

**DOCUMENTATION OF A NUMERICAL CODE FOR
THE SIMULATION OF VARIABLE DENSITY
GROUND-WATER FLOW IN THREE DIMENSIONS**

By Logan K. Kuiper

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CONVERSION FACTORS

For use of readers who prefer to use metric units, conversion factors for terms used in this report are listed below:

<u>Multiply</u>	<u>By</u>	<u>To obtain</u>
cubic foot (ft^3)	0.02832	cubic meter (m^3)
foot per day (ft/d)	0.3048	meter per day (m/d)
pound, avoirdupois	453.6	gram (g)

**DOCUMENTATION OF A NUMERICAL CODE
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ABSTRACT

This report documents a numerical code for the simulation of variable density time dependant ground-water flow in three dimensions. The ground-water density, although variable in space, is assumed to be approximately constant in time and known. The Integrated Finite Difference grid elements in the code follow the geologic strata in the modeled area. If appropriate, the determination of hydraulic head in confining beds can be deleted to decrease computation time. The strongly implicit procedure (SIP), successive over-relaxation (SOR), and eight different preconditioned conjugate gradient (PCG) methods are used to solve the approximating equations.

The use of the computer program that performs the calculations in the numerical code is emphasized. Detailed instructions are given for using the computer program, including input data formats. An example simulation and Fortran listing of the program are included.

INTRODUCTION

This report documents a numerical code for the simulation of variable density time dependant ground-water flow in three dimensions. The ground-water density, although variable in space, is assumed to be approximately constant in time and known. The Integrated Finite Difference grid elements in the code are six sided and rectangular when viewed from the vertical direction. The sides of these grid elements are planar, but their top and bottom surfaces follow the curvature of the geologic strata in the modeled area.

The strongly implicit procedure (SIP), successive over-relaxation (SOR), and eight different preconditioned conjugate gradient methods (PCG) (Kuiper, written commun., 1984) are used to solve the approximating equations.

The ground-water flow equation with constant density is used for most ground-water flow studies. In many problems the variation in ground-water density ρ is sufficiently small that it can be neglected. For certain situations, however, it is necessary to treat ρ as a function of water pressure, salt concentration, and temperature.

In some cases, particularly in a confined aquifer, the pressure at a point may change considerably with time, even though the density, temperature, and salt concentration of the water change very little. This is possible, since water density is more weakly dependent upon pressure than it is upon temperature and salt concentration. Density changes that occur due to thermal and salt transport are much slower than those that occur due to pressure changes. Thus if one is interested in the simulation of pressure for a short time period, it is a permissible approximation to regard the density as being time independent and to use the ground-water flow equation by itself without the solute transport or heat conduction equation. In this case, the density $\rho(x,y,z)$ is regarded as being time independent and is determined either by measurement, model calibration, or other procedures, much the same as the hydraulic conductivity. After a certain time period, depending upon the circumstances, pressure changes may pass to a state of quasi-equilibrium. This may occur in a time period which is sufficiently small that density changes, due to thermal and salt transport, are insignificant. A good approximation to this quasi-equilibrium solution is the solution of the steady state ground-water flow equation, again with density $\rho(x,y,z)$ independent of time. Numerical solutions of this type, although valid only for the restricted conditions given above, are far less expensive in terms of computational cost than are those for more general situations which also solve the coupled solute transport and/or heat condition equations. In this report, as with Bennett (1980) and Weiss (1982), ground-water density ρ is assumed to be a known function of spatial position.

THEORETICAL DEVELOPMENT

The basic development of the numerical code documented in this report has been presented by Kuiper (1983), and will not be presented here. Approximating equations (17) and (28) of Kuiper (1983), for steady-state flow, are:

$$F \approx A_x \hat{K}'_{uu} \left[\frac{\Delta h}{\ell} + \frac{B}{\ell \rho_0} \right] + \dots \quad (M/T) \quad (1)$$

$$F_z \approx (\Delta x_i \Delta y_j) \hat{K}'_{ww} \left[\frac{\Delta h}{b'} + \frac{\rho_{i,j,k} b_{i,j,k} + \rho_{i,j,k+1} b_{i,j,k+1}}{2b' \rho_0} \right] \quad (M/T) \quad (2)$$

Equation (1) gives an approximation to the flow into the side of a grid element i,j,k from a horizontally adjacent grid element $i+1,j,k$. The quantity ℓ is the distance in the i direction between the center of grid element i,j,k and grid element $i+1,j,k$, Δh is the difference in the pressure head h between the two grid element centers, A_x is an approximation to the area of the common side shared by the two grid elements, and \hat{K}'_{uu} is the weighted harmonic mean of the hydraulic conductivity for the two grid elements. The quantity B is an approximation to the integral of $\rho \Delta z$ from the center of grid element i,j,k to the center of grid element $i+1,j,k$. The fluid density is ρ and Δz is the increment of vertical distance z , measured positive upwards. In equation (2), F_z is an approximation to the flow downward into the top of grid element i,j,k from grid element $i,j,k+1$. The terms in equation (2) are completely analogous to those in equation (1). The vertical distance between the two grid element centers is b' , and $b_{i,j,k}$ and $b_{i,j,k+1}$ are the vertical thicknesses of grid elements i,j,k and $i,j,k+1$ respectively. Note that the harmonic mean has been taken of the hydraulic conductivity rather than transmissivity.

