MATHEMATICAL MODEL OF UNSTEADY GROUNDWATER FLOW THROUGH AQUIFERS AND CALIBRATION VIA A NON-LINEAR OPTIMIZATION TECHNIQUE

H. M. V. Samani

Department of Civil Engineering
Shahid Chamran University of Ahwaz
Ahwaz, Iran

M. Kolahdoozan

Department of Civil Engineering
Bradford University
England

Abstract In this study, the general partial differential equation of unsteady groundwater flow through non-homogeneous and anisotropic aquifer was solved by the fully implicit finite difference method with control volume approach. The calibration of permeability and storage coefficients as model parameters was performed by a transformation technique and application of Powell's non-linear optimization method. The developed model has been found efficient in terms of convergence and accuracy. Capability of the model, has also been demonstrated by being applied to a real aquifer.

Key Words Nonhomogeneous, Anistoropic, Aquifer, Transmissivity, Storage Coefficient, Optimization, Objective Function, Constraint, Calibration, Control Volume Approach

چکیده در این تحقیق، معادله دیفرانسیلی عمومی جریان غیر ماندگار آبهای زیرزمینی در سفره های غیر همگن و غیر همسان بوسیله روش تفاضلهای محدود غیر صریح کامل در حجم کنترل حل گردیده است. کالیبراسیون ضرایب نفوذپذیری و ذخیره در نقاط مختلف بعنوان پارامترهای مسئله با استفاده از تکنیک تبدیل و اعمال روش پاول در بهینه یابی غیر خطی انجام شده است. مدل تهیه شده از نقطه نظرهای همگرائی و دقت کارآئی خوبی داشته است. توانائی مدل با اعمال آن به سفره واقع به اثبات رسیده است.

INTRODUCTION

One of the essential issues in water resourses management is to study the groundwater storage and movement in aquifers. Mathematical modeling can be introduced to predict the groundwater table variation due to water pumping from an aquifer.

Applying Darcy's law with continuity equation to a soil element of an aquifer in cartesian coordinates and using Dupuits principle, yields the governing equation of groundwater flow which is as follows:

$$\frac{\partial}{\partial x}\left(K_x d \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y d \frac{\partial h}{\partial y}\right) = S \frac{\partial h}{\partial t} + R \qquad (1)$$

where

x and y = coordinates of the aquifer in the plane:

K_x and K_y = permeabilities in x and y directions respectively;

d = thickness of the aquifer ;

h = hydraulic head

S = storage coefficient or specific yield coefficient;

R = recharge or vertical seepage discharge per unit area.

Equation 1 in its general form has no exact analytical solution. Analytical solutions to the one and two-dimensional forms of Equation 1 with different simple initial and boundary conditions in homogeneous and isotropic porous media were introduced in the literature [1-3]. A number of simplifying assumptions are required to solve the unsteady groundwater flow analytically. These assumptions, however, are sometimes far from the real conditions. Analytical solutions are thus not directly applicable to most field problems. Consequently, to solve field problems, it is preferable to use numerical techniques because they allow for a more generalized treatment with fewer assumptions.

The simplest, and probably the most commonly used triangle based finite element approach is the control volume Galerkin finite element method which has been employed by Dassarguds [4], Cordes and Kinzelbach [5], Fung, Hiebert, and Nghiem [6] and Durlofsky [7]. The disadvantage of this method is that the whole system of equations has to be solved once simultanously. Another common numerical method in the literature is the one in which the spacial derivatives are discretized by the Galerkin finite elements method and for the time derivatives a fully implicit finite difference scheme is used [8]. This method is accurate and inconditionally stable but has the same disadvantages of the preceding method.

The finite difference technique is one of the common numerical methods used to solve Equation 1. In this study, the fully implicit finite difference method with a control volume approach [9] was used. The non-linear system of equations obtained through the analysis was solved by the line by line sweeping method in four directions [9]. This method is unconditionally stable, accurate, fast, and needs less memory than the finite element method because the solution of the equations is done line by line not all at once. The formulation of this method is almost similar to the Galerkim finite element method except the weighting function which is considered equal to unity.

The other important issue in mathematical modeling of groundwater flow in an aquifer is the model calibration. The calibration should be done in such a way that the differences between calculated and observed heads will be minimized.

The trial and error method of calibration has been the most common one [10-16]. Since, the number of parameters is usually large, the trial and error method needs a large number of runs and usually has a low accuracy. Some researchers attempt to improve the trial and error technique by introducing a policy for correcting the parameters after each trial run [17-19]. Simple optimization techniques such as linear and quadratic programing were used by Kleinecke [20] and Hefez et al. [21].

In this research, to calibrate the model a non-linear optimization method for both confined and unconfined aquifers with a zoning technique is introduced.

