

Identifying the Parameters of an Aquifer Cell Model

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Cell models are commonly used for forecasting water levels in aquifers. Calibration of such models is achieved through identification of their parameter values, the transmissivities and storativities of all cells, using historical data. Several methods of formulating the identification as a linear or quadratic programming problem are presented. Examples are given, results of the various methods compared, and the sensitivity of these results to errors in the data is discussed. Inflows or outflows during historical periods may also be determined by the same methods; an example for a real aquifer is presented.

INTRODUCTION

The problem of identifying the parameters of an aquifer model is known also as the inverse problem. Here identification of parameters means the determination of the distributions of storativity $S = S(x, y)$ and transmissivity $T = T(x, y)$ of an aquifer in which we assume two-dimensional flow in the horizontal plane. The complete distributions are required if one wishes to forecast the future regime in the aquifer in response to various imposed activities of pumping and recharge.

An indirect way of obtaining the sought distributions is by some trial and error technique of adjusting the various parameters until an acceptable agreement is reached between the response of the model and that of the aquifer itself under some specified operation regime. A prerequisite for the application of this approach is the availability of hydrological data (e.g., water levels and rates of pumping, discharge of springs, artificial recharge, and natural replenishment) for some period in the past called the identification or calibration period. Sometimes, certain parts of the historical hydrological data mentioned above are not known. In this case we may regard the missing information items also as unknown parameters, the values of which have to be determined during the identification procedure. The natural replenishment of an aquifer is often considered such an unknown parameter. Unless otherwise specified, we shall consider henceforth the problem of identifying the distributions of S and T only.

The main disadvantage of a trial and error technique is that it does not involve an algorithm for seeking the solution systematically. In recent years, advanced mathematical methods have been developed and implemented for determining unknown model parameters. Among these one may mention the works of *Deininger* [1969], *Vemuri and Karplus* [1969], *Korganoff* [1970], *Coats et al.* [1970], *Emsellem and de Marsily* [1971], *Kleinecke* [1971], and *Neuman* [1973]. The present work is another attempt in this direction.

In this work the aquifer is represented by a finite difference model, and linear and quadratic programming procedures are employed as tools for identifying its parameters. The proposed methods have been tested on synthetic models, the parameters of which were a priori known. This technique made it possible to check results and compare the different methods. The application of the proposed techniques to cases of practical interest is now under way and will be reported separately.

FINITE DIFFERENCE MODEL

Various numerical models of groundwater systems may be employed. Essentially, the models considered in this paper deal with flow in a confined aquifer or in a phreatic one in which the spatial variations of the water table are small with respect to the thickness of the aquifer. It is assumed that the aquifer is isotropic and that the flow in it is essentially two-dimensional in the horizontal (x, y) plane.

The continuity equation for this model is

$$\frac{\partial}{\partial x} \left(T \frac{\partial \phi}{\partial x} \right) + \frac{\partial}{\partial y} \left(T \frac{\partial \phi}{\partial y} \right) + r - p = S \frac{\partial \phi}{\partial t} \quad (1)$$

where $T = T(x, y)$ is the transmissivity of the aquifer, $S = S(x, y)$ is the storativity of the aquifer, $\phi = \phi(x, y, t)$ indicates the elevation of the water table or the piezometric surface, $r = r(x, y, t)$ represents inflow per unit (horizontal) area (e.g., by artificial and natural replenishment), and $p = p(x, y, t)$ represents withdrawal from the aquifer per unit (horizontal) area (e.g., by pumping).

The flow domain is subdivided into a network of rectangular cells (Figure 1) which serve in constructing the finite difference representation of (1).

In the cell model the continuous variables transform into discrete ones in the following way:

$$x \rightarrow x_i \quad i = 1, 2, \dots, I \quad (2)$$

$$y \rightarrow y_j \quad j = 1, 2, \dots, J \quad (3)$$

$$t \rightarrow t^n \quad n = 0, 1, 2, \dots, N \quad (4)$$

$$\phi(x, y, t) \rightarrow \phi_{i,j}^n \quad (5)$$

$$p(x, y, t) \rightarrow p_{i,j}^{n+1/2} = (p_{i,j}^{n+1} + p_{i,j}^n)/2 \quad (6)$$

$$r(x, y, t) \rightarrow r_{i,j}^{n+1/2} = (r_{i,j}^{n+1} + r_{i,j}^n)/2 \quad (7)$$

$$T(x, y) \rightarrow T_{i,j} \quad (8)$$

$$S(x, y) \rightarrow S_{i,j} \quad (9)$$

In Figure 1 the centers of the cells are indicated in order to emphasize the fact that any property of the cell is represented by a single value which is assigned to its center. Note that the value of the transmissivity is also assigned to the centers of the cells and not to the border lines between adjacent cells, as is sometimes done. The number of transmissivity values, which are to be identified, is equal to the number of cells, whereas assignment of values to cell boundaries would result in roughly twice this number.

Two finite difference schemes, commonly used for

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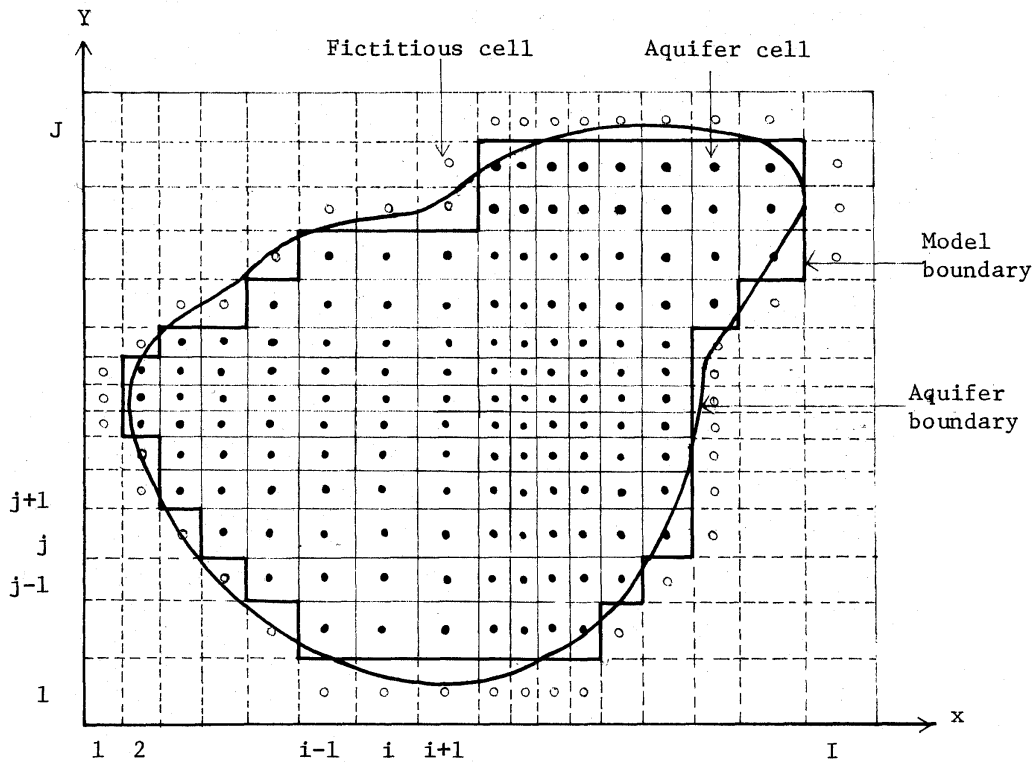


Fig. 1. An aquifer model divided into cells.

forecasting groundwater levels, are presented below. Figure 2 shows the nomenclature used for a typical cell (*i, j*) in the finite difference equations.