With the substitutions $h' = h+z$ and $\rho' = \rho - \rho_0$, the terms in the brackets in equations (1) and (2) remain the same except that fresh-water head h' replaces pressure head h , and ρ' replaces ρ . With this alteration, multiplication by -1, and division by $\rho_0 = 1 \text{ gm/cm}^3$, equations (1) and (2) may be written in matrix form as:

$$Mh' = \hat{q} \quad (L^3/T) \quad (3)$$

Matrix M has seven diagonals corresponding to the $i,j,k-1$, $i,j-1,k$, $i-1,j,k$, i,j,k , $i+1,j,k$, $i,j+1,k$, $i,j,k+1$ grid element locations. Component i,j,k of vector \hat{q} includes the sum of all sources of mass (divided by ρ_0) that arise in grid element i,j,k . Such sources of mass include ground-water pumping from wells, as a negative quantity, and also the dissolution of solutes from the porous media. From equation (1), and since $K = K'/\rho_0$, the $i+1,j,k$ location diagonal of matrix M is equal to the quantity $-A_x \hat{K}_{xx}/\ell$, where the notations K_{uu} , K_{vv} , and K_{ww} (Kuiper, 1983) are replaced by K_{xx} , K_{yy} , and K_{zz} in this report. Similar equalities pertain to the $i-1,j,k$, $i,j-1,k$, and $i,j+1,k$ diagonals. The second term in equation (1), with \hat{K}'_{uu} replaced by \hat{K}_{uu} , is part of vector \hat{q} . The $i,j,k+1$ diagonal of matrix M is equal to the quantity $-(\Delta x \Delta y_j) \hat{K}_{zz}/b$ from equation (2). The $i,j,k-1$ diagonal is equal to the $i,j,k-1$ location equivalent of this same quantity. The second term in (2) with \hat{K}'_{ww} replaced by \hat{K}_{ww} is part of vector \hat{q} . The center diagonal of M is equal to the negative of the sum of the six off-center diagonals.

Equation (3) is modified for time dependant flow. Component i,j,k of matrix equation (3) expresses the conservation of mass for grid element i,j,k . Using the backward difference for the time derivative, $[(dV)S_s(\rho/\rho_0)/\Delta t](h')^{n-1}$, for grid element i,j,k , is added to the i,j,k component of mass recharge vector \hat{q} . The dV , S_s , and ρ , are the volume, specific storage, and water density for grid element i,j,k . The Δt is the time interval between times n and $n-1$. The expression $[(dV)S_s(\rho/\rho_0)/\Delta t]$ is added to the center diagonal of matrix M .

For any grid element, the computer model allows for mass discharge which, when the hydraulic head H is greater than some chosen value H_e , increases linearly with h' . When such discharge is taking place, vector \hat{q} and the center diagonal of matrix M receive additional terms, as with the addition of time dependancy.

MODEL APPLICATION

Grid Elements

Figure 1 shows a side view example of the grid element system, and figure 2 shows a top view.

In figures 1 and 2, the modeled region lies within the total volume taken up by grid elements I, J, K for $2 \leq I \leq 10$, $2 \leq J \leq 5$; and $2 \leq K \leq 6$. There are: nine columns numbered $I = 2, 3, \dots, 10$; four rows numbered $J = 2, 3, 4, 5$; and five layers numbered $K = 2, 3, \dots, 6$. In the computer program, grid elements are not identified using I, J, K , but rather by a single subscript:

$$IJ = I + (NI10)(J-2) + (NIJ10)(K-2)$$

where $NIJ10 = (NI10)(NJ10)$. $NI10$, $NJ10$, and $NK10$ are the total number of columns, rows, and layers in the modeled region. In the example in figures 1 and 2, $NI10 = 9$, $NJ10 = 4$, and $NK10 = 5$. IJ has the values $2, 3, \dots, 181$. Confining bed grid elements are identified by

$$IJLB = I + (NI10)(J-2) + (NIJ10)(KLB-2)$$

where KLB denotes confining bed layer. In figure 1, KLB has the values 7 and 8. $IJLB$ has the values 182, 183, ..., 253.