NUMERICAL METHOD

Integrating Equation 1 on the control volume of the node i, j shown in Figure 1 gives:

$$\int_t^{t+\Delta t}\int_s^n\int_w^e \frac{\partial}{\partial x}\left(K_x d\frac{\partial h}{\partial x}\right) dx\, dy\, dt + \int_t^{t+\Delta t}\int_w^e\int_s^n \frac{\partial}{\partial y}\left(K_y d\frac{\partial h}{\partial y}\right) dy\, dx\, dt = \int_t^{t+\Delta t}\int_s^n\int_w^e S\frac{\partial h}{\partial t} dt\, dx\, dy + \int_t^{t+\Delta t}\int_s^n\int_w^e R\, dx\, dy\, dt \qquad (2)$$

Assuming constant R and S and using the fully implicit scheme for the spacial derivatives yields:

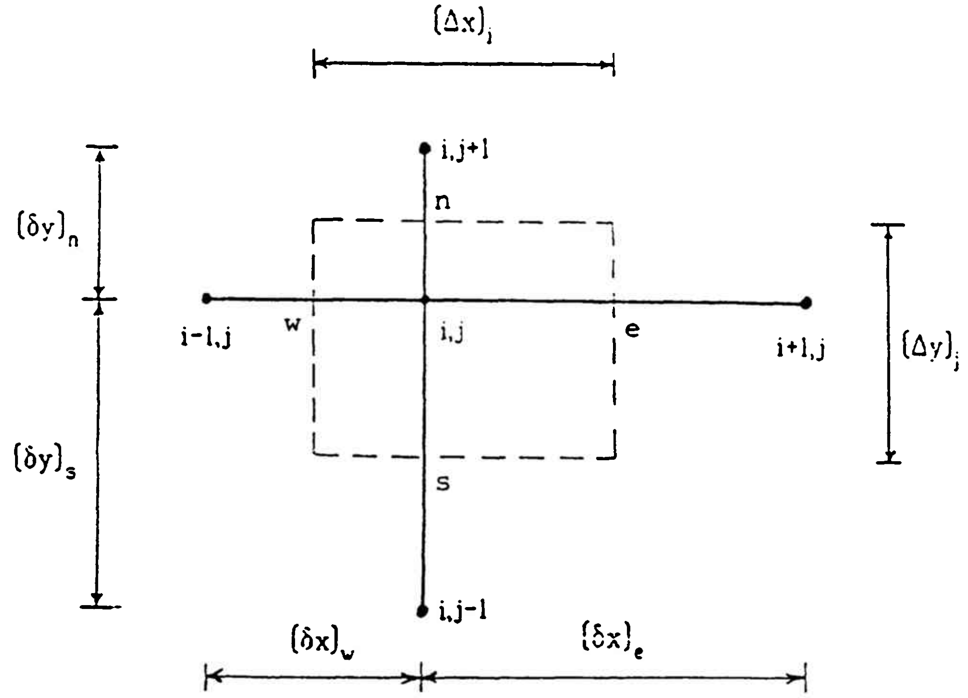


Figure 1. Control Volume of node i,j.

$$\left[\frac{1}{2}K_{xe}\left\{\frac{(h_{i+1,j}^{m+1})^2-(h_{i,j}^{m+1})^2}{(\delta x)_e}\right\}-\frac{1}{2}K_{xw}\left\{\frac{(h_{i,j}^{m+1})^2-(h_{i-1,j}^{m+1})^2}{(\delta x)_w}\right\}\right](\Delta y)_j-$$

$$\left[K_{xe}z_e\frac{h_{i+1,j}^{m+1}-h_{i,j}^{m+1}}{(\delta x)_e}+K_{xw}z_w\frac{h_{i,j}^{m+1}-h_{i-1,j}^{m+1}}{(\delta x)_w}\right](\Delta y)_j+$$

$$\left[\frac{1}{2}K_{yn}\left\{\frac{(h_{i,j+1}^{m+1})^2-(h_{i,j}^{m+1})^2}{(\delta y)_n}\right\}-\frac{1}{2}K_{ys}\left\{\frac{(h_{i,j}^{m+1})^2-(h_{i,j-1}^{m+1})^2}{(\delta y)_s}\right\}\right](\Delta x)_i-$$

$$\left[K_{yn}z_n\frac{h_{i,j+1}^{m+1}-h_{i,j}^{m+1}}{(\delta y)_n}+K_{ys}z_s\frac{h_{i,j}^{m+1}-h_{i,j-1}^{m+1}}{(\delta y)_s}\right](\Delta x)_i=$$

$$S_{i,j}\frac{h_{i,j}^{m+1}-h_{i,j}^{m}}{\Delta t}(\Delta x)_i(\Delta y)_j+R_{i,j}(\Delta x)_i(\Delta y)_j \qquad (3)$$

in which

K_{xe} and K_{xw} = permeabilities of the control volume in x-direction at points e and w respectively;

K_{yn} and K_{ys} = Permeabilities of the control voume in y-direction at points n and s respectively;

m = time index;

z_e, z_w, z_n and z_s represent heights of the impervious bed from datum of points e, w, n and s respectively.