The first finite difference model to be employed is the implicit scheme:

$$\frac{1}{\Delta x_i} \left(\frac{T_{i+1,j} + T_{i,j} \cdot \phi_{i+1,j}^{n+1} - \phi_{i,j}^{n+1}}{2 \Delta x_{i+1/2}} - \frac{T_{i-1,j} + T_{i,j} \cdot \phi_{i-1,j}^{n+1} - \phi_{i,j}^{n+1}}{2 \Delta x_{i-1/2}} \right)$$

$$+ \frac{1}{\Delta y_j} \left(\frac{T_{i,j+1} + T_{i,j} \cdot \phi_{i,j+1}^{n+1} - \phi_{i,j}^{n+1}}{2 \Delta y_{j+1/2}} - \frac{T_{i,j-1} + T_{i,j} \cdot \phi_{i,j-1}^{n+1} - \phi_{i,j}^{n+1}}{2 \Delta y_{j-1/2}} \right) + r_{i,j}^{n+1/2} - p_{i,j}^{n+1/2} = S_{i,j} \frac{\phi_{i,j}^{n+1} - \phi_{i,j}^n}{\Delta t^{n+1/2}} \quad (10)$$

As seen from (10) the average transmissivity is used for computing the rate of flow between two adjacent cells.

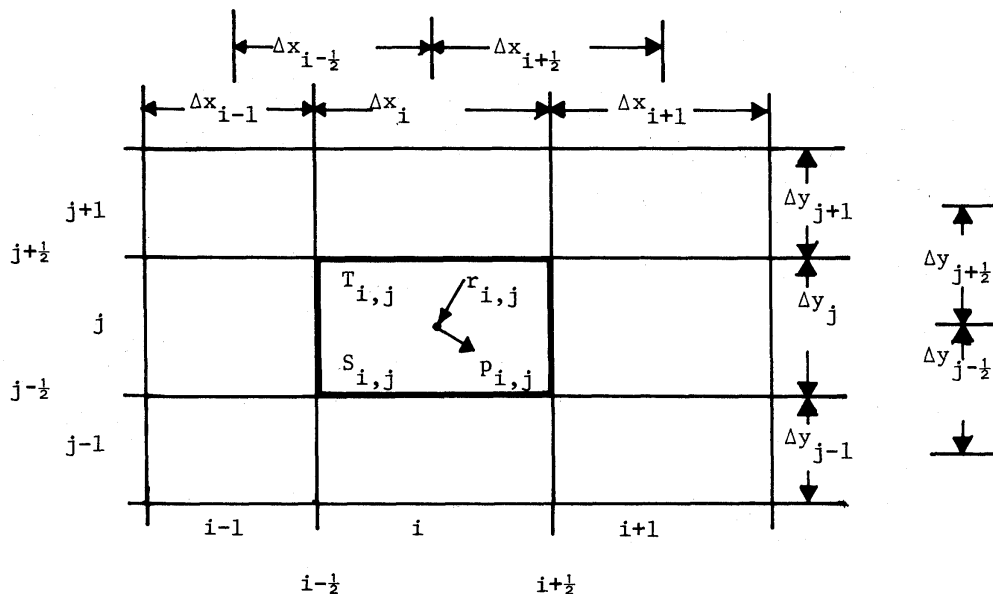


Fig. 2. Nomenclature for a typical cell.

The second scheme is based on the Crank-Nicholson method [Von Rosenberg, 1969]:

$$\begin{aligned} & \frac{1}{\Delta x_i} \left(\frac{T_{i+1,j} + T_{i,j} \cdot \phi_{i+1,j}^{n+1/2} - \phi_{i,j}^{n+1/2}}{2} \right. \\ & \quad \left. - \frac{T_{i-1,j} + T_{i,j} \cdot \phi_{i-1,j}^{n+1/2} - \phi_{i,j}^{n+1/2}}{2} \right) \\ & + \frac{1}{\Delta y_j} \left(\frac{T_{i,j+1} + T_{i,j} \cdot \phi_{i,j+1}^{n+1/2} - \phi_{i,j}^{n+1/2}}{2} \right. \\ & \quad \left. - \frac{T_{i,j-1} + T_{i,j} \cdot \phi_{i,j-1}^{n+1/2} - \phi_{i,j}^{n+1/2}}{2} \right) \\ & + r_{i,j}^{n+1/2} - p_{i,j}^{n+1/2} = S_{i,j} \frac{\phi_{i,j}^{n+1} - \phi_{i,j}^n}{\Delta t^{n+1/2}} \end{aligned} \quad (11)$$

where spatial gradients are computed at the midpoint of the time interval. For example,

$$\phi_{i,j}^{n+1/2} = \frac{\phi_{i,j}^n + \phi_{i,j}^{n+1}}{2} \quad (12)$$

BOUNDARY CONDITIONS

One has to specify the appropriate boundary conditions when (10) or (11) is written for a boundary cell. The possible boundary conditions are a given potential, an impervious boundary, and a given flux across the boundary. To introduce the boundary conditions in the finite difference model, we have used fictitious cells, located outside the model boundary (see Figure 1). The transmissivity of each such cell was made equal to that of the aquifer cell to which it is adjacent, and the values of ϕ in the fictitious cell were manipulated to introduce the appropriate boundary condition into the model. This leaves the number of transmissivities to be identified equal to the number of cells. The methods for specifying the boundary conditions are detailed elsewhere [Hefez et al., 1972].

STATEMENT OF IDENTIFICATION PROBLEM FOR A CELL MODEL

The identification problem can be stated as follows: Determine $T_{i,j}$ and $S_{i,j}$ for each cell of the model, using the equations obtained by writing either (10) or (11) for every cell and for every time interval during the calibration period. The following characteristics have to be specified for the particular problem at hand: shape of model, its division into cells, boundary conditions in terms of values of ϕ in the fictitious cells, initial values of ϕ , values of ϕ in all cells at the beginning and end of each time interval, and inputs and outputs (artificial and natural recharge, pumping, spring discharge, etc.) for all cells and for all time intervals.

The method of solution proposed here enables several relaxations relative to the above requirements: (1) when information is missing in some cells, one can identify the parameters for only part of cells; (2) it is possible to identify unknown discharge rates; (3) when boundary conditions are unknown, one may identify parameters for all cells except the storativity in cells adjacent to the unknown boundary; and (4) it is possible to identify all parameters when water levels are known for only part of the historical period in some cells.

IDENTIFICATION AS AN OPTIMIZATION PROBLEM

For the sake of simplicity, let us first assume that data are available for all cells at all times, i.e., ϕ , p , and r are known for all i, j , and n . Denoting the number of cells by C , the number

of sought parameters is $2 \cdot C$, while the number of available equations is $N \cdot C$, where N is the number of time intervals included in the calibration period. The equations are linear in the unknowns T and S and can be solved as a system of linear equations provided that the number of equations is equal to the number of unknowns and provided that all equations are independent of each other. Obviously, the first condition is satisfied when $N = 2$, i.e., for two time intervals. In cases of parameter identification of practical interest, however, we usually have information for more than two time intervals, i.e.,

$$N > 2 \quad (13)$$

which means that the number of equations is larger than the number of unknowns.

If we wish to solve the problem as one of solving $2 \cdot C$ equations in $2 \cdot C$ unknowns, we have to pick two specific time intervals, which brings up the questions of which ones to choose and whether each pair of chosen intervals will yield the same solution. The answer to the last question is in general negative. This stems from the fact that in the equations, water levels and parameter values are those of a model, whereas the information we use is that of water levels in the field. This discrepancy introduces a certain noise in each equation. Each equation becomes an approximation, and hence a different solution will be derived from any subset of equations. Obviously, we should be interested in making use of all the information available, assuming that as we use more information, a better solution will be obtained.

Hence the problem becomes one of obtaining the best set of parameters, i.e., that set which will satisfy the equations most closely, closeness being defined in some exact sense. In other words, we are faced here with the problem of obtaining the optimal solution of the given set of equations. In what follows we shall show that by choosing the criterion according to which we determine how closely the equations are satisfied, we determine the type of optimization problem we have on hand.