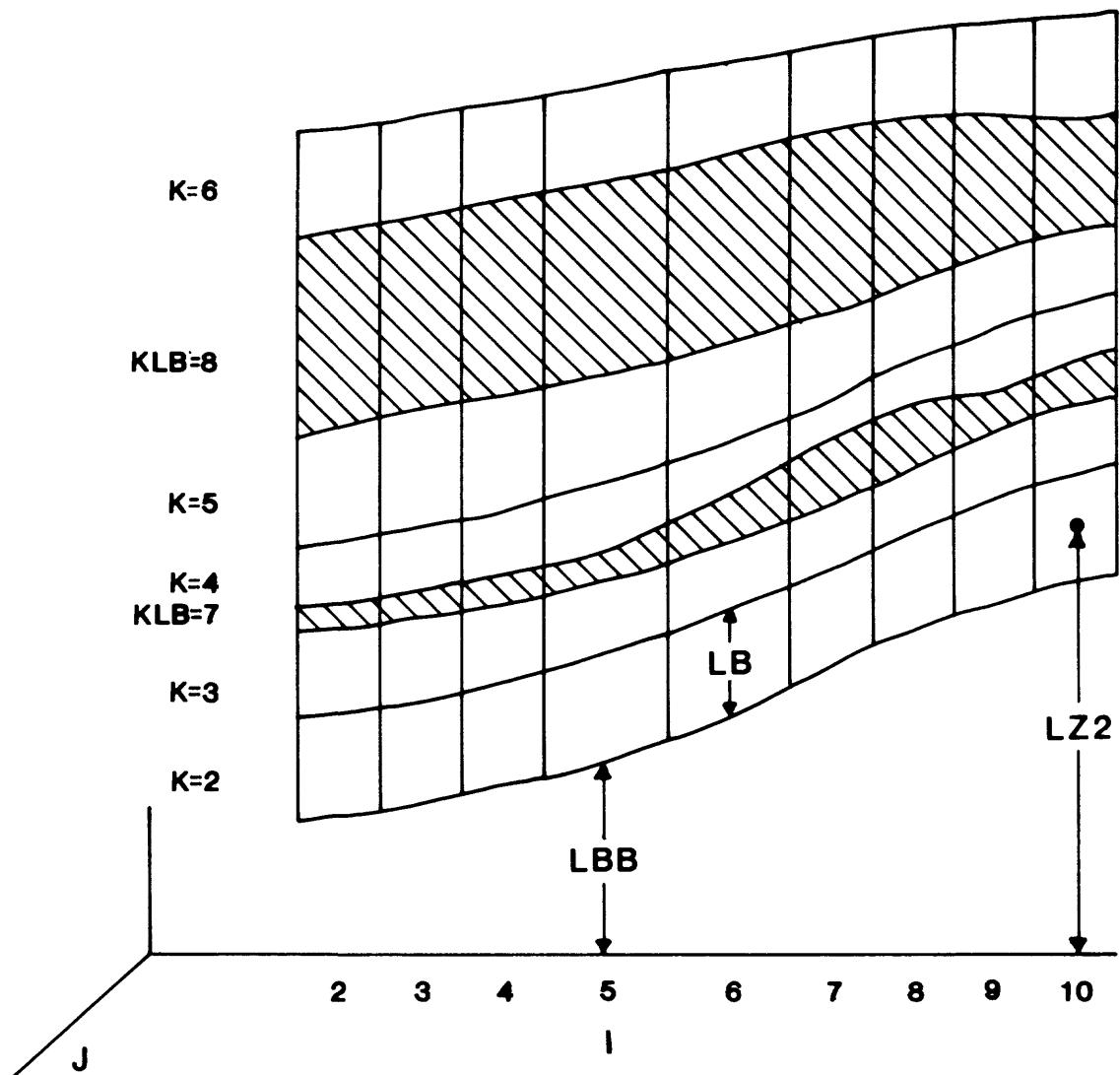
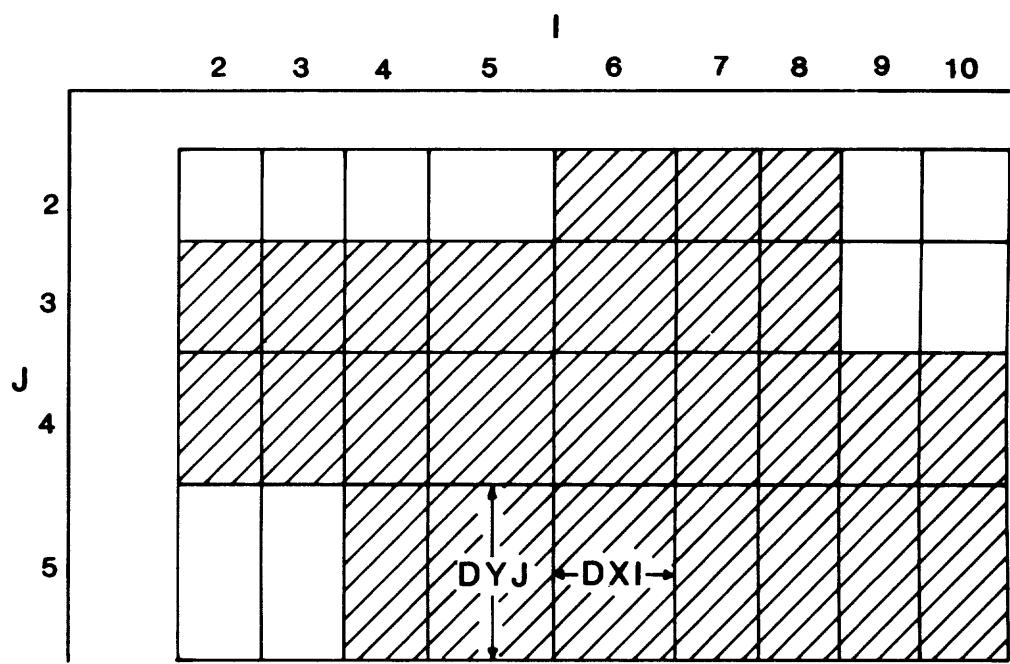


Figure 1.--Side view of grid elements.



