Aquifer Simulation Model for Use on Disk Supported Small Computer Systems

by T. A. PRICKETT and C. G. LONNQUIST
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by T. A. Prickett and C. G. Lonnquist

ABSTRACT

A generalized digital computer program listing is given that can simulate two-dimensional flow of groundwater in heterogeneous aquifers under nonleaky and/or leaky artesian conditions. A special feature of the program is that a large simulation (up to an estimated 10,000 node problem) can be accomplished on a disk supported small computer with only 4000 words (32 bits per word) of core storage.

The computer program can handle time varying pumpage from wells, natural or artificial recharge rates, the relationships of water exchange between surface waters and the groundwater reservoir, the process of groundwater evapotranspiration, and the mechanism of flow from springs.

A finite difference approach is used to formulate the equations of groundwater flow. A modified alternating direction implicit method is used to solve the set of resulting difference equations.

The discussion of the digital technique includes the necessary mathematical background, the documented program listing, sample computer input data, and explanations of job setup procedures. The program is written in FORTRAN and will operate with any consistent set of units.

INTRODUCTION

The use of digital computers in groundwater resource evaluation has been firmly established for several years. Computers are available that allow solution of large sets of simultaneous equations that are involved in studying cause and effect relationships in heterogeneous aquifer systems with a wide variety of source
and sink functions and boundary conditions. In addition, listings of computer programs are readily available for solution of groundwater problems (see for example Tyson and Weber, 1964; Prickett and Lonnquist, 1968a, 1968b, and 1971; and Pinder, 1970). However, these programs require a relatively large computer in terms of core storage (in excess of 64,000 words for a typical regional problem).

When a groundwater hydrologist needs a computer analysis, his first problem is to make arrangements for the use of computer facilities. In general, large computers are available through arrangements made with universities and commercial data processing firms. On the other hand, there are substantial numbers of small computers (less than 32,000 words of core storage) to be found in local private firms, universities, and state agencies. Quite often, the small computer facilities are cheap to rent and have time available, and thus present another possibility for getting the job processed.

The purpose of this report is to present a computer program for solving a large groundwater problem on a small computer and thus eliminate the absolute need of a large computer. This is accomplished by writing a program (which requires only a small amount of core storage) to be used on a disk supported small computer. The disk unit serves as the main storage device as opposed to core storage on large computers.

A generalized computer program is presented that will simulate two-dimensional nonsteady-state flow problems in heterogeneous aquifers under nonleaky and/or leaky artesian conditions. This program includes time varying pumpage from wells, natural or artificial recharge rates, the relationships of water exchange between surface waters and the groundwater reservoir, the process of groundwater evapotranspiration, and the mechanism of flow from springs. The program is written to operate with any consistent set of units.

A finite difference approach that is identical to that taken by Prickett and Lonnquist (1971) has been adopted in formulating the equations of groundwater flow. A brief mathematical background is given that describes the modified iterative alternating direction implicit method of solving the equations. This is followed by the documented program listing, sample computer input data, and an explanation of the job setup procedures.
Parts of this report are abstracted from Bulletin 55, written by Prickett and Lonnquist (1971), since the mathematics and job setup are basically the same. For a full understanding of the validity of the method described here, the reader should refer to the more detailed explanation in Bulletin 55.

The computer program in this report is written in FORTRAN for use on an IBM 1130 disk supported computer with only 4000 words (32 bits per word) of core storage. However, the program will operate, with modifications, on other computers such as a CDC model SC 1700, Datacraft model 602V5, Digital Equipment Corporation model PDP-11/10, Microdata Corporation model 810, and Varian Data Machines model 620/L-100.

The program operates most efficiently on computers which have between 4000 and 32,000 words of core storage. Beyond this range other programs should be considered to take advantage of additional core storage.