So far we have assumed that the only unknown parameters are T and S and that all the information for the calibration period is available. When information is missing for any cell during any time interval, the number of equations will be reduced.

STATEMENT OF THE IDENTIFICATION AS A LINEAR OR QUADRATIC PROGRAMING PROBLEM

It was shown above how the identification problem is reduced to one of seeking the optimal solution to a set of equations. We shall now be more specific and state the problem on hand as one of linear or quadratic optimization. We shall show several alternatives for defining the objective function and discuss the differences among them.

Let us first rewrite the model equation (11) in a form which will emphasize that T and S are the unknowns to be identified:

$$\begin{aligned} & a_{i,j}^{n+1/2} \cdot T_{i,j-1} + b_{i,j}^{n+1/2} \cdot T_{i-1,j} + c_{i,j}^{n+1/2} \cdot T_{i,j} + d_{i,j}^{n+1/2} \\ & \quad \cdot T_{i+1,j} + e_{i,j}^{n+1/2} \cdot T_{i,j+1} + f_{i,j}^{n+1/2} \cdot S_{i,j} \\ & = p_{i,j}^{n+1/2} - r_{i,j}^{n+1/2} \end{aligned} \quad (14)$$

The coefficients in this equation are

$$a_{i,j}^{n+1/2} = \frac{-1}{2\Delta y_j} \cdot \frac{\Delta \phi_{i,j-1/2}^{n+1/2}}{\Delta y_{j-1/2}} \quad (15)$$

$$b_{i,j}^{n+1/2} = \frac{-1}{2\Delta x_i} \cdot \frac{\Delta \phi_{i-1/2,j}^{n+1/2}}{\Delta x_{i-1/2}} \quad (16)$$

$$c_{i,j}^{n+1/2} = \frac{1}{2\Delta x_i} \left(\frac{\Delta\phi_{i+1/2,j}^{n+1/2}}{\Delta x_{i+1/2}} - \frac{\Delta\phi_{i-1/2,j}^{n+1/2}}{\Delta x_{i-1/2}} \right) + \frac{1}{2\Delta y_j} \left(\frac{\Delta\phi_{i,j+1/2}^{n+1/2}}{\Delta y_{j+1/2}} - \frac{\Delta\phi_{i,j-1/2}^{n+1/2}}{\Delta y_{j-1/2}} \right) \quad (17)$$

$$d_{i,j}^{n+1/2} = \frac{1}{2\Delta x_i} \cdot \frac{\Delta\phi_{i+1/2,j}^{n+1/2}}{\Delta x_{i+1/2}} \quad (18)$$

$$e_{i,j}^{n+1/2} = \frac{1}{2\Delta y_j} \cdot \frac{\Delta\phi_{i,j+1/2}^{n+1/2}}{\Delta y_{j+1/2}} \quad (19)$$

$$f_{i,j}^{n+1/2} = \frac{\phi_{i,j}^{n+1} - \phi_{i,j}^n}{\Delta t^{n+1/2}} \quad (20)$$

Equation (10) can be treated in a similar manner. In order to simplify the presentation, while emphasizing the various optimization criteria, (14) may be further reduced to the following compact form:

$$\sum_{m=1}^5 g_m \cdot T_m + f_{i,j}^{n+1/2} \cdot S_{i,j} = p_{i,j}^{n+1/2} - r_{i,j}^{n+1/2} \quad \forall i, j, n \quad (21)$$

where the sum is taken over the five terms which include transmissivity, i.e.,

$$\sum_{m=1}^5 g_m \cdot T_m = a_{i,j}^{n+1/2} \cdot T_{i,i-1} + b_{i,j}^{n+1/2} \cdot T_{i-1,i} + c_{i,j}^{n+1/2} \cdot T_{i,j} + d_{i,j}^{n+1/2} \cdot T_{i+1,i} + e_{i,j}^{n+1/2} \cdot T_{i,j+1} \quad (22)$$

Even when the optimal solution is obtained and inserted back into the equations, only in part of the set of equations (21) will equality hold between the right- and left-hand sides. In the remaining equations a difference, or deviation, will be observed between the two sides of the equation. We shall use the absolute values of these deviations and their squares in order to define five different possible criteria for approaching an agreement between the two sides of the equations.

Criterion A: the maximum absolute deviation. Let X denote the maximum absolute deviation occurring in one equation (21), i.e., for all cells and all time intervals. We may therefore state that all other deviations are less than or equal to X :

$$\left| \sum_{m=1}^5 g_m \cdot T_m + f_{i,j}^{n+1/2} \cdot S_{i,j} - p_{i,j}^{n+1/2} + r_{i,j}^{n+1/2} \right| \leq X \quad \forall i, j, n \quad (23)$$

This inequality may be replaced by two equivalent inequalities:

$$\sum_{m=1}^5 g_m \cdot T_m + f_{i,j}^{n+1/2} \cdot S_{i,j} - p_{i,j}^{n+1/2} + r_{i,j}^{n+1/2} \leq X \quad \forall i, j, n \quad (24)$$

$$\sum_{m=1}^5 g_m \cdot T_m + f_{i,j}^{n+1/2} \cdot S_{i,j} - p_{i,j}^{n+1/2} + r_{i,j}^{n+1/2} \geq -X \quad \forall i, j, n$$

Using this criterion the identification problem may now be stated as the following optimization problem: determine the unknown values of $S_{i,j}$, $T_{i,j}$, and X from

$$\min F = X \quad (25)$$

subject to the constraints

$$\sum_{m=1}^5 g_m \cdot T_m + f_{i,j}^{n+1/2} \cdot S_{i,j} - X \leq p_{i,j}^{n+1/2} - r_{i,j}^{n+1/2} \quad \forall i, j, n \quad (26)$$

$$\sum_{m=1}^5 g_m \cdot T_m + f_{i,j}^{n+1/2} \cdot S_{i,j} + X \geq p_{i,j}^{n+1/2} - r_{i,j}^{n+1/2} \quad \forall i, j, n$$

and to the nonnegativity restrictions

$$T_{i,j}, S_{i,j}, X \geq 0 \quad \forall i, j \quad (27)$$

This is a typical statement of a linear programming problem in which there are $(2C + 1)$ decision variables and $2CN$ constraints (not counting the physical restrictions expressed by (27)). One should note that X is regarded here as a decision variable and it alone appears in the objective function.

Criterion B: the sum of the absolute values of the maximum deviations in all time intervals. For each time interval we have C (equal to number of cells) balance equations, with different deviations between the two sides. Let $Y^{n+1/2}$ denote the maximum absolute value of all deviations corresponding to the $(n + \frac{1}{2})$ time interval. We may then state that all other deviations for the time interval are smaller than or equal to $Y^{n+1/2}$, i.e., for each $n = 0, \dots, N - 1$,

$$\left| \sum_{m=1}^5 g_m \cdot T_m + f_{i,j}^{n+1/2} \cdot S_{i,j} - p_{i,j}^{n+1/2} + r_{i,j}^{n+1/2} \right| \leq Y^{n+1/2} \quad \forall i, j \quad (28)$$

The number of maximum deviations $Y^{n+1/2}$ is equal to the number of time intervals in the calibration period.

The second linear identification problem can therefore be stated: determine $T_{i,j}$, $S_{i,j}$, and $Y^{n+1/2}$ such that the sum of the absolute values of the maximum deviations in all time intervals will reach a minimum:

$$\min F = \sum_{n=0}^{N-1} Y^{n+1/2} \quad (29)$$

subject to the constraints

$$\sum_{m=1}^5 g_m \cdot T_m + f_{i,j}^{n+1/2} \cdot S_{i,j} - Y^{n+1/2} \leq p_{i,j}^{n+1/2} - r_{i,j}^{n+1/2} \quad \forall i, j, n \quad (30)$$

$$\sum_{m=1}^5 g_m \cdot T_m + f_{i,j}^{n+1/2} \cdot S_{i,j} + Y^{n+1/2} \geq p_{i,j}^{n+1/2} - r_{i,j}^{n+1/2} \quad \forall i, j, n$$

and the nonnegativity restrictions

$$T_{i,j}, S_{i,j}, Y^{n+1/2} \geq 0 \quad \forall i, j, n \quad (31)$$

Here we have $(2C + N)$ decision variables and $2CN$ constraints of type (30). Again, T and S do not appear in the objective function.