EXPLANATION

**MAXIMUM HORIZONTAL EXTENT
OF MODELED REGION**

Figure 2.--Top view of grid elements.

The solution procedure in the numerical code assumes that no flow can pass through the boundary surface surrounding the modeled region. By fixing the rate of water withdrawal or injection from grid elements adjacent to the boundary surface, specified flow boundary conditions can be simulated. By fixing the hydraulic head in grid elements adjacent to the boundary, specified hydraulic head boundary conditions can be simulated.

In the computer program, grid elements, and confining bed grid elements, which lie outside of the modeled region, are flagged with NT=0. When a grid element has NT=0, it is dropped from the calculations in the solution procedure, thus reducing the computation time. Figure 2 shows the maximum horizontal extent of the modeled region. Because the modeled region may have different values of I and J for each layer, some of the grid elements or confining bed grid elements, which lie in the cross-hatched area in figure 2, lie outside of the modeled region.

For the computer program, values of ρ' may have any value outside of the modeled region. Values for LB and LBB in figure 1, in the cross-hatched area in figure 2, even when outside of the modeled region, should have values such that the computer program, when summing values of LB and LBB, obtains the correct elevations for LZ2 in figure 1 for the grid elements and confining bed grid elements within the modeled region. Values for LB, and LBB, may have any value outside of the cross-hatched area in figure 2.

When a layer, or confining bed layer, pinches out, LB is set to zero, and a non-zero value for K_{zz} (see page D-2) is used. This prescription for LB and K_{zz} causes a pinched-out grid element or confining bed grid element to offer no resistance to the flow of water through the elements' top and bottom surfaces, but prevents any flow through the elements' sides.

Fresh-Water Head

In the development by Kuiper (1983), the approximating equations (1) and (2) are written using pressure head $h = p/\rho_0 g$, where p is pressure, $\rho_0 = 1 \text{ gm/cm}^3$, and g is the acceleration of gravity. When equations (1) and (2) are altered using fresh-water head $h' = h+z$ and $\rho' = \rho - \rho_0$, and then divided by ρ_0 , they become equation (3).

When a cased well extends to a point at elevation z and at which the ground water has pressure p and density ρ , the water rises inside the well bore a distance $p/\rho g = h \rho_0/\rho$. Since the hydraulic head H is the elevation of the formation water in the well bore:

$$H = \frac{h}{\frac{\rho}{\rho_0}} + z$$

or

$$H = \frac{h' - z}{\left(\frac{\rho'}{\rho_0} + 1 \right)} + z \quad (4)$$

The computer program solves matrix equation (3) written with fresh-water head h' as the unknown. Any fixed hydraulic head values (MHD values in the computer program) are first converted to fixed h' values, using equation (4) evaluated at the center of the grid element, before the solution procedure is started. After a solution is obtained, the newly found h' values (XX values in the computer program) are converted to hydraulic head values, using equation (4), before they are printed. Hydraulic head values are input into the computer program and are also obtained as output, even though fresh-water head h' is used in the solution procedure.

Confining Beds

Confining bed grid elements, by definition, have zero hydraulic conductivity in the I and J directions, and thus do not allow any water to pass through their sides. Their specific storage is zero, and they do not have any wells, or any sources or sinks of mass of any type.

Figure 1 shows two confining beds, between the $K = 3$ and $K = 4$ layers and also between layers $K = 5$ and $K = 6$. The vertical dimension and ρ' for confining bed and regular grid elements are input in the computer program using the data sets LB and LRO respectively. For the example in figures 1 and 2, 180 values of LB(IJ) and LRO(IJ) for IJ = 2, 3, ..., 181 are read in. In addition, 72 values of LB(IJLB) and LRO(IJLB) for IJLB = 182, 183, ..., 253 are read in. The LB(IJ) and LB(IJLB) values are read in as one continuous array of 252 values, with the confining bed grid elements following the regular grid elements. In like manner, LRO(IJLB) values follow LRO(IJ) values. This same procedure is used to read in values for NT(IJ) and NT(IJLB), which are needed for the computation of hydraulic conductivity.

When more than one confining bed exists between two aquifer layers, they must be combined into one effective confining bed with the z component of K equal to $(K_{zz})_{eff}$, and with the same total vertical dimension LB, by using:

-1

$$\frac{(K_{zz})_{eff}}{LB} = \left[\sum_{i=1}^n \left(\frac{b_i}{K_{zz}} \right)_i \right]^{-1} \quad (5)$$

The number of adjacent confining beds is n. Confining bed i has vertical dimension b_i , and $(K_{zz})_i$ for the z component of K. The total thickness, or vertical dimension, of the adjacent confining beds is $\sum_{i=1}^n b_i = LB$. The ground-water density ρ_{eff} , for the effective confining bed, is found using:

$$(LB) \rho_{eff} = \sum_{i=1}^n \rho_i b_i \quad (6)$$

Recharge

Component IJ of mass recharge vector \hat{q} in equation (3), with units (L^3/T), includes the sum of all sources of mass (divided by ρ_0) that occur in grid element IJ. Such sources of mass include ground-water pumping from wells, as a negative quantity, and also the dissolution of solutes from the porous media. Vector \hat{q} is denoted by the quantities $YQ(IJ)$ in the computer program. The user must specify the mass recharge rates $YQ(IJ)$, one for each grid element IJ, but may also specify mass recharge rates $Q2(I,J,K)$ with which one must give the associated locations I, J, and K. If values for $Q2(I,J,K)$ are specified, the computer program adds these values to those given for $YQ(IJ)$.