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BRIEF MATHEMATICAL BACKGROUND

The partial differential equation (Jacob, 1950) governing the nonsteady-state, two-dimensional flow of groundwater may be expressed as

\[
\frac{\partial}{\partial x}(\nabla^2 h) + \frac{\partial}{\partial y}(\nabla^2 h) = S \frac{\partial h}{\partial t} + Q
\]

(1)
where

\[ T_x = \text{aquifer transmissivity in the x direction} \]
\[ T_y = \text{aquifer transmissivity in the y direction} \]
\[ S = \text{aquifer storage coefficient} \]
\[ h = \text{head} \]
\[ t = \text{time} \]
\[ Q = \text{source or sink functions expressed as net flow rates per unit area} \]

A numerical solution of equation 1 can be obtained through a finite difference approach. The finite difference approach first involves replacing the continuous aquifer system parameters with an equivalent set of discrete elements. Secondly, the equations governing the flow of groundwater in the discretized model are written in finite difference form. Finally, the resulting set of finite difference equations is solved numerically with the aid of a digital computer.

A finite difference grid is superposed over a map of an aquifer as illustrated in figure 1. The aquifer is thus subdivided into volumes having dimensions \( m \Delta x \Delta y \), where \( m \) is the thickness of the aquifer. The differentials \( \Delta x \) and \( \Delta y \) are approximated by the finite lengths \( \Delta x \) and \( \Delta y \), respectively. The area \( \Delta x \Delta y \) should be small compared with the total area of the aquifer to the extent that the discrete model is a reasonable representation of the continuous system. The intersections of grid lines are called nodes and are referenced with a column \( (i) \) and row \( (j) \) coordinate system colinear with the x and y directions, respectively.

Figure 1. Finite difference grid

The general form of the finite difference equation governing the flow of groundwater in the discretized model is then given by
Since there is an equation of the same form as equation 2 for every node of the digital model, a large set of simultaneous equations must be solved for the principal unknowns $h_{i,j}$. A modified form of the iterative alternating direction implicit method given by Prickett and Lonnquist (1971) is used to solve the set of simultaneous equations.

\[
T_{i,j}^1 (h_{i-1,j} - h_{i,j})/\Delta x + T_{i,j}^2 (h_{i,j+1} - h_{i,j})/\Delta x^2 + T_{i,j}^1 (h_{i,j+1} - h_{i,j})/\Delta y + T_{i,j}^2 (h_{i,j-1} - h_{i,j})/\Delta y^2
= S_{i,j} (h_{i,j} - h_{i,j})/\Delta t + Q_{i,j}/\Delta x\Delta y
\]  

(2)

where

- $T_{i,j}^1$ = aquifer transmissivity between nodes $i,j$ and $i,j+1$
- $T_{i,j}^2$ = aquifer transmissivity between nodes $i,j$ and $i+1,j$
- $h_{i,j}$ = calculated heads at nodes $i,j$ at the end of a time increment measured from an arbitrary reference level
- $h_{i,j}^{\phi}$ = calculated heads at nodes $i,j$ at the end of the previous time increment measured from the same reference level defining $h_{i,j}$
- $\Delta t$ = time increment elapsed since last calculation of heads
- $S_{i,j}$ = aquifer storage coefficient at node $i,j$
- $Q_{i,j}$ = net withdrawal rate if positive, or net accretion rate if negative at node $i,j$

Since there is an equation of the same form as equation 2 for every node of the digital model, a large set of simultaneous equations must be solved for the principal unknowns $h_{i,j}$. A modified form of the iterative alternating direction implicit method given by Prickett and Lonnquist (1971) is used to solve the set of simultaneous equations.

**Modified Iterative Alternating Direction Implicit Method (MIADI)**

Briefly, the MIADI method involves first, for a given time increment, reducing the large set of simultaneous equations down to a number of small sets. This is done by solving the node equations, by Gauss elimination, of an individual row of the model while all terms related to the nodes in the two adjacent rows are held constant. After all row equations have been processed row by row, attention is focused on solving the node equations, again by Gauss elimination, of an individual column while all terms related to the two adjacent columns are held constant. Finally, after all equations have been solved column by column, an 'iteration' has been completed. The above process is repeated a sufficient number of times to
achieve convergence, and this completes the calculations for the given time increment. The calculated heads are then used as initial conditions for the next time increment. This total process is repeated for successive time increments until the desired simulation is completed.