Criterion C: the sum of the absolute values of the maximum deviations in all cells. Denote by $Z_{i,j}$ the maximum of the absolute values of the deviations occurring in the N equations of a cell. We may then state that for each cell the absolute values

of the deviations in all the balance equations will be smaller than or at most equal to $Z_{i,j}$, i.e., for each (i, j) ,

$$\left| \sum_{m=1}^5 g_m \cdot T_m + f_{i,j}^{n+1/2} \cdot S_{i,j}^{n+1/2} - p_{i,j}^{n+1/2} + r_{i,j}^{n+1/2} \right| \leq Z_{i,j} \quad \forall n \quad (32)$$

Accordingly, the third linear optimization problem may now be stated: determine $T_{i,j}$, $S_{i,j}$, and $Z_{i,j}$ so as to minimize the objective function F :

$$\min F = \sum_i \sum_j Z_{i,j} \quad (33)$$

subject to the constraints

$$\sum_{m=1}^5 g_m \cdot T_m + f_{i,j}^{n+1/2} \cdot S_{i,j} - Z_{i,j} \leq p_{i,j}^{n+1/2} - r_{i,j}^{n+1/2} \quad \forall i, j, n \quad (34)$$

$$\sum_{m=1}^5 g_m \cdot T_m + f_{i,j}^{n+1/2} \cdot S_{i,j} + Z_{i,j} \geq p_{i,j}^{n+1/2} - r_{i,j}^{n+1/2} \quad \forall i, j, n$$

and the nonnegativity restrictions

$$T_{i,j}, S_{i,j}, Z_{i,j} \geq 0 \quad \forall i, j \quad (35)$$

The number of decision variables here is $3C$, and the number of constraints of type (34) is $2CN$.

Criterion D: the sum of absolute values of all deviations. Denote by $U_{i,j}^{n+1/2}$ the absolute value of the deviation for each equation, i.e., for each i, j , and n ,

$$\left| \sum_{m=1}^5 g_m \cdot T_m + f_{i,j}^{n+1/2} \cdot S_{i,j} - p_{i,j}^{n+1/2} + r_{i,j}^{n+1/2} \right| = U_{i,j}^{n+1/2} \quad (36)$$

The identification can now be stated as a linear programming problem in the following way: determine the values of $T_{i,j}$, $S_{i,j}$, and $U_{i,j}^{n+1/2}$ such that the objective function F will attain a minimum

$$\min F = \sum_n \sum_i \sum_j U_{i,j}^{n+1/2} \quad (37)$$

subject to the constraints

$$\sum_{m=1}^5 g_m \cdot T_m + f_{i,j}^{n+1/2} \cdot S_{i,j} - U_{i,j}^{n+1/2} \leq p_{i,j}^{n+1/2} - r_{i,j}^{n+1/2} \quad \forall i, j, n \quad (38)$$

$$\sum_{m=1}^5 g_m \cdot T_m + f_{i,j}^{n+1/2} \cdot S_{i,j} + U_{i,j}^{n+1/2} \geq p_{i,j}^{n+1/2} - r_{i,j}^{n+1/2} \quad \forall i, j, n$$

and the nonnegativity restrictions

$$T_{i,j}, S_{i,j}, U_{i,j}^{n+1/2} \geq 0 \quad \forall i, j, n \quad (39)$$

Here the number of unknowns is $C(N+2)$ and the number of constraints of type (38) is $2CN$. Since the absolute value of the deviation is defined by the equality (36), in the optimal

solution only one of each pair of constraints will be binding, while the other will actually be redundant. In order to avoid this unnecessary redundancy which will only burden the solution, let us modify the criteria defined above, which will be denoted as $D/1$, and define an alternative criterion $D/2$.

Let the deviation in each equation be expressed as a difference between the values of two positive variables:

$$\sum_{m=1}^5 g_m \cdot T_m + f_{i,j}^{n+1/2} \cdot S_{i,j} - p_{i,j}^{n+1/2} + r_{i,j}^{n+1/2} = V_{i,j}^{n+1/2} - W_{i,j}^{n+1/2} \quad (40)$$

The deviation itself may be either positive or negative, depending on the magnitudes of V and W . The linear optimization problem may now be restated: determine the values of $T_{i,j}$, $S_{i,j}$, $V_{i,j}^{n+1/2}$, and $W_{i,j}^{n+1/2}$ such that objective function F will attain a minimum:

$$\min F = \sum_n \sum_i \sum_j (V_{i,j}^{n+1/2} + W_{i,j}^{n+1/2}) \quad (41)$$

subject to the constraints

$$\sum_{m=1}^5 g_m \cdot T_m + f_{i,j}^{n+1/2} \cdot S_{i,j} - V_{i,j}^{n+1/2} + W_{i,j}^{n+1/2} = p_{i,j}^{n+1/2} - r_{i,j}^{n+1/2} \quad \forall i, j, n \quad (42)$$

and the nonnegativity restrictions

$$T_{i,j}, S_{i,j}, V_{i,j}^{n+1/2}, W_{i,j}^{n+1/2} \geq 0 \quad \forall i, j, n \quad (43)$$

In this form there are $2C(N+1)$ decision variables and NC constraints of type (42). In the optimal solution, at least one of each pair for a cell, V and W , will vanish. The advantage of introducing this modified form of the criterion is that the number of constraints has been cut in half, resulting in a significant reduction in computational effort.

Criterion E: the sum of the squares of the deviations. A quadratic objective function may be defined by taking the sum of the squares of the deviations between the two sides of the equations for all cells and all time intervals. The optimization problem will then be stated: determine the values of $T_{i,j}$ and $S_{i,j}$ such that the objective function F will attain a minimum:

$$\min F = \sum_n \sum_i \sum_j \left(\sum_{m=1}^5 g_m \cdot T_m + f_{i,j}^{n+1/2} \cdot S_{i,j} - p_{i,j}^{n+1/2} + r_{i,j}^{n+1/2} \right)^2 \quad (44)$$

subject to the nonnegativity restrictions

$$T_{i,j}, S_{i,j} \geq 0 \quad \forall i, j \quad (45)$$

This is a typical quadratic programming problem, with a quadratic objective function and linear constraints.

The main difference between this and the previous optimization problems is that here the balance equations appear as part of the objective function, whereas the constraints are only the physical (nonnegativity) ones.

SOLUTION OF THE LINEAR AND THE QUADRATIC PROGRAMMING PROBLEMS

The solution of linear programming problems can be obtained by using ready made reliable computer programs, which are nowadays supplied as a routine by computer manufacturers. In the present work, use was made of IBM's program

TABLE 1. Comparison of the Optimization Problems

	Linear Criteria					Quadratic Criterion
	A	B	C	D/1	D/2	E
Number of variables	$2C + 1$	$2C + N$	$3C$	$C(N + 2)$	$2C(N + 1)$	$2C$
Number of constraints	$2CN$	$2CN$	$2CN$	$2CN$	CN	
Number of variables in the objective function	1	N	C	CN	$2CN$	$2C$

MPS/360. Prior to using the program the data have to be prepared in an appropriate manner. For this purpose a computer program composed of two stages has been prepared. In the first stage the data of the identification problem (water levels, pumping and recharge rates, boundary conditions, etc.) are read in, and the coefficients for the objective function and the constraints are computed and stored in a proper format on a disk, to be later used as input for the linear programming program. In the second stage the MPS/360 program (available in the computer library) reads the data from the disk and solves for the optimal values of the sought parameters (details and a listing of the program are contained in the report by Hefez *et al.* [1973]).