Using harmonic means of neighbour node permeabilites for the control voume boundary point permeabilities, introducing arithmatic means for elevations of them and considering:

$d_{i,j} = h_{i,j} - z_{i,j}$

Equation 3 after some simplifications will be as follows:

$$T_1\left(h_{i+1,j}^{m+1}-h_{i,j}^{m+1}\right)-T_2\left(h_{i,j}^{m+1}-h_{i-1,j}^{m+1}\right)+T_3\left(h_{i,j+1}^{m+1}-h_{i,j}^{m+1}\right)-T_4\left(h_{i,j}^{m+1}-h_{i,j-1}^{m+1}\right)=S_{i,j}\frac{h_{i,j}^{m+1}-h_{i,j}^{m}}{\Delta t}+R_{i,j} \qquad (4)$$

where

$$T_1=\frac{2K_{i+1,j}K_{i,j}}{K_{i+1,j}+K_{i,j}}\,\frac{d_{i,j}+d_{i+1,j}}{2}\left[\frac{2}{(\delta x)_e\{(\delta x)_e+(\delta x)_w\}}\right];$$

$$T_2=\frac{2K_{i,j}K_{i-1,j}}{K_{i,j}+K_{i-1,j}}\,\frac{d_{i,j}+d_{i-1,j}}{2}\left[\frac{2}{(\delta x)_w\{(\delta x)_e+(\delta x)_w\}}\right];$$

$$T_3=\frac{2K_{i,j+1}K_{i,j}}{K_{i,j+1}+K_{i,j}}\,\frac{d_{i,j}+d_{i,j+1}}{2}\left[\frac{2}{(\delta y)_n\{(\delta y)_n+(\delta y)_s\}}\right];$$

$$T_4 = \frac{2K_{i,j}K_{i,j-1}}{K_{i,j}+K_{i,j-1}} \frac{d_{i,j}+d_{i,j-1}}{2}\left[\frac{2}{(\delta y)_s\left((\delta y)_n+(\delta y)_s\right)}\right];$$

$$R_{i,j} = \frac{(Qpump_{i,j} - Qar_{i,j})}{\left(\frac{(\delta x)_e+(\delta x)_w}{2}\right)\left(\frac{(\delta y)_n+(\delta y)_s}{2}\right)} - Qper_{i,j}$$

in which

$Qpump_{i,j}$ = pump discharge at node i,j;

$Qar_{i,j}$ = recharge discharge at node i,j;

$Qper_{i,j}$ = vertical seepage discharge into the aquifer at node i,j per unit area.

Applying Equation 4 to all nodes of the aquifer grid and introducing initial and boundary conditions, a system of non-linear equations results. These equations were solved by the iterative line by line sweeping method in four directions [9] in which the tridiagonal matrix algorithm is introduced to solve the equations for every line.

ANALYTICAL CHECKS

To check the accuracy of the model, problems which have exact analytical solutions were selected. These problems were solved by the developed model. Then results were compared to analytical exact solutions.

Example 1

A confined homogeneous and isotropic aquifer as shown schematically in Figure 2 is considered. The aquifer has the following characteristics:

$S = 0.003,\qquad T = 0.001\ \frac{m^2}{s},\qquad Q_p = 0.25\ \frac{m^3}{s}$

where, T, is the transmissivity of the aquifer and Q_p is the pump discharge.

The analytical solution of the water drawdown in the well given by Theis [22] and numerical results computed by the developed model are illustrated in

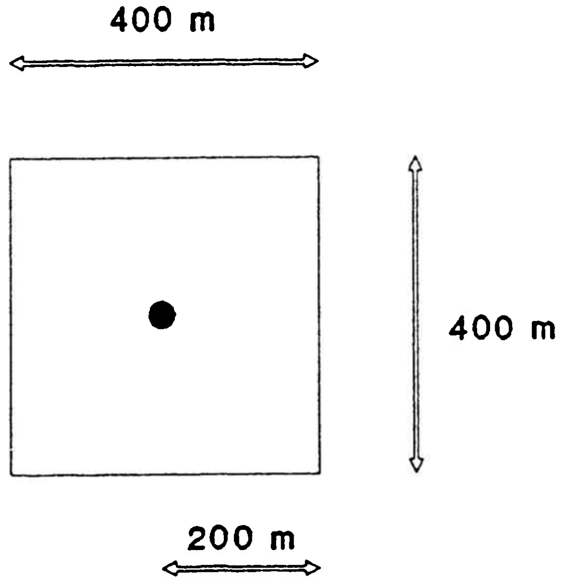


Figure 2. Aquifer of Eample 1.

Figure 3. Head versus distance from the well center after 5000 seconds are also introduced in Figure 4. Results show good accords between analytical and numerical methods.

Example 2

A semi-infinite homogeneous and isotropic aquifer confined above and below by impermeable layers as shown in Figure 5 is considered. The aquifer is bounded at x equal to zero by a fully penetrating hydraulically connected stream or lake; the aquifer is extended to infinity in the positive x-direction. Initially, t = 0, the head in the aquifer is at equilibrium and assumed to be everywhere equal to h_0. At time, t = 0, the lake level is raised to a new elevation equal to H_0. The head along the aquifer in x-direction is to be predicted at different times. The analytical solution of this problem is given by Carslaw and Jaeger [23] as:

$$\frac{h}{H_0} = \mathrm{erfc}\left(\frac{x}{2}\sqrt{\frac{S}{Tt}}\right) \qquad (5)$$