Equation 2 may be rewritten to illustrate the general form for calculations by rows. As a first simplification it is assumed that the finite difference grid is made up of squares such that $\Delta y = \Delta x$. (The case where $\Delta y$ does not equal $\Delta x$ can be treated by methods outlined by Prickett and Lonnquist, 1971.) Equation 2 is then expanded, the signs reversed, and terms of $h_{i,j}$ grouped together to yield

$$-T_{i-1,j} h_{i-1,j} + h_{i,j} (T_{i-1,j} + T_{i,j} + T_{i,j-1} + T_{i,j+1}$$

$$+ S_{i,j} \Delta x^2 / \Delta t) - T_{i,j} h_{i,j+1} = (S_{i,j} \Delta x^2 / \Delta t) h_{i,j}$$

$$+ T_{i,j-1} h_{i,j-1} + T_{i,j+1} h_{i,j+1} - Q_{i,j}$$

Equation 3 is of the form

$$A Ah_{i-1,j} + B Bh_{i,j} + CCh_{i+1,j} = DD$$

where

$$AA = -T_{i-1,j}$$

$$BB = T_{i-1,j} + T_{i,j} + T_{i,j-1} + T_{i,j+1} + S_{i,j} \Delta x^2 / \Delta t$$

$$CC = -T_{i,j}$$

$$DD = (S_{i,j} \Delta x^2 / \Delta t) h_{i,j} + T_{i,j-1} h_{i,j-1} + T_{i,j+1} h_{i,j+1} - Q_{i,j}$$

A similar set of equations can be written for calculations by columns.

The key to the manner in which the small storage computer is used lies in the fact that data from only three rows or columns are needed in core at any one time to solve the above mentioned equations. The logic of the following computer program is such that data for all equations of the model are stored on a disk. Then special instructions are used to transfer appropriate data between the disk and core storage for individual row or column calculations as the simulation proceeds. An explanation of the mechanics of the transfers between disk and core storage is included in a later section.
Figure 2. Aquifer simulation model for disk supported computer
Figure 2. (Concluded)
The aquifer simulation program listing given in figure 2 was coded in FORTRAN to solve the sets of row node equations 3"3d.

Figure 3 illustrates the parameters included in the simulation program. Briefly, the program is intended for use when analyzing cause and effect relationships involving drawdowns or heads in a nonsteady, heterogeneous and/or homogeneous aquifer system under nonleaky and leaky artesian conditions. Programming techniques involving time varying pumpage from wells, natural or artificial recharge rates, the relationships of water exchange between surface waters and the groundwater reservoir, the process of groundwater evapotranspiration, and the mechanism of flow from springs.

Figure 3. Generalized aquifer cross section showing simulation program parameters
are also included. Under these conditions it is possible to include special boundaries such as irregular barrier or recharge boundaries (constant head) and constant withdrawal or recharge rates.

The program listing of figure 2 is written in such a way that it will operate with any consistent set of units. However, the comment cards preceding the actual program list the variables in the gallon-day-foot system of units. This system of units is made consistent (exterior to the program) by working with a so-called storage factor defined as

\[ SF_{i,j} = 7.48S_{i,j} \Delta x \Delta y \]

where

\[ SF_{i,j} = \text{storage factor for node located at model coordinates } i, j, \text{ in gallons per foot (gal/ft)} \]

\[ S = \text{the aquifer storage coefficient for artesian conditions, a fraction} \]

\[ 7.48 = \text{number of gallons in a cubic foot of water, in gallons per cubic foot (gal/ft}^3) \]

\[ \Delta x, \Delta y = \text{finite difference grid intervals, in feet} \]

The storage factor of equation 4 is substituted for the terms \( S_{i,j} \Delta x^2 \) in equations 3, 3b, and 3d, which transforms these equations so that all combinations of terms have consistent units of gallons per day (gpd). To work with a consistent set of units such as in the metric system the user merely drops the constant 7.48 from equation 4.

### Job Setup

The computer job setup will first be explained in general and then in more detail as necessary.