The quadratic programming problem was solved in the present work by a computer program suggested by Kunzi *et al.* [1968], which is based on Wolfe's [1959] method. The program underwent significant modifications before it could be applied (details and a listing of the program also appear in the report by Hefez *et al.* [1973]).

COMPARISON OF OPTIMIZATION CRITERIA

The five criteria presented above differ from each other and will therefore result in different values for the optimal parameters of the given cell model. This is so in spite of the fact that all criteria are based on the same data and the same balance equations. Since we are interested in only one solution, we shall have to decide which criterion to use.

A first approach for selection among the various criteria may be based on the degree of difficulty of computing the solution. Table 1 summarizes some of the differences among the optimization problems set up according to the five criteria.

If the five criteria were theoretically equivalent to each other, the choice of the one to be used could be based on such technical considerations as computer time, computer memory, etc. This is especially true for models involving a large number of cells C and a large number of time intervals N , as these numbers determine the numbers of variables and constraints.

From Table 1, one can see that among the linear criteria, criterion A involves the least number of variables, whereas the second form of criterion D involves the least number of constraints.

It is of interest to note that in the quadratic criterion E the numbers of constraints and of variables are the least. This may lead one to assume that this criterion will also be the most efficient from the point of view of computer memory and computation time. However, the solution of the quadratic programming problem is much more complicated in comparison with that of linear programming so that one cannot really estimate the required memory and computing time on the basis of the numbers of variables and constraints alone. It should also be emphasized that reliable and efficient computer programs are readily available for the solution of linear

programming problems, whereas this is not usually the case for quadratic programming.

In all five criteria, one has to compute the balance equations for all cells and for all time intervals. In the linear problems no further computations are necessary in order to form the objective function and the constraints. In the quadratic programming case, on the other hand, one has also to compute the coefficients appearing in the objective function by squaring and summing up balance equations.

A better basis for choice relates to the differences in the results obtained by employing the different criteria. Kleinecke [1971] reports very poor results obtained by using criterion E. He chose criterion C as the best, arguing without proof that this criterion is better than D. He reached this conclusion by comparing the results of the analysis with those obtained by using an electric analog.

In the present work, a comparison among the different criteria was made by identifying the parameters of a number of synthetic models. Here a synthetic model is one whose parameters are known a priori, and hence for which we can forecast the water levels for the calibration period. These water levels are, in turn, used as input data for identifying the model parameters. The parameters thus obtained are then compared with the known parameters of the model. The deviations of the computed parameters from the known values resulting from the use of each criterion presented above facilitate the comparison among the criteria. From this comparison, some results of which are presented below, it is suggested that the best criteria are D and E in which the objective function incorporates the sum of all the deviations.

RESULTS

Example 1: Identifying the Parameters of a Synthetic Nonrectangular Model

This example deals with the identification of a synthetic nonrectangular model of 24 cells (Figure 3). The following questions were studied by use of this model: the differences between the five criteria, the differences between the two finite difference schemes, (10) and (11), and the sensitivity of the solution to errors in values of ϕ .

Because of the large amount of data we shall present here only the main details. The cells of the model were numbered as shown in Figure 3. The dimensions of all cells are $\Delta x = 1000$ m and $\Delta y = 1500$ m. The duration of the calibration period was 2 years, during which a specified schedule of summer pumping and winter recharge was implemented. The recharge took place in all cells. Pumping took place only in the cells whose numbers are circled in Figure 3.

In the forecasting stage the water levels for the calibration period were computed by using 6-day intervals. However, for the identification problem, water levels at 60-day intervals

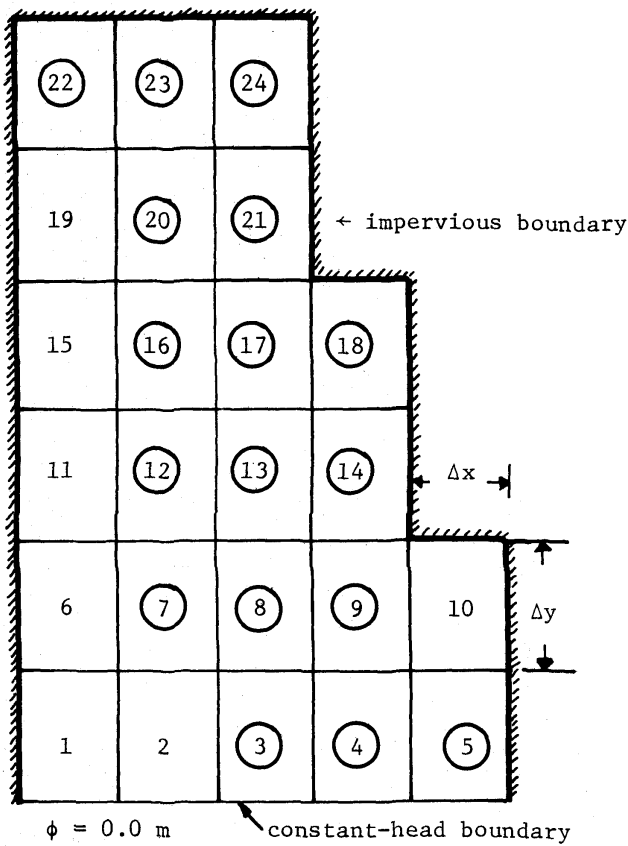


Fig. 3. The model studied in example 1.

were used. This resulted in 12 time intervals for the identification problem.

The true values of the parameters (used to obtain the water levels in the model) were $T = 3000 \text{ m}^2/\text{d}$ and $S = 10\%$ in all cells. Following are some results and conclusions derived from the example.

Tables 2 and 3 show the results obtained for T and S , respectively, using the five criteria and the forecasting equation (11). Examination shows that the best results were obtained when criterion E was used, and that the results obtained by using the second form of criterion D are better than those obtained by the use of criterion A, B, or C.

In order to examine the effect of the choice of a finite difference scheme, we compare the results of using criterion D/2 as shown in Tables 2 and 3 with those shown in Table 4 (first two columns) which were obtained with the same criterion but with the scheme of (10). The main difference is that the values of storativity in all cells as shown in Table 4 are lower than the true value of 10%. Better results are obtained in this example (and in additional ones) when the scheme of (11) was used.

Analysis of results. Before using the model, with parameter values determined by the identification process, one should estimate the degree of accuracy to be expected when the model is used to forecast future water levels. There are several ways for doing this: (1) use the model to compute water levels for some historical period, the data of which were not used in the identification, compare the results with measured data, and draw conclusions; (2) perform a statistical analysis of the deviations between computed and measured water levels for the calibration period and assume that the same statistical behavior of the deviations will occur in forecasting future water levels; (3)

TABLE 2. Identified Transmissivity Values for Example 1

Cell	Criterion				
	A	B	C	D/2	E
1	2947	3020	3033	2980	2997
2	2807	2970	2933	2977	2971
3	3106	2923	3025	2952	2970
4	2972	2854	3104	2942	2967
5	3081	2958	3006	3050	3018
6	2735	3012	3037	3027	3018
7	2499	2898	2896	2995	2971
8	3088	2977	3086	2937	2994
9	2813	2790	2999	3036	2997
10	3523	3133	3025	3131	3062
11	3022	3078	3033	2994	3000
12	2897	2989	2830	2983	2980
13	2981	2801	2877	2979	2954
14	3380	2945	3260	3018	3034
15	2267	2893	3017	3014	3012
16	2187	2786	2888	3043	2981
17	3324	2940	3264	3029	3007
18	3126	2652	3138	3087	3002
19	2940	3260	3037	2989	3002
20	3004	3020	2758	2966	2947
21	3173	2759	2848	3086	2978
22	2503	2755	2936	2958	3001
23	2381	2612	2981	3111	3073
24	3464	2793	3098	2924	2972
$ \Delta T _{\max}$	733	388	264	131	73
$\sum \Delta T $	5362	3824	2217	1072	544
$\sum \Delta T /24$	223	159	93	45	23

Values are given in square meters per day.

examine the sensitivity of the parameter values computed in the identification process to 'noise' in the data.