Head Dependant Discharge

For any grid element the computer model allows for mass discharge which, when the hydraulic head H is greater than some chosen value H_e , increases linearly with H . The rate of mass discharge (L^3/T) from a grid element is given by $Aa(H-H_e)$ when $H>H_e$, and is zero when $H<H_e$. H is the hydraulic head in the grid element and A is the area of the grid element, $((DXI(I) \times DYJ(J))$. In the computer program, $XXE(IJ)$ is H_e , measured relative to the center of the grid element. $ALN(IJ)$, with units ($1/T$) specifies the quantity a .

The discharge may be used for a variety of purposes. It lends itself readily to evaporation which is sometimes assumed to begin when the hydraulic head rises to within a certain distance from ground surface. It can also be used to simulate discharge into a stream. In this case $Q2$ (or YQ) would also be used, to arrive at a net discharge of $Aa(H-H_e)-Q2$ for $H>H_e$, and $Q2$ for $H<H_e$. By choosing H_e to be less than any H that could possibly exist in the grid element being considered, the net discharge becomes $Aa(H-H_e)-Q2 = Aa[H-(H_e+Q2/Aa)]$. H_e and $Q2$ should be chosen such that H_e+Q2/Aa is equal to the stream elevation.

SOLUTION METHODS

Strongly Implicit Procedure

The strongly implicit procedure (SIP) for the solution of equation (3) uses the basic iterative equations (10), (14), and (15) of Weinstein and others (1969). In the numerical code, Weinstein's equation (10) is used with $\alpha_1 = \alpha_2 = \alpha_3 = \alpha_m$ where

$$(1 - \alpha_m) = (1 - \alpha_{\max})^{m/C-1} \quad m = 0, 1, \dots, (C-1)$$

C is the number of iteration parameters in a cycle, and is denoted by LENGTH in the computer program. In the computer program, one may choose $(1 - \alpha_{\max})$ to be WMAX by reading in a non-zero value for WMAX, or let the program calculate a value:

$$(1 - \alpha_{\max}) = (\text{XYFC}) (\text{XY}) \quad (7)$$

where

$$\text{XY} = \left(\frac{\pi^2}{2} \right) \frac{1}{\text{NCNT}} \sum_{IJ} \min \left[\frac{1}{(NI10)^2 (1+XM(IJ))}, \frac{1}{(NJ10)^2 (1+YM(IJ))}, \frac{1}{(NK10)^2 (1+ZM(IJ))} \right] \quad (8)$$

where

$$XM = \frac{B+H+Z+S}{D+F} \quad (9)$$

$$YM = \frac{D+F+Z+S}{B+H} \quad (10)$$

$$ZM = \frac{D+F+B+H}{Z+S} \quad (11)$$

where Z, B, D, F, H, and S are the diagonals $i,j,k-1$, $i,j-1,k$, $i-1,j,k$, $i+1,j,k$, $i,j+1,k$, and $i,j,k+1$ diagonals in the matrix M, using the notation in the computer program. The sum in IJ is over all the grid elements in the modeled region except those that have fixed head. NCNT is the number of such grid elements. The factor XYFC in equation (7) may be varied from 1.0 in an attempt to accelerate the convergence of SIP. Weinstein's equation (15) is modified by multiplying the right hand side by β' (Trescott and Larson, 1977). This iteration parameter, called HMAX in the computer program, may also be varied from 1.0 to accelerate convergence. For a given problem, the best choice for XYFC, and HMAX will depend a great deal upon whether one is using direction reversal in the J direction, the J and K directions, or only the K direction, corresponding to L9 = 1, 2, and 3 in the computer program. It will also depend upon the value used for LENGTH, the number of iteration parameters.

Increasing HMAX or decreasing XYFC usually tends to accelerate convergence unless instability arises. In the case of instability one should either decrease HMAX, increase XYFC, or do both. The best choice for the SIP parameters L9, LENGTH, HMAX, and XYFC will depend upon the particular problem being solved. Generally speaking, problems with a large number of grid elements for which the head is fixed, tend to be more stable and allow values of HMAX > 1.0

The user of the computer program is encouraged to experiment somewhat with selecting L9, LENGTH, HMAX, and XYFC, particularly with L9, HMAX, and XYFC. Good starting values are LENGTH = 5, HMAX = 1.0, and XYFC = 1.0. HMAX will usually have values between 0.5 and 1.5, and XYFC between 0.01 and 100. If one uses WMAX, and thus bypasses equations (7) through (11) and the use of XYFC, its value will usually lie between 0.000001 and 0.1. Decreasing WMAX usually tends to accelerate convergence unless instability arises.