The aquifer system properties are discretized by superposing a finite difference grid over maps of the aquifer system as shown in figure 4. The total dimensions of the grid are defined by NC, the number of columns of the model, and by NR, the number of rows of the model. Next, a parameter card and default value card are prepared according to the formats illustrated in figures 5a and b. The default value card provides data for simulating an NC by NR aquifer system model having homogeneous properties with identical initial heads and net withdrawal rates.
Figure 4. Plan view of finite difference grid over map of aquifer system

Figure 5. Input data formats for computer program
A node card deck is then prepared according to the format illustrated in figure 5c. The node card deck contains one card for each node that has any aquifer system properties differing from those defined on the default value card. Finally, pumping schedule cards are prepared according to the card format illustrated in figure 5d.

The program deck, parameter card, default value card, node card deck, and pumping schedule deck are assembled in the order illustrated in figure 6. Appropriate computer installation job control cards are included and the program is ready to run. The computer output will be in the form of printed numerical values of heads for all nodes at the end of every time increment according to FORMAT statement 355 of the program shown in figure 2.

Preparation of Data Cards

Parameter Card. Enter numerical values for NSTEP, DELTA, and ERROR according to the format given in figure 5a. A general rule for choosing an initial DELTA is to decide at what minimum TIME drawdowns or heads of interest occur and then precede this time by at least six time increments. Choose an initial value of ERROR from the following formula

\[
\text{ERROR} = \frac{Q \times \text{DELTA}}{10 \times \text{SF1}}
\]

where

- \(Q\) = total net withdrawal rate of model, in gpd
- \(\text{DELTA}\) = initial time increment, in days
- \(\text{SF1}\) = average storage factor of model, in gpd/ft

The computer program is then 'tested' by making a few preliminary runs with different values of ERROR, with a final value being chosen at the point where reduction in that term does not significantly change the solution.
Default Value Card. After entering values of NC and NR on the card, enter the most commonly occurring values of the aquifer system parameters.

Node Card Deck. It should be emphasized that the node deck contains one card for each node that has any aquifer system properties differing from those defined on the default value card. If a node card is included, all values must be punched on it even if some of the values are equal to the default values.

Leaky Artesian Conditions. Calculate recharge factors $R_{i,j}$ in gallons per day per foot (gpd/ft) from the following formula

\[
R_{i,j} = \left(\frac{P'}{m'}\right)Ax\Delta y
\]

where

- $P'$ = vertical hydraulic conductivity of confining bed, in gallons per day per square foot (gpd/ft²)
- $m'$ = thickness of confining bed, in feet

The recharge factor defines the slope of the line given in figure 3b.

Appropriate source bed heads RH, elevations of the top of the aquifer RD, and recharge factors are entered on the default value card and any differing values on the node cards.

Induced Infiltration. Calculate recharge factors (in gpd/ft) from the following formula

\[
R_{i,j} = \left(\frac{P'}{m'}\right)A_s
\]

where

- $P'$ = hydraulic conductivity of the streambed, in gpd/ft²
- $m'$ = thickness of streambed, in feet
- $A_s$ = area of the streambed assigned to node, in square feet

The recharge factor defines the slope of the line shown in figure 3c. Appropriate values of stream water surface elevations RH, elevations of the bottom of the streambed RD, and recharge factors calculated from equation 7 are entered on node cards.

Evapotranspiration. Find the slope of the line shown in figure 3d by calculations with field data. The value of the slope of that line is then entered on node cards in the space reserved for the recharge factor. Set values of both RD and RH equal to one another. RD is defined as the elevation of the water table below which the effects of evapotranspiration cease.
Flow from Springs. Determine a recharge factor (slope of the line shown in figure 3e) from field data of flow versus head changes in the vicinity of the spring. A recharge factor may also be found empirically by matching simulated with observed spring flows. The elevation at which water flows from the spring is recorded in both RH and RD.