While the first and/or second way should be performed in practical cases, it is instructive to examine results obtained by

TABLE 3. Identified Storativity Values for Example 1

Cell	Criterion				
	A	B	C	D/2	E
1	11.7	11.3	11.6	11.6	11.5
2	11.7	11.2	11.4	11.2	11.3
3	11.6	12.1	10.6	11.5	11.6
4	12.2	12.0	12.0	12.0	11.6
5	11.1	12.0	11.4	11.5	11.4
6	9.7	10.0	9.8	9.9	9.9
7	10.2	10.6	10.7	10.7	10.6
8	9.8	10.0	9.9	10.2	10.0
9	9.2	9.5	9.2	9.4	9.6
10	10.3	9.8	10.0	9.8	10.1
11	10.0	9.8	9.8	9.9	9.9
12	10.2	9.7	9.4	9.7	9.8
13	9.3	10.0	9.4	10.3	10.1
14	9.4	9.6	9.5	10.0	9.7
15	9.9	10.2	10.0	9.9	9.9
16	9.7	9.8	9.9	9.8	9.8
17	10.3	9.8	10.3	9.8	9.8
18	10.1	10.1	10.5	10.0	10.1
19	9.9	9.8	9.8	9.9	9.9
20	10.1	10.2	10.1	10.4	10.2
21	10.3	10.0	10.3	10.0	9.9
22	10.1	10.3	10.3	10.0	10.1
23	9.4	10.1	9.4	9.9	10.0
24	10.3	10.0	10.1	10.0	10.0
$ \Delta S _{\max}$	2.2	2.1	2.0	2.0	1.5
$\sum \Delta S $	13.9	12.3	13.2	11.4	10.4
$\sum \Delta S /24$	0.58	0.51	0.56	0.48	0.44

Values are given in percent.

TABLE 4. Effect of Noise on Identified Parameters

Cell	Without Noise		With Noise ± 2 cm		With Noise ± 5 cm	
	T	S	T	S	T	S
1	3055	6.4	2867	8.0	2823	9.0
2	3050	6.2	2933	6.2	2597	6.0
3	3027	6.2	2737	8.4	2316	8.7
4	3017	6.3	2880	9.2	2220	14.5
5	3053	6.5	2991	5.7	2748	4.7
6	3010	8.0	2828	7.4	2591	6.2
7	2989	7.7	2703	7.5	1957	7.8
8	2962	7.8	2779	9.6	2396	9.9
9	2946	7.8	2929	7.3	2162	9.0
10	3000	8.1	2942	8.3	2387	9.0
11	3011	9.2	2717	9.7	2551	10.2
12	2948	9.3	3255	10.0	3149	11.0
13	2943	9.1	2473	8.8	1722	8.2
14	2993	9.5	2648	9.0	2050	8.5
15	2980	9.5	2819	9.8	2610	9.6
16	2964	9.6	2546	9.2	1506	9.1
17	2938	9.4	2617	9.1	1894	9.6
18	2877	9.7	3186	10.3	2157	10.6
19	2958	9.7	2501	9.1	1954	8.2
20	2928	9.6	3536	10.3	3306	10.7
21	2922	9.8	2611	9.4	1571	9.6
22	2921	9.7	2995	9.7	2327	10.6
23	2958	9.7	2435	10.2	638	11.0
24	2960	9.9	2321	9.9	1668	10.4
$\max \Delta $	123	3.8	679	4.3	2362	5.3
$\sum \Delta$	1036	35.3	6705	29.5	19310	35.9
$\sum \Delta/24$	43	1.49	281	1.24	808	1.50

the third way and draw general conclusions on the robustness of the identification process, i.e., the stability of computed values to random noise in the data.

Sensitivity to errors in values of ϕ . Table 4 summarizes results of the identification performed on the synthetic aquifer of example 1 under the following conditions: (1) the criterion is $D/2$, the forecasting scheme is (10), and there are no errors in the data for ϕ ; (2) same as the first except that errors in values of ϕ are introduced as a random noise, uniformly distributed over the range ± 2 cm; (3) same as the second except that the range of the noise is ± 5 cm.

These perturbations in the data are representative of the degree of error to be expected in water level data used in the model. These errors may be due to measurement errors and to the way in which one value per cell is obtained by averaging data of several observations. The magnitude of the noise represents only a very small relative error in the water levels themselves, which may be of the order of several feet to hundreds of feet. More important, though, are the relative errors introduced in the spatial and temporal gradients, which make up the coefficients in the constraints of the optimization problem. Typical differences between water levels in adjacent cells are of the order of tens of centimeters, and changes in water levels over 60 days are of similar magnitude. Thus the noise in water level data, which does not seem very significant in itself, may result in very substantial errors in the gradients, as much as 100% and more.

The deviations of the computed transmissivities are much more affected by the noise than the storativities. The greatest effect is in cells 16–24, where the gradients are smallest.

Inflow and outflow rates as unknowns. So far, only the transmissivity and storativity have been considered as unknown parameters which have to be identified. However, in certain problems of practical interest, inflow and/or outflow rates in certain cells and/or during certain time intervals are also not

known a priori and have to be determined as part of the calibration procedure. As an example, let the natural replenishment be added to the list of parameters whose values are being sought. Let $q_{i,j}^{n+1/2}$ denote the natural replenishment in the cell (i, j) during the time interval $(n, n + 1)$. In the balance equation (11) this discharge rate was included in the inflow rate:

$$r_{i,j}^{n+1/2} = (r')_{i,j}^{n+1/2} + q_{i,j}^{n+1/2} \quad (46)$$

where r' is the known part of the inflow. By inserting (46) into (21), we obtain

$$\begin{aligned} \sum_{m=1}^5 g_m \cdot T_m + f_{i,i}^{n+1/2} \cdot S_{i,i} + q_{i,i}^{n+1/2} \\ = p_{i,i}^{n+1/2} - (r')_{i,i}^{n+1/2} \end{aligned} \quad (47)$$

This equation is still linear; hence the techniques described above are applicable here also except that (47) will be used instead of (11). Following is a numerical example in which the winter natural replenishment was identified for the Yarkon-Taninim aquifer in Israel.

Example 2: A Single-Cell Model of the Yarkon-Taninim Aquifer

Data for this model were provided by the research and development team of the Hydrological Department of Water Planning for Israel (Tahal) Ltd. The objective of this model is to represent the regime of the aquifer and to enable the incorporation of the model in a comprehensive model dealing with the operation of the entire Israel National Water Scheme. For this purpose a single-cell model was found sufficient. The model is presented here, to give an example of identification of a real aquifer, and to give an example of identifying an inflow rate in addition to the storativity of the aquifer. Figure 4 gives

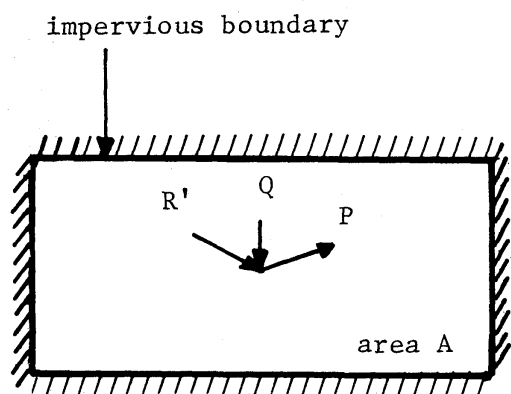


Fig. 4. A single-cell model of the Yarkon-Taninim aquifer.

a schematic representation of the model with its inflows and outflows. (Transmissivities play no role in a single-cell model.)

The balance equation (47) for the single-cell aquifer can be rewritten in the form

$$S \cdot A \cdot \frac{\Delta\phi^{n+1/2}}{\Delta t^{n+1/2}} + Q^{n+1/2} = P^{n+1/2} - (R')^{n+1/2} \quad (48)$$

where Q is the natural replenishment during the time interval $(n, n + 1)$ and R' are all other inflows during that same period.