Analytical and numerical results are shown in

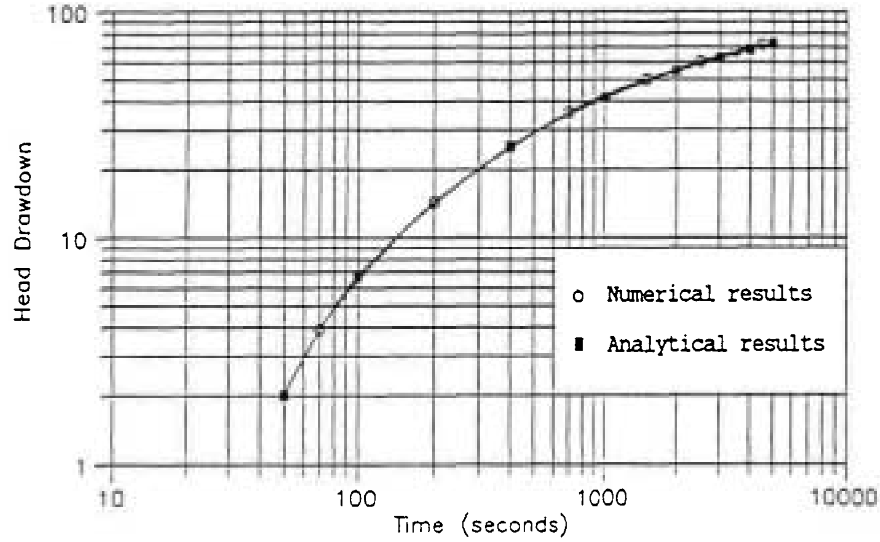


Figure 3. Numerical and analytical results of the aquifer.

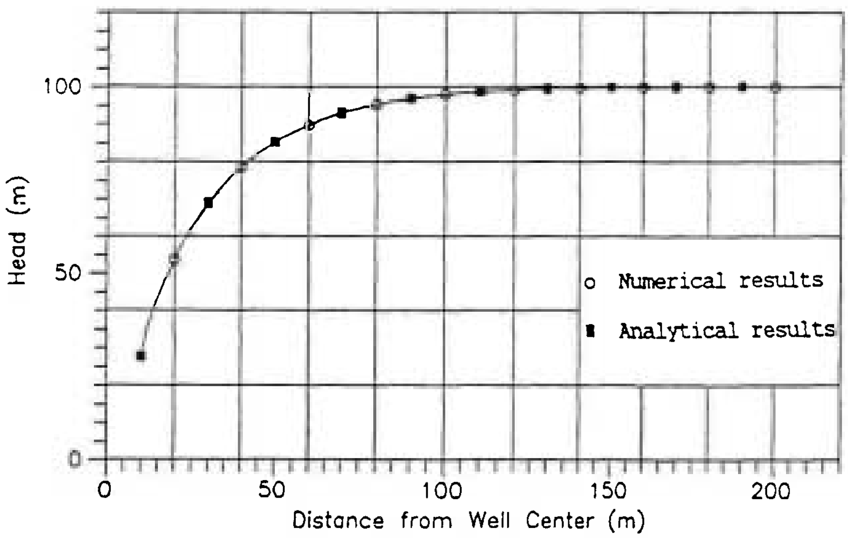


Figure 4. Head versus distance from the center of the well after 5000 seconds.

Figures 6 and 7. It is apparent that the accuracy of the model is quite satisfactory.

CALIBRATION OF THE MODEL

If measurements of aquifer permeability and storage coefficients are available at every nodal point in an aquifer, prediction of the water table variation would be a straightforward procedure. In practice, the data base on which models must be designed is often very sparse. Besides, the variation of effective stresses and pore pressures in aquifers due to the drawdown of heads causes soil parameters to be varied. Therefore, it is almost always necessary to calibrate the model

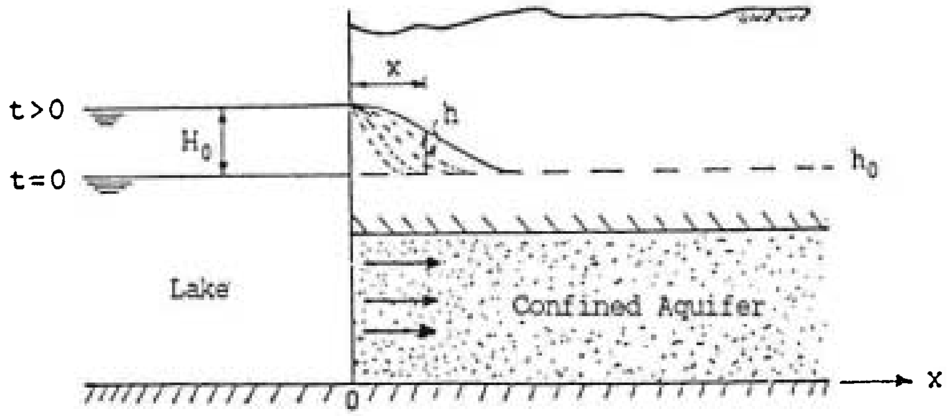


Figure 5. Semi infinite confined aquifer beside a lake.

