N4 - Control variable. If to N4 is assigned any value different than 1, the parameter b is assumed to be known "a priori", and in the process of minimization it will be taken as a constant.

NP - Number of data points corresponding to the pumping test data that will be considered in the analysis.

3. X1 - Distance between the initial water table and the observation point in the observation well. Leave blank if the average drawdown between the two points is pretended.

X2 - Distance between the initial water table and the bottom of the perforations in the observation well. Leave blank if the drawdown at a point is pretended.

X3 - Distance between the initial water table and the top of perforations in the observation well. Leave blank if the drawdown at a point is pretended.

Y_4 - Distance between initial water table and bottom of perforations in pumping well.

Y_5 - Distance between initial water table and top perforations in pumping well.

Y_6 - Aquifer thickness.

Y_7 - Dkrr - Symbol used for Krr, the variable X(3), which is given by $K_D r^2$.

Y_8 - First time increment. It is the time corresponding to the first data recorded in the pumping test.

Y_9 - Tss - Symbol used for the variable X(2), which is given by $\frac{T}{Sr^2}$, where T is the transmissivity of the aquifer, S is the storage coefficient corresponding to the first response of the aquifer to the pumping, and r is the distance between the observation well and the pumping well.

4. TT(I), I = 1, NP - Values of the time since pumping started corresponding to each data point recorded during the test.

5. W(I), I = 1, NP - Values of the weights assigned to each data point.

6. HD(I), I = 1, NP - Values of the drawdowns recorded during the pumping test.

7. M - Number of the equations of constraints which will be imposed on the variables in the minimization procedure.

   N - Number of variables.

   NIBR - Number of iterations the minimization routine is allowed to perform before returning to the main program.

   EPS - Tolerance limit that will be taken by the subroutine BDSUB as the smaller value significantly different than zero.

   TOLX - Tolerance limit that will be taken by the subroutine MGFN as the smaller value significantly different than zero in the analysis of the X(I) values.

TOLB - Tolerance limit that will be taken by the subroutine MGFN as the smaller value significantly different than zero in the analysis of the vector B, of the equations defining the linear constraints.

TOLFX - Tolerance limit that will be taken by the subroutine MGFN as the smaller value significantly different than zero in the analysis of the values of the objective function between two successive iterations.

8. X(I), I = 1, N - Initial solution for each of the N variables, considering the same four ones corresponding to the hydraulic parameters of the aquifer to be estimated, plus the "dummy" variables used in the linear constraint system analysis.

9. A(I,J) - Where I takes the values from 1 to M and J takes the values from 1 to N. Matrix of the coefficients of the variables corresponding to the linear constraint system.

10. B(I) - Constraint vector.

11. SC - Storage coefficient of the aquifer.

RR - Square of the distance from the pumping to the observation well.

Q - Discharge pumped from the pumping well.

Output Statements

The first six output statements are executed in the main program before the minimization subroutine is called.

1. HD(I), I = 1, NP;
2. TT(I), I = 1, NP;
3. W(I), I = 1, NP;
4. A(I,J), I = 1, M, J = 1, N
5. β(I), I = 1, M;
6. SC

   RR

   Q.

The next output statements are executed during the minimization process, by the subroutines COMFN and PDSUB, which are called by the minimization subroutine as the process of the minimization is performed.

The first subroutine to be called is COMFN, (which computes the value of the objective function for the estimates given by the minimization subroutine. It first prints the headings under which the parameters will be printed. These headings are:

SD - Dimensionless drawdown (computed accordingly to Neuman"s theoretical model).

DTS - Dimensionless time with respect to the storage coefficient S. It is given by TTS.TT(I).

TYS - Dimensionless time with respect to the specific yield Sy.

DET - Sigma, given by the ratio S/Sy.

BETA - β, given by the ratio krr/b^2.

PD - It is l_D, given by the ratio l/b, where l is the distance between the initial water table and the bottom of perforations in the pumping well, and b the aquifer thickness.

DD - It is d_D, given by the ratio d/b, where d is the distance from the initial water table to the top of perforations in the pumping well.

ZD - It is Z_D, given by the ratio between z/b, where z is the distance from the bottom of the aquifer to the observation point, in the observation well.

Z_{D1} - It is Z_{D1}, given by the ratio between z_1/b, where z_1 is the distance from the bottom of the aquifer to the bottom of perforations, in the observation well.

Z_{D2} - It is Z_{D2}, given by the ratio between z_2/b, where z_2 is the distance from the bottom of the aquifer to the top of perforations in the observation well.

Under these headings, and each time COMFN is called, the values of variables X(1) are printed.

The evaluation of the drawdown corresponding to each data point is then executed. Before the printing of the dimensionless drawdown for each time increment, some of the values obtained by the numerical evaluation of the theoretical function of the drawdown are printed, in a four column display.

Immediately after the printing of the eight parameters above mentioned, for each data point (namely AVRG, DTS, TYS, DET, BETA, PD, ZD_1, Z_{D2}), a line of four values is printed. The first value is the theoretical drawdown, the second the real drawdown, the third the dimensionless real drawdown (corresponding to the observed value), and the fourth, the dimensionless theoretical drawdown. These theoretical values were evaluated for the estimates given at that point by the minimization subroutine. The purpose of this printing is to give the user an immediate idea about the behavior of the function for the estimates used at that point, compared with the behaivor of the aquifer recorded in the observed values of drawdown versus time.

After the printing of the eight parameters above mentioned for the last data point, the values of X(I) are again printed in the next line, as well as, and by its respective order, the value of KH, the horizontal hydraulic conductivity and the value of FX.

Each time the subroutine PDSUB is called, the derivative of the drawdown s, evaluated according to its theoretical model, in order to each of the parameters, are evaluated and printed for each time increment from the initial time.

In the headings printed each time each derivative is going to be evaluated, in the place of S_D, is printed the symbol DER N(K), K being the derivative being called at that point. In the first column of the eight characters, the derivatives will be printed, where in the subroutine COMFN the dimensionless drawdown was printed.

After the evaluation of the derivative of s for all the data points, the values of X(I), I = 1, N, are again printed.

The minimization procedure will always end after COMFN is called, and once the process is finished, the value of the parameter KR is printed, being a normal return to be defined by the value of 1 assigned to KR, that will be then the last value to be printed. If another number instead of 1 is printed, that means that error returns from the minimization subroutine have happened and the user is advised to read the comment statements printed in the beginning of the program, to identify what the cause of this error return could be.

The consideration of one, two, three, or four parameters to be estimated, according to the instructions given in the main program, can be chosen by the user.

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