In (48) the storage capacity $S \cdot A$ (equal to the product of storativity and area of cell) appears as a single unknown parameter. Obviously, if A is known, one can regard S as the parameter to be identified; $Q^{n+1/2}$ are a series of n unknown inflows from precipitation (and from other unidentified sources).

The calibration period, which included the 11 years from 1958 to 1969, was divided into summer and winter seasons. Each season of 6 months served as a time interval in the calibration process. Table 5 summarizes the data used for the identification in this example. Table 6 shows the results obtained for $S \cdot A$ and the $Q^{n+1/2}$ using criteria A, B, and E.

It was a priori assumed that natural replenishment occurs only during winter. An attempt was also made to identify the parameters separately from the winter balance equation and from the summer ones. The results in Table 6 indicate that the same $S \cdot A$ value of 85.3 was obtained from the summer equations as from the full set of equations. However, the result for $S \cdot A$ obtained from the use of the winter equations alone is

TABLE 5. Data for the Identification Procedure of Example 2

Season	$\Delta\phi$, m	Precipitation, 10^6 m^3	Pumping Minus Recharge $P - R'$, 10^6 m^3
Summer 1958	-2.80	0	244.2
Winter 1958-1959	1.30	497.7	165.9
Summer 1959	-2.36	0	216.5
Winter 1959-1960	0.80	394.4	138.3
Summer 1960	-2.52	0	230.7
Winter 1960-1961	1.78	570.5	145.5
Summer 1961	-2.62	0	198.5
Winter 1961-1962	2.30	654.1	136.6
Summer 1962	-2.63	0	275.5
Winter 1962-1963	1.03	418.4	158.6
Summer 1963	-2.65	0	204.3
Winter 1963-1964	3.07	737.4	145.1
Summer 1964	-2.85	0	243.5
Winter 1964-1965	4.47	824.5	95.8
Summer 1965	-2.68	0	206.9
Winter 1965-1966	1.72	520.0	95.1
Summer 1966	-3.72	0	266.2
Winter 1966-1967	4.36	968.2	120.5
Summer 1967	-2.30	0	221.7
Winter 1967-1968	2.14	540.2	130.4
Summer 1968	-2.94	0	249.9
Winter 1968-1969	4.42	883.4	117.5

meaningless. As in this case the number of unknowns exceeds the number of equations by one. The use of criterion E (minimization of the sum of the squares of the deviations) yielded results similar to those of criterion B or D.

POSSIBLE IMPROVEMENTS: WEIGHTING TERMS IN THE OBJECTIVE FUNCTION

There is a possibility of modifying the objective function by assigning different weights to certain terms in the objective function. The weights actually reflect the importance of each deviation, both in time and in space. Weights can be used in all criteria, except criterion A which has only a single term.

For criterion B we write, instead of (29),

$$\min F = \sum_{n=0}^{N-1} w^{n+1/2} \cdot Y^{n+1/2} \quad (49)$$

For criterion C, instead of (33),

TABLE 6. Identified Storage Capacity and Natural Replenishment of Example 2

Parameter	Units	Criterion A (or C)			Criterion B (or D)	Criterion E
		Summer Equations	Winter Equations	All Equations		
Value of the optimal objective function	10^6 m^3	234	0	806	233	7865
$S \cdot A$	$10^6 \text{ m}^3/\text{m}$	85.3	0	85.3	85.4	84.2
Q , 1958-1959	10^6 m^3		166	226	277	275
Q , 1959-1960	10^6 m^3		138	155	207	206
Q , 1960-1961	10^6 m^3		146	246	298	295
Q , 1961-1962	10^6 m^3		137	282	333	330
Q , 1962-1963	10^6 m^3		159	195	247	245
Q , 1963-1964	10^6 m^3		145	356	407	404
Q , 1964-1965	10^6 m^3		96	426	478	472
Q , 1965-1966	10^6 m^3		95	191	242	240
Q , 1966-1967	10^6 m^3		121	441	493	488
Q , 1967-1968	10^6 m^3		130	262	313	311
Q , 1968-1969	10^6 m^3		118	443	495	490

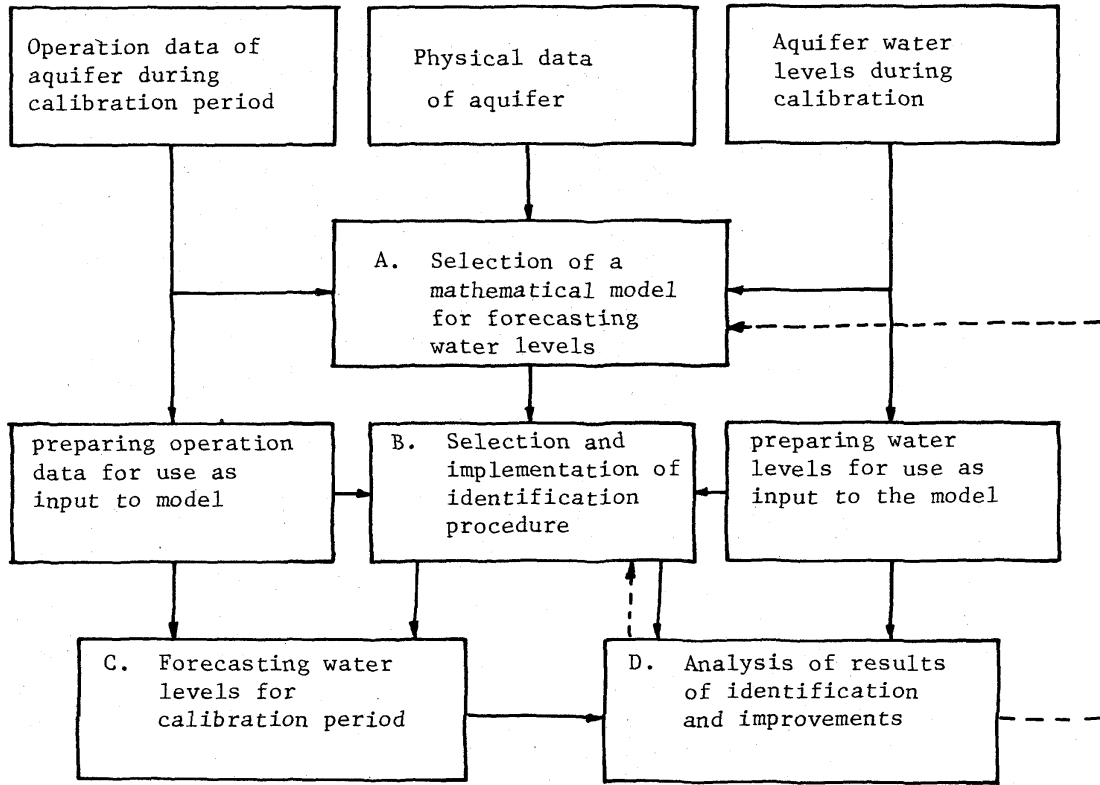


Fig. 5. General flow chart for the identification procedure.

$$\min F = \sum_i \sum_j w_{i,j} \cdot Z_{i,j} \quad (50)$$

For criterion D/1, instead of (37),

$$\min F = \sum_n \sum_i \sum_j w_{i,j}^{n+1/2} \cdot U_{i,j}^{n+1/2} \quad (51)$$

For criterion D/2, instead of (41),

$$\min F = \sum_n \sum_i \sum_j w_{i,j} (V_{i,j}^{n+1/2} + W_{i,j}^{n+1/2}) \quad (52)$$

For criterion E, instead of (44),

$$\min F = \sum_n \sum_i \sum_j w_{i,j}^{n+1/2} \left(\sum_{m=1}^5 g_m \cdot T_m + f_{i,j}^{n+1/2} \cdot S_{i,j}^{n+1/2} - p_{i,j}^{n+1/2} + r_{i,j}^{n+1/2} \right)^2 \quad (53)$$

The method for assigning weights has not been finalized, nor experimented with, during the phase of the work reported herein. We propose that weights can be assigned by one or more of the following considerations: (1) cell areas, i.e., when cells differ considerably in their area, one may assign a higher weight to smaller cells, since they usually indicate a higher concentration of wells with known data; (2) cells in which the information available seems less reliable may be assigned a low weight; (3) cells in sensitive areas, where the reliability of the computed results is important, may be assigned a high weight.