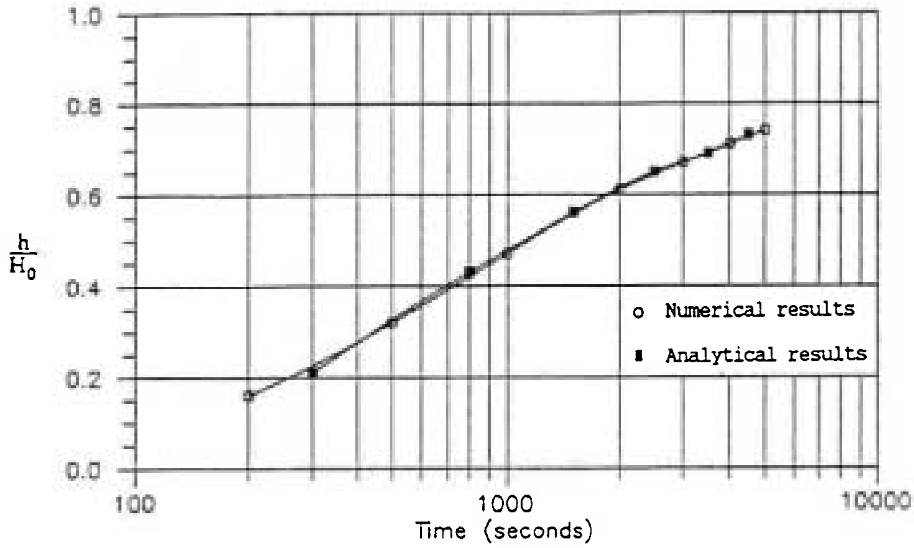


Figure 6. Relative head versus time at x= 10m.

against historical records of pumping rates and drawdown pattern. However, the parameters may reach a relative equilibrium after a period of time in which they might be considered as constants.

Parameters which should be determined through the calibration of the model are permeabilities, or transmissivities and storage coefficients at nodal points of the aquifer grid. The calibration in this study can be performed as follows:

Heads at different points in the aquifer should be measured after a reasonable period of time in which parameters had been reached to a relative equilibrium.

Using initially guessed parameters, the model should be run to obtain computed heads. Of course, the measured and computed heads will be different due to the error of parameter estimation. Considering the function:

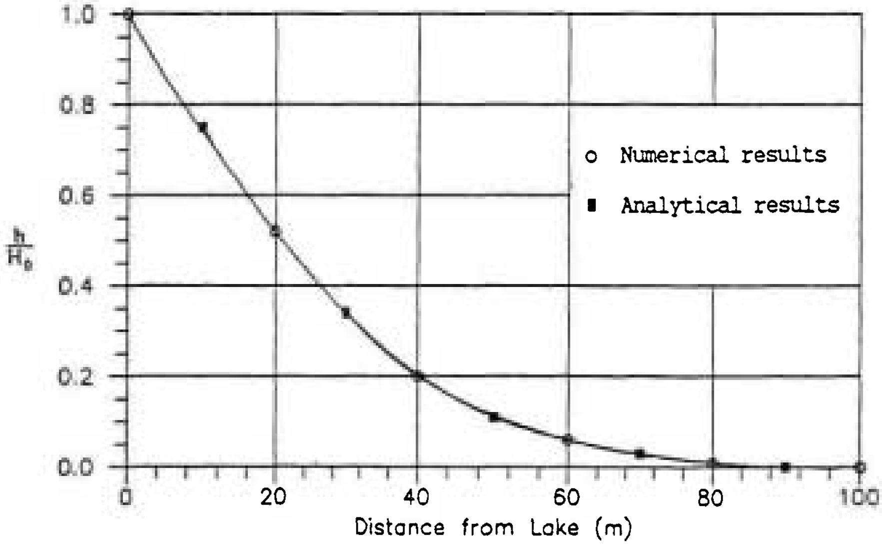


Figure 7. Relative head versus x after 5000 seconds.

$$F = \sum_{j=1}^{n_1} \sum_{i=1}^{m_1} \left(h_{i,j\,meas.} - h_{i,j\,comp.} \right)^2 \tag{6}$$

in which

m_1 = number of nodes in x-direction

n_1= number of nodes in y-direction

$h_{i,j\,meas.}$ = Measured head at node i, j

$h_{i,j\,comp.}$ = Computed head at node i, j

It is not necessary to employ all nodal heads for computing F. The best choice of parameters is the one which minimizes the function F. Minimization of F can be achieved by using optimization techniques. The method used in this study is powell's method with transformation [24]. In this technique transformations are considered in which problems of constrained optimization can be reduced to a form with no constraints explicitly appearing so that they are then suitable for solution by powell's conjugate directions of non-linear optimization method [25]. Powell's method efficiently solves non constrained optimization problems. The numerical model and the optimization method are combined as shown in the flow-chart of Figure 8.