Successive Over-Relaxation

The successive over-relaxation method (SOR) repeatedly finds values for the unknown variable XX at node points spaced along a single line with the adjacent values of the unknown XX taken to be known.

An 8 by 10 2-dimensional example is as follows. Values are first found at J=1, I=1 to 8, then J=2, I=1 to 8, etc., etc. The 8 equations for XX(I=1 to 8,J) contain values for XX(I=1 to 8,J-1) and XX(I=1 to 8,J+1), which are treated as known quantities. After a sweep is made across the solution area finding values along the 10 rows, a sweep is made finding values along the 8 columns: First I=1, for J=1 to 10, then I=2, for J=1 to 10, etc.

If the solution region is 3-dimensional, values would probably also be found in the K-direction.

The computer program allows one to omit calculating values in any one or two of the I, J, and K directions. The program omits the directions specified by NSKP1 and NSKP2. Directions I, J, and K correspond to 1, 2, and 3. For example: NSKP1=0 and NSKP2=1 causes the I direction to be skipped. Setting NSKP1=2 and NSKP1=3 causes both the J and K directions to be skipped.

Two relaxation parameters, RELX1 and RELX2, are used. Over-relaxation corresponds to these parameters having values greater than 1.0 and under-relaxation to values less than 1.0. RELX1 is applied after each single line of values is found, in each of the I, J, and K directions. RELX2 is applied after a full set (up to 3 if all of the I, J, and K directions are used, i.e., NSKP1=NSKP2=0) of sweeps is made over the solution region. Over-relaxed or under-relaxed values for XX are calculated using values of XX just prior to the last full set of sweeps, and the newly calculated XX values which were produced by the last full set of sweeps. The actual relaxation parameter used is RELX3 where:

```
RELX3 = 1.0      when ICNT = 1-5  
        = RELX2    when ICNT = 6-20  
        = RELX2 - COEF(INCT - 20) when ICNT ≥ 21
```

ICNT is the count of the number of full sets of sweeps, and is output as the number of "iterations used" by the computer program. COEF is selected to decrease RELX3 from RELX2 sufficiently fast to counter the possibly destabilizing effect of large values for RELX3 near convergence.

Preconditioned Conjugate Gradient

The preconditioned conjugate gradient (PCG) methods (Hageman and Young, 1981; Kershaw, 1978; Kuiper, 1981; Kuiper, written commun., 1984) are easier to use than SIP or SOR because they require very few convergence parameters only ITMAX, ERR, and XX10 need to be selected.

PCG methods solve nonlinear problems differently than SIP and SOR. For this reason the computer program uses the PCG methods differently, with regard to water discharge from a grid element when $H > H_e$, than it uses SIP or SOR. When using the PCG methods $Aa(H - H_e)$ (see the head dependant discharge section) is evaluated as $Aa(H^n - H_e)$, during the iterations finding the solution for XX^{n+1} , h' at time step $n+1$. For SIP and SOR however $Aa(H - H_e)$ is evaluated as $Aa(H^{n+1} - H_e)$. For this reason the PCG methods may give slightly different results. They will give the same results as SIP, or SOR, when such water discharge from a grid element does not occur.

For ISOR = 2, 3, ..., 9 the PCG methods: incomplete Cholesky conjugate gradient types 1,2, and 3, ICCG(1), ICCG(2), and ICCG(3); Richardson, RFCG; point Jacobi conjugate gradient, Pt. J. CG; block Jacobi conjugate gradient, Blk. J. CG; SIP conjugate gradient, SIPCG; and symmetric factorization procedure conjugate gradient, SFPCG are used. These eight methods are described by Kuiper (written commun., 1984). Usually the ICCG, SIPCG, and SFPCG methods perform better than the others. In general the PCG methods are much faster than either SIP (Kuiper, written commun., 1984) or SOR.

Convergence

In the computer program, iteration is terminated when either

$$\max_{(over IJ)} \left| \begin{array}{c} XX^{ICNT} - XX^{(ICNT-1)} \\ XX^{(ICNT-1)} - XX^{(ICNT-2)} \end{array} \right| + < ERR \quad (L) \quad (12)$$

or

$$\max_{(over IJ)} \left| [M]XX^{ICNT} - YQ \right| < XX10 \quad (L^3/T) \quad (13)$$

or $ICNT \geq ITMAX$. $ICNT$ is the iteration counter, and $ITMAX$ is the maximum number of iterations. In the first iteration stop, inequality (12), ERR should be chosen sufficiently small that any further decrease fails to produce any real and desirable increased accuracy in the answers for hydraulic head.

In the second iteration stop, inequality (13), $[M]$, XX , and YQ denote matrix M , h' , and vector \hat{q} in equation (3). This maximum residual error iteration stop, is in general strongly preferred to the use of (12), since (12) does not guarantee that the errors in the components of XX^{ICNT} are less than ERR , in fact they may be much larger. On the other hand, using (13) places the limit $XX10$ on the maximum error of the equations being solved, namely those of matrix equation (3).