Variable Pumping Rates. Set up a stepwise pumping schedule, as exemplified in figure 7, for each well of the model. The computer program can manipulate positive (pumping), negative (recharge), or zero withdrawal rates. Between changes in pumping rates, the computer program operates with nonuniform time steps within each period of pumping. However, DELTA is reset to its initial value at each change in pumping rate.

Once the pumping schedules have been set up, enter the rates and well location coordinates on node cards and on pumping schedule cards according to the formats of figure 5c and d. The first pumping rate of the schedule is entered into Q by including a node card. Subsequent pumping rates are entered on pumping schedule cards, their rates becoming effective after the time step number, ISTEP, equals the value entered as ISP. With the schedule of figure 7, for example, the pumping rate P₁ would be included on a node card and two pumping schedule cards would be prepared with ISP equaling 9 for rate P₂ and ISP equaling 15 for rate P₃. The pumping schedule deck must be in order of increasing ISP and row number, and preceded and followed by a blank card.
The basic operation of the computer program is explained in the following discussion according to the listing of figure 2 and the flow chart given in figure 8.

The computer program consists of a MAIN section and the three subroutines, PARM, NODE, and OUT. The storage requirements, including arrays, are only 2520 words for MAIN, 313 words for PARM, 202 words for NODE, and 392 words for OUT. For clarity the total program will be explained in the order of the subroutines first and the main section last.

Figure 8. Flow chart for computer program
Subroutine PARM

The first statement of this subroutine defines the structure of the disk storage. Storage space is allocated for a 50 by 50 model or 2500 nodes. Each node has 10 variables for storage, denoted as a 'record.' Since each variable requires 2 words when using an IBM 1130 computer, 20 words per record must be specified on the disk to store the 10 variables per node. The U indicates that the disk input/output functions are unformatted. The term ID1 is used as the 'pointer' for reading and writing on the disk.

Figure 9 illustrates how the disk storage configuration is set up from data specified on the parameter and default value cards. A simple 4 by 5 finite difference grid is used as an example. One should note that a 'frame' of extra rows and columns has been set up around the simulated model. In storing the default values on the disk pack, the transmissivities within the frame are set equal to zero. This has been done so that boundary transmissivities are automatically set to zero at the beginning or end of a row or column.

Subroutine NODE

This subroutine reads the node cards and places the data in the appropriate locations on the disk. In addition, if any of the node cards contain data which are in contact with the frame, then the aquifer transmissivities are reset to zero in the frame.

Subroutine OUT

This subroutine prints the simulation results, predicts future heads, and reads new net withdrawal rate values in preparation for the next time step. To save core storage, the pumping schedule cards are read only as they are needed. The computer operator should be made aware of this feature since he might, out of curiosity, remove the cards during the simulation and cause the computation to stop.

MAIN Program

The dimension statement reserves core storage sufficient for three rows or three columns of data from models that contain not more than 50 rows and 50 columns.
The G and B arrays (Prickett and Lonnquist, 1971) are used in both the row and column calculations and must be dimensioned to the maximum row or column limits.

Figure 10 illustrates the computer core storage configuration with the first three rows of data in core for the example model of figure 9. The largest portions of the MAIN program are devoted first to statements transferring the proper rows or
columns of data back and forth between the disk and core. Secondly, a series of statements are included to determine the core storage location of the row or column along which heads are to be calculated. This second series of statements has to do with what is termed 'revolving subscript specification' to be explained as follows.

The third subscript in the DIMENSION statement S array reserves three block locations of row or column data with numbered subscripts 1, 2, and 3. At the beginning of the simulation the first three rows of data are transferred from the disk into these 3 block locations. The data from row one goes in location 1, that from the second row in 2, and that from the third row in 3. As calculations of heads progress row by row, data are transferred between the disk and available core storage. The new row data are transferred into the block location vacated by unnecessary row data. The sequence of the row data in the three S array block locations is as follows. The data for a row along which heads are to be calculated follows a core storage sequence (J2) of 2, 3, 1, 2, 3, 1, etc. The adjacent row data needed for calculation of heads follow a sequence which is one step behind or ahead of the above sequence; namely, for one adjacent row the sequence (J1) is 1, 2, 3, 1, 2, 3, etc., and for the other adjacent row the sequence (J3) becomes 3, 1, 2, 3, 1, 2, etc. Therefore, the formulation of the MIADI program section can be completely generalized by revolving the S array subscripts J1, J2, and J3 from 1 through 3 as described above. A similar description can be given for calculations along columns.