In the problems dealt with in this study, derivatives

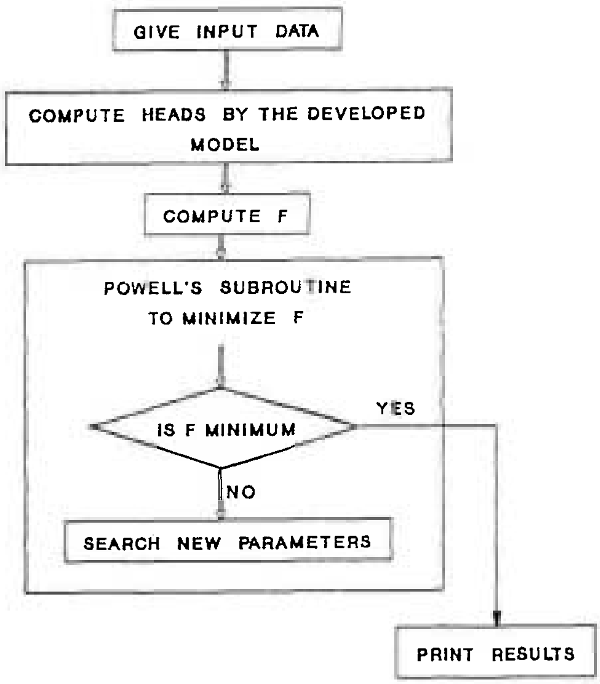


Figure 8. Calibration program flow-chart.

of the objective function F with respect to the parameters are not determinable in a simple way. This makes Powell's method more useful because it does not require calculation of the derivatives. Besides, the method is quite fast, especially when the initial guess of parameters is reasonable.

To demonstrate the accuracy of the numerical model combined with calibration, a problem with known parameters which has an exact analytical solution is selected.

Heads calculated from the analytical solution with known parameters are considered to be the measured heads, h_{meas}. Then, the same problem can be solved by the developed numerical model to compute heads, h_{comp}. The calibration program will determine the parameters so that the function, F, is minimized.

The following example is considered to demonstrate the capability and accuracy of the calibration program.

Example 3

Considering a homogeneous and isotropic aquifer with a well in the center of that as shown in Figure 9.

$$S = 0.003, \qquad T = 0.001\ \frac{m^2}{s}, \qquad Q_p = 0.25\ \frac{m^3}{s}$$

Parameters computed by the calibration program where:

$$T = 0.001\ \frac{m^2}{s} \qquad \text{and} \qquad S = 0.0029$$

The above parameters minimize the function F and, therefore, they give the best fit to the analytical solution points when using the numerical model.

Referring to Figure 10, it is obvious that the parameters are very close to the real ones which assures accuracy of the calibration model.

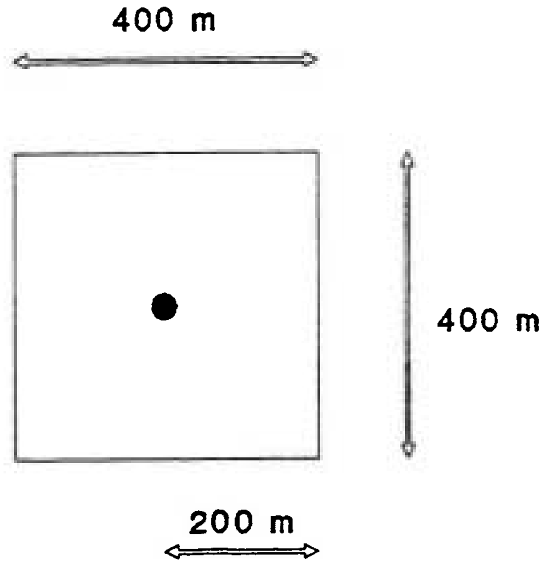


Figure 9. Aquifer of example 3.

ANALYSIS OF A REAL PROBLEM

To demonstrate the capability of the developed model with calibration in real cases, Rokh plain located at Khorasan province in Iran is considered. This plain is one of the most important groundwater resourses in the region. Figure 11 shows Rokh plain with locations of wells. The aquifer is unconfined, non-homogeneous and anisotropic with dimensions of about 12 km × 26 km.

Initial conditions for the heads are introduced in Figure 12. Heads in the whole plain and discharges at boundaries after one year are given for the purpose of calibration. Since, the number of parameters is large, it is reasonable to divide the whole region to a number of zones as shown in Figure 13. This reduces the number of parameters considerably.

Zoning of the aquifer can be done on the basis of field tests and measurements in which zones with almost similar parameters might be obtained.

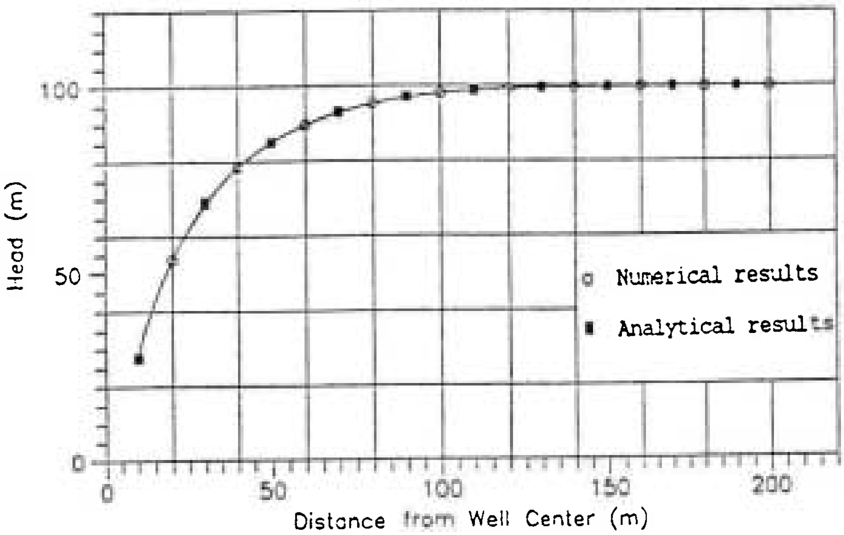


Figure 10. Head versus distance from well center after 5000 seconds related to example 3.