Users may wish to set IWRT = 1 in order to obtain a convergence watching output from the computer program. For each iteration, this output prints fresh-water head XX at three locations of one's choice: IJ = NW1, NW2, and NW3. Also printed for each iteration are the maximum change in XX:

$$\max_{(over IJ)} \left| XX^{ICNT} - XX^{(ICNT-1)} \right|$$

the location I,J,K at which this maximum change occurred, $XX(I,J,K)^{ICNT}$, and the maximum residual error

$$\max_{(over IJ)} \left| [M]XX^{ICNT} - YQ \right|$$

If a clear idea of the convergence process is desired, $XX(NW1)$, $XX(NW2)$, and $XX(NW3)$, the maximum change in XX, and the maximum residual error, should be graphed as functions of the iteration counter ICNT.

If one wishes to use iteration stop (12), ERR should be given an appropriate value and XX10 should be set to zero. Set ERR = 0 and choose an appropriate value for XX10 if (13) is to be used. In general, however, iteration terminates when (12), or (13), or $ICNT \geq ITMAX$, or certain internal stops are satisfied.

Computation Time

The amount of computation needed for one iteration is proportional to the number of elements in the modeled region of the problem being solved. Thus it is appropriate that the amount of time needed for computation be set equal to:

$$(\text{CPU time}) = (\theta) (\text{number of grid elements})(\text{number of iterations}) \quad (14)$$

The quantity θ is CPU time per node iteration, and is in effect defined by equation (14). For a desired solution accuracy, as determined by XX10 or ERR, the number iterations should be minimized by proper selection of the parameters L9, LENGTH, HMAX, and XYFC, for SIP and the parameters RELX1, RELX2, and COEF, for SOR. The PCG methods do not have any parameters that affect the number of iterations required to obtain a given accuracy. The quantity θ has a different fixed value for each of the ten solution methods, SIP, SOR, and the eight PCG methods. It cannot be changed by the computer program user, but when using SOR it is proportional to the number of sweeps taken per iteration.

WATER DENSITY CALCULATIONS

Values of water density can be entered for each grid element, or values of density can be calculated for those grid elements for which values for pressure, molality, and temperature are entered. The same option pertains to the confining bed grid elements. Calculations of density in the model are limited to temperatures between 0°C and 75°C.

When LLRO = 0, only the values entered for LRO(IJ) = $(\rho'/\rho_0)_{I,J,K}$ and LRO(IJLB) = $(\rho'/\rho_0)_{I,J,KLB}$, where $\rho' = \rho - \rho_0$, are used. When LLRO = 1, read-in values for LRO(IJ) and LRO(IJLB) are replaced by calculated values, whenever such values are available. These calculated values are determined and made available only for those IJ or IJLB for which the pressure is specified to be greater than zero. A blank or zero is entered in the pressure data array when no calculation of LRO is desired and the read-in value for LRO is to be used. ρ/ρ_0 is determined using the method of Potter and Brown (1977):

$$(\rho/\rho_0) = \frac{1000 + M_2 m}{\frac{1000}{(\rho_w/\rho_0)} + A_0 m + B_0 m^3/2 + C_0 m^2} + \delta(P, m, T) \quad (15)$$

where ρ_w is the density of pure water at the temperature and pressure of the ground-water sample, $M_2 = 58.488$ is the molecular weight of NaCl, and m is molality of the ground-water sample. Equation (15) for ρ/ρ_0 approximates data for NaCl solutions and is assumed to be an adequate approximation to ρ/ρ_0 for ground water.

Values for the parameters A_o , B_o , and C_o (Potter and Brown, p. 35, 1977) are: $A_o = 12.43, 16.62, 18.00, 18.18$; $B_o = 3.07, 1.773, 1.66, 1.19$; and $C_o = -0.02, 0.098, 0.002, 0.12$; for water temperature T equal to 0, 25, 50, and 75°C . A_o , B_o , and C_o are approximated by third order polynomial interpolation for $0 \leq T \leq 75^\circ\text{C}$. These polynomials, one for each of the parameters A_o , B_o , and C_o , are exact at $T = 0, 25, 50$, and 75°C . With $\delta = 0$, equation (15) is solved for ρ_w with ρ taken from Potter's table 1 with $m = 1$ and 6, giving $(\rho_w)_{m=1}$ and $(\rho_w)_{m=6}$. The value taken for ρ_w for use in (15) is $\hat{\rho}_w = [(\rho_w)_{m=1} + (\rho_w)_{m=6}] / 2$. This is done for $T = 0, 25, 50$, and 75°C , giving four values for $\hat{\rho}_w$ from which $\hat{\rho}_w(T)$ is obtained using a third order interpolation polynomial as described above. The term δ is pressure, molality, and temperature dependent, and is a small perturbation to the main term in equation (15):

$$\delta(P, m, T) = \frac{am+b}{10^3} (P/\text{bar}) \quad \text{for } 0 \leq P \leq 100 \text{ bar} \quad (16)$$

$$\delta(P, m, T) = \frac{am+b}{10^3} + [\frac{-84(x-1)}{10^5} + 3.75] [(P/\text{bar}) - 100] \quad \text{for } 100 \text{ bar} \leq P$$

where $a = -0.75(x-1) + .25$, and $b = 3.5(x-1) + 2$, where $x = T/25^\circ\text{C}$ and P is pressure. For $P \leq 500$ bar, $m \leq 6$, and $0 \leq T \leq 75^\circ\text{C}$, equations (15) and (16) fit the tabular data for ρ of Potter and Brown (1977) to within the allowable error tolerances they specify.