EXAMPLE PROGRAM CHECKOUT PROBLEM

A small test problem is included to check out the program of this report for use on various small core storage disk supported computers.

As illustrated in figure 11, two wells are pumping in a finite aquifer near a river. Initial heads in the aquifer and river are set equal to zero, the chosen arbitrary head reference level. It is assumed that the two wells are to be pumped at the rates shown in the schedules of figure 12. The river shown in figure 11 is 50 feet wide, has a streambed thickness of 0.3 feet, hydraulic conductivity of 1.2 gpd/ft², and a streambed bottom elevation of 0.8 feet below the reference level.
A square ($\Delta y = \Delta x$) finite difference grid interval of 1000 feet is assumed, and the computer model then is 5 columns by 7 rows in size. Data from figure 11 indicate that the coordinates of well 1 are $i = 3$, $j = 3$, and the coordinates of well 2 are $i = 4$, $j = 5$.

The recharge factors for the streambed of the river are, by equation 7

$$ R_{i,j} = \left( \frac{P'\cdot m'}{m'} \right) A_s = \left( \frac{1.2}{0.3} \right) 1000 \times 50 $$
$$ R_{i,j} = 200,000 \text{ gpd/ft} $$

where $A_s$ is the area of the streambed simulated at each node discretized into 50-foot widths by 1000-foot lengths along row 6 of the model.

The storage factor for the entire model is by equation 4

$$ S_{i,j} = 7.48 S_{i,j} \Delta x \Delta y $$
$$ S_{i,j} = 7.48 \times 1.003 \times 10^{-3} \times 1000 \times 1000 $$
$$ S_{i,j} = 7500 \text{ gal/ft} $$

The data deck setup for the above hypothetical test model is given in figure 13. A sample time-drawdown curve for an observation point located at model grid point $i = 3$, $j = 7$ is given in figure 14. A sample printout of all model heads for $\text{TIME} = 2.20 \text{ days}$ is given in figure 15.

**COMPUTATION TIME COMPARISONS**

The example program checkout problem of this report, and other equivalent ones, have been run on IBM 1130 disk supported computers with core storage of 8000 and 16,000 words. In addition, the same problems have been run, all in core storage, with the programs given by Prickett and Lonnquist (1971) on IBM 360 models 75 and 40 computers. Comparisons for needed central processor times are as follows.

<table>
<thead>
<tr>
<th>Computer</th>
<th>Time (seconds)</th>
</tr>
</thead>
<tbody>
<tr>
<td>360/75 (in core)</td>
<td>6</td>
</tr>
<tr>
<td>360/40 (in core)</td>
<td>25</td>
</tr>
<tr>
<td>1130 (16,000 words)</td>
<td>150</td>
</tr>
<tr>
<td>1130 (8000 words)</td>
<td>460</td>
</tr>
</tbody>
</table>
Figure 11. Example aquifer problem

Figure 12. Example pumping schedules for program checkout problem

Figure 13. Data deck setup for example problem

Figure 14. Time drawdown curve for example problem

Figure 15. Numerical printout for example problem
It should be pointed out that the above times do not allow for reading cards or printing the results. Also from a user's standpoint, a factor which does not show up in the above table is actual turnaround time, which is the time between handing the cards to the operator and receiving the printed output. Turnaround time can vary considerably from one computer installation to another. For instance, turnaround time for the 360/75, operated through a remote job entry terminal, at best was about 10 minutes. This time can be compared with about 5 minutes turn-around for the 1130 with 16,000 words of storage. The main cause of the difference here is that the 360/75 computer is processing several jobs simultaneously whereas the 1130 is working on only one job.

It is obvious that the small computer consumes large amounts of central processor time, but it does allow problem solving with small core storage.

REFERENCES