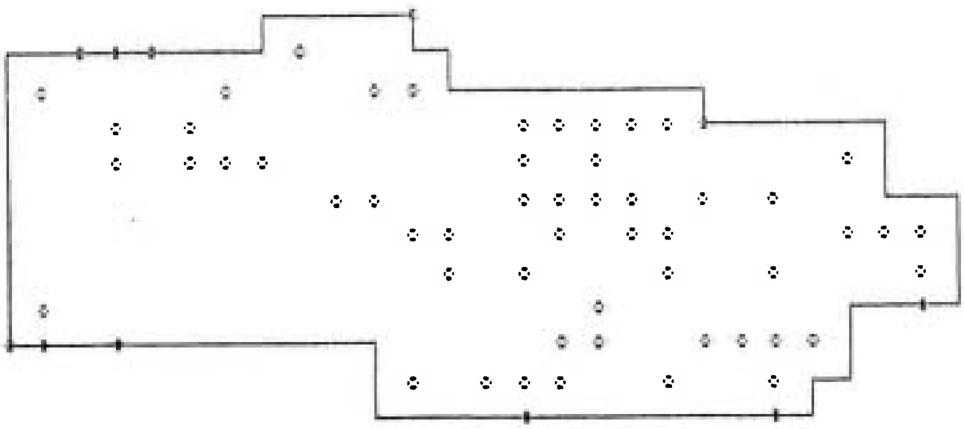


Figure 11. Rokh plain with locations of wells.

Computed and measured head contour lines of Rokh plain after one year are introduced in Figures 14 and 15 respectively. It is apparent that computed and observed results show very good accords.

Parameters estimated by the calibration process which are introduced in Figure 16 can be used to predict the situation of the water table and water balance in the future.

SUMMERY AND CONCLUSION

A mathematical model was developed in which the fully implicit finite difference method with control volume approach is introduced to solve the non-linear transient flow equation in non-homogeneous and anisotropic aquifers. In this approach a grid with variable increments can be used. This enables us to

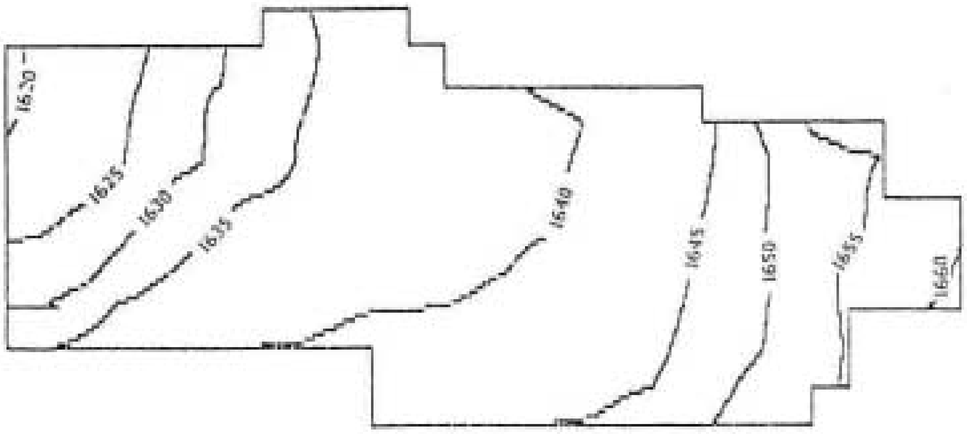
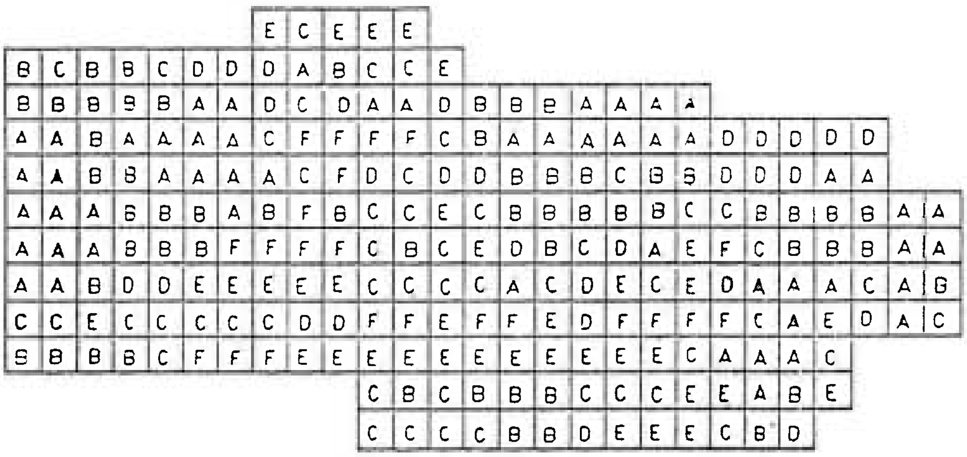


Figure 12. Head contour-lines at the begining of the study



K → A = 20.0 B = 14.4 C = 8.6 D = 4.0 E = 3.0 F = 1.9 (m/day)

S → A = 39.5 B = 23.0 C = 12.4 D = 7.9 E = 2.2 F = 1.8 %

Figure 13. Zoning of Rokh plain aquifer.

employ small increments in sensitive regions to increase accuracy. The non-linear discretized equations were sloved by the line by line sweeping method in four directions which is a combination of the tridiagonal matrix algorithm with Gauss-Seidel line by line iterative algorithm. In general, the convergence of the model was found to be fast. If small time step is chosen, the number of itrations can be reduced to one.