As already stated above, this subject requires further investigation before the use of weights can be made systematic.

FLOW CHART FOR THE CALIBRATION PROCEDURE

In addition to the solution of a linear or quadratic programming problem the identification procedure involves several additional steps. These are summarized in the flow chart shown in Figure 5. The chart indicates four main steps in the identification procedure: (1) selection of a mathematical model to be used for forecasting water levels in the aquifer; (2) calculating the values of the parameters of the model using the data of the calibration period (prior to using these data they have to be prepared in a form accepted by the identification program (nodes, time intervals, etc.)); (3) forecasting water levels for the calibration period, making use of the derived aquifer parameters and the information of operation during the calibration period; (4) analysis of deviation between the response of the aquifer (e.g., water levels) and that of the model and a sensitivity analysis of the solution to possible errors in the data. This may lead to the introduction of weighting coefficients and to an improvement in the model response.

The full arrows in Figure 5 show the direction of information flow during the various steps. The dashed arrows show possible routes to be taken by the analyst.

Figure 6 shows the same flow chart in a somewhat different form, with more details. The operations are shown in a chronological order, separating those performed by man from those performed by the computer. In this form one can clearly see the importance of the engineer's or planner's decisions. Although the computations are carried out by the computer, and they yield the solution, it is the analyst's guidance of the process which determines what the solution will be.

SUMMARY

Although the evaluation of the identification methods proposed here was based mainly on the analysis of synthetic

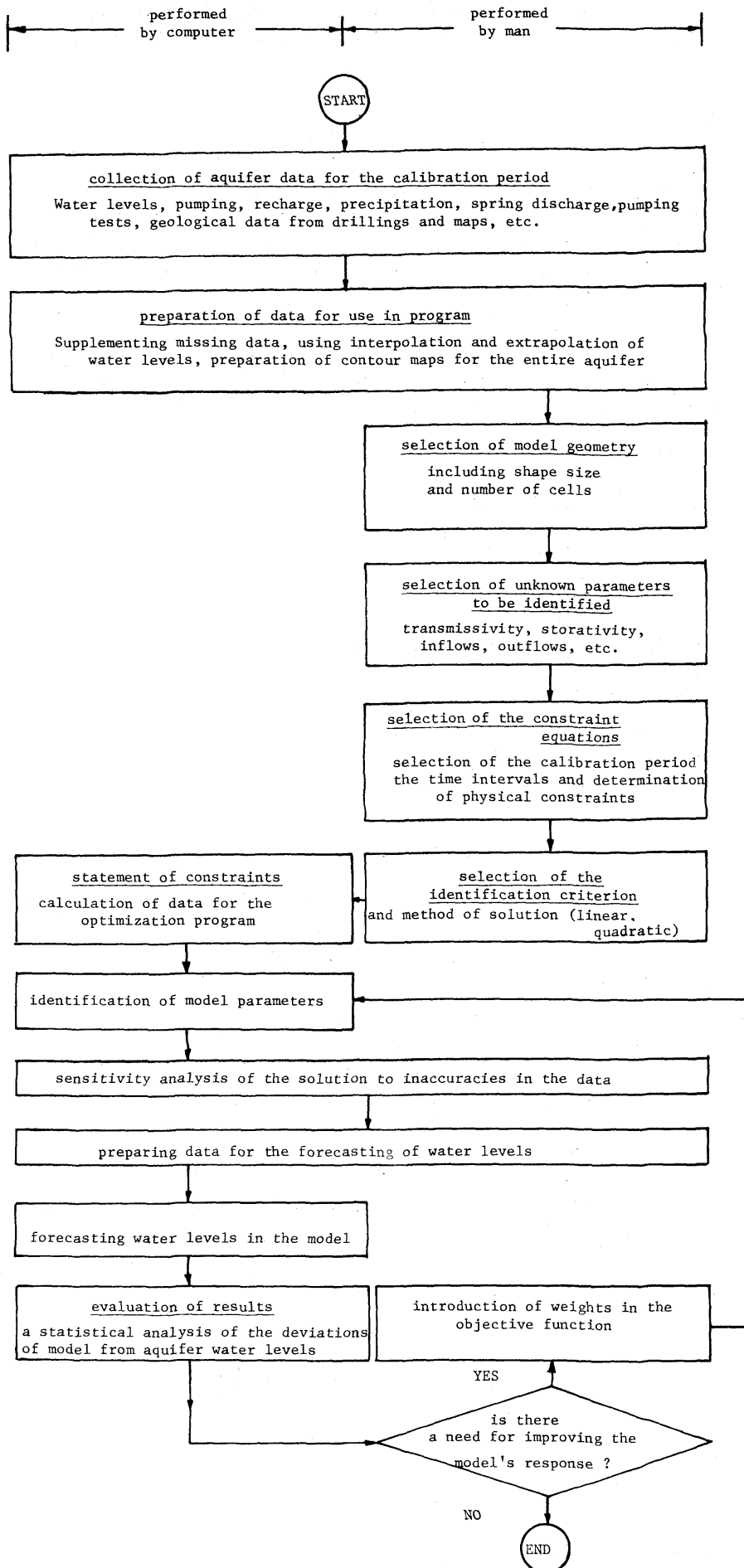


Fig. 6. Detailed flow chart for identification of model parameters.

models and not on real aquifer situations, one may reach several intermediate conclusions already at the present stage of the development.

Complete identification procedure. The procedure of identifying model parameters does not terminate with their computation by a method which guarantees the best fit between model and aquifer discharge rates. It is recommended to seek a solution which will also result in an optimal fit between model and aquifer water levels. This conclusion stems from the fact that the water levels for the calibration period are known to a higher degree of certainty than the various discharges. Accordingly, once the parameters have been identified, one must continue as follows: (1) use the parameters to forecast the water levels for the calibration period; (2) carry out a statistical analysis of the deviations of the computed water levels from the observed ones; (3) recompute the parameters by introducing weights in the objective function; (4) repeat steps 1 and 2 with the computed values of the parameters (repeat until a satisfactory agreement is reached between aquifer and model water levels); and (5) finally, carry out an analysis of the sensitivity of the solution to possible error or changes in the water levels in the various inflow and outflow rates during the calibration period.

Balance equations. The ultimate objective of the model, once all its parameters have been identified, is to forecast future water levels in the aquifer in response to various natural and planned activities. It is therefore desirable to identify the same model which we shall later use for forecasting. The alternating direction implicit (ADI) method has been found to be very efficient for forecasting future aquifer water levels [Hefez et al., 1972]. Unfortunately, this scheme is impractical for the identification of parameters. It has been demonstrated in the present work that (11) is closest to the ADI scheme and may be used in the identification process.

Criteria for identifying the parameters. Five different criteria were presented here. Four were based on the absolute value of the difference between the two sides of the balance equations, and one was based on the square of this difference. By using synthetic models, the best criteria were shown empirically to be those in which the sum of absolute deviations (or squares of them) for all balance equations was used as the objective function.

Linear and quadratic programming. The identification problem as stated in the present work is solved as a linear or a quadratic programming problem. The solution in the latter case is much more complicated, whereas the solution of the linear

programming problem is based on readily available computer programs. One advantage, however, of the quadratic programming problem is that the size of the problem (number of constraints) and the needed computer memory are independent of the number of time intervals included in the calibration period.

Identification of inflows and outflows. It is possible to identify inflows such as from natural replenishment and outflows by the identification procedure described here.

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