Calibration of the model to estimate the aquifer parameters is achieved by using powell's non-linear optimization method with a transformation techinque

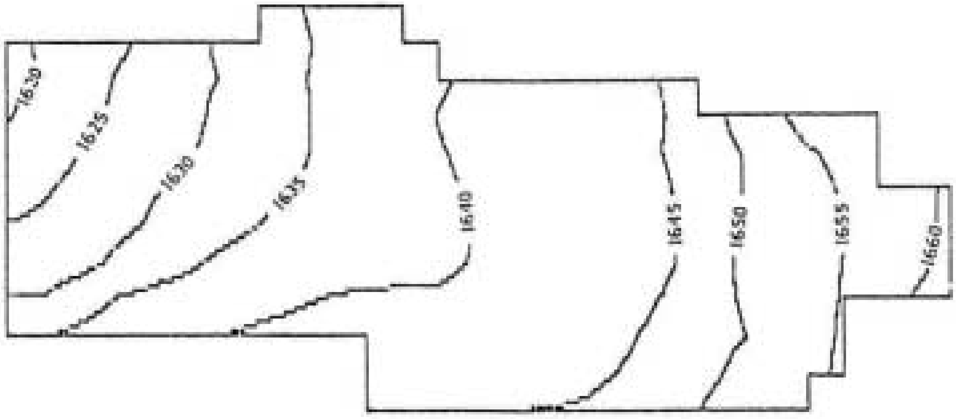


Figure 14. Computed contour-lines in Rokh plain after one year.

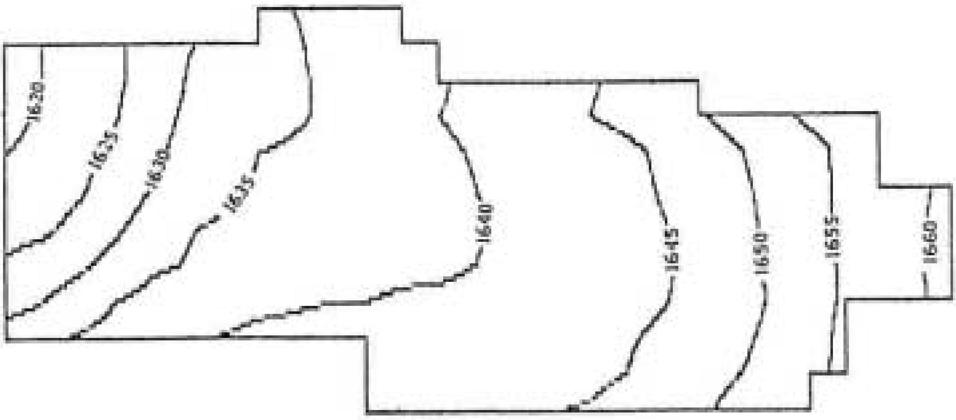


Figure 15. Measured contour-lines in Rokh plain after one year.

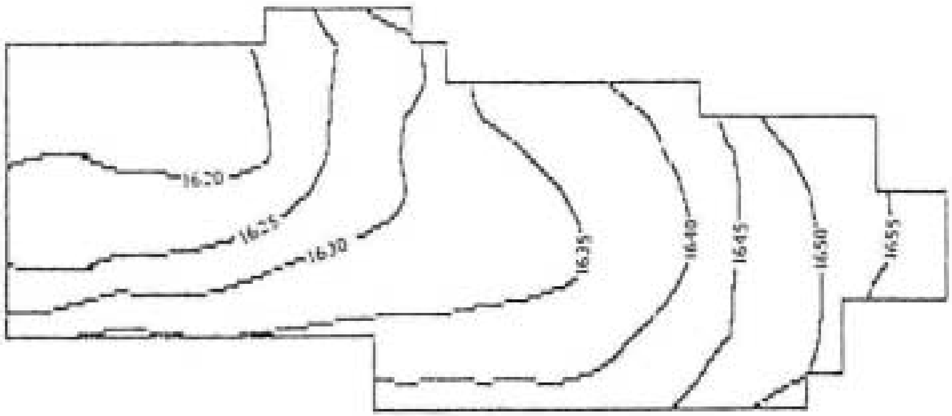


Figure 16. Computed contour-lines in Rokh plain after 10 years.

to change the constrained optimization problem to unconstrained one. This technique does not require objective function derivatives calculations. The method has been satisfactory from convergence and accuracy point of views.

Number of parameters can be reduced considerably by dividing the region into zones in which the parameters for every single zone are similar. The model was applied to analyse a real problem. Results of the analysis were quite satisfactory.

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