Pressure P is given by $P = \rho g l'$, where l' is the length of the column of water with density ρ that would exist in a well bore extending to the center of the grid element in which ρ is to be determined. Thus equation (15), along with equation (16), becomes an equation to be solved for ρ once l' , m , and T have been specified. This can be done readily with several iterations of equation (15) using $\rho = \rho^{n+1}$ left of the equality and $\rho = \rho^n$ in δ , with n the iteration number.

UNITS

The user may use any consistent set of units for all variables except: l' , used to give water pressure $P = \rho g l'$ for calculating water density ρ , must be in feet; water temperature T , also used for calculating water density ρ , must be in degrees celsius. Hydraulic conductivity K has units (L/T). Thus, for example, if the length and time units were chosen to be feet and days respectively, then K would be expressed in ft/d. Specific storage has units (1/L). All mass flow rates, such as the mass recharge rates YQ or $Q2$, and also those through grid element sides, express the mass of water moving per unit time divided by $\rho_0 = 1 \text{ gm/cm}^3$, and consequently have units (L^3/T). For example, a value of $50 \text{ ft}^3/\text{d}$ for the mass flow rate through a particular grid element side means that the mass of water passing though the side per day is equal to the mass of 50 ft^3 of a fluid with density 1 gm/cm^3 , or approximately $(50) (62.43)$ pounds. This would correspond to less than 50 ft^3 of water if the density of the water exceeds ρ_0 . Suppose a well pumps (from a grid element) at a volumetric rate of $1000 \text{ ft}^3/\text{d}$, as measured in the field and suppose that the density of the water pumped is ρ . Then the rate at which mass is being removed is $(1000 \text{ ft}^3/\text{d})\rho$. Thus the value to be used for YQ or $Q2$ is $-(1000 \text{ ft}^3/\text{d})(\rho/\rho_0)$. The minus sign occurs because YQ and $Q2$ are defined to be positive for recharge. Thus, field measured volumetric flow rates need to be multiplied by (ρ/ρ_0) to arrive at the mass flow rates used in the computer program. This situation arises because the basic flow equations as solved in the computer program conserve mass rather than volume.

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ATTACHMENT A

COMPUTER PROGRAM

This section explains the Fortran computer program. It should be used in conjunction with the Fortran program listing in Attachment E.

Main program (MAN0080 - MAN7690)

Explanation of program

0080-0180

The array variables DD, BB, ZZ, SV, XXS, ALN, XXE, XXSTR, YQ1, DT, E2, F2, G2, VV, XX, YQ, MHD, and LZ2 have a dimension size equal to the total number of grid elements plus 2: $[(NI10)(NJ10)(NK10)+2]$. The array variables LB, LRO, and NT, have a dimension size equal to the total number of grid elements and confining bed grid elements plus 2: $[(NI10)(NJ10)(NK15)]+2$. The dimension size of array variable LBB is $[(NI10)(NJ10)+2]$. The dimension size of these array variables should be adjusted by the computer program user in the main program as well as in the subroutines. The dimension size of the other array variables are probably sufficiently large and can be left at the values shown.

The use of the IMPLICIT REAL*8 statement is optional. Removing this statement will decrease the storage requirement of the computer program but may cause certain outputs, such as water flow rates, to become less accurate. The user should try deleting the IMPLICIT REAL*8 statement to see whether any decrease in accuracy is experienced. In general, the use of the statement is recommended.

0200-0230 Data for use in the determination of water density from water pressure, molality and temperature.

0240-0250 Initialize MAQ1 to 0.

0270-0370 Read group I data.

0380-0530 Determine various integer parameters related to the number of grid elements and confining bed grid elements.

0570-0630 Read and write MHD.

0640-1050 If LLRO = 1 read ℓ' , m, T, and determine ρ for those grid elements having $\ell' > 0$. Temporarily place ρ in LB.

1060-1110 Read and write LRO. These written values will have been determined from ℓ' , m, and T, if LLRO = 1 and $\ell' > 0$.

1120-1170 Read and write LBB.

1180-1230 Read and write LB.

1240-1340 If IEVP = 1, read and write XXE(IJ) and ALN(IJ).

1350-1410 Read and write initial hydraulic head.

1420-1450 Read and write SV.

1460-1510 If IKZZ = 1, read XKZZ.

1520-1550 Remove pinched-out nodes when appropriate.

1560-1770 Read and write FCNT, DDK, BBK, and NT.

1790-1830 Read and write MAQ1, if there are any confining beds.

1840-2010 Read and write DXI and DYJ.

2020-2060 Read and write NI, NJ, NK, and Q2.

2090-2180 Initialize various arrays to zero.

2210-2760 Determine LZ2 and initial or fixed XX, put recharge rates Q2 into YQ. If IEVP = 1, modify XXE and ALN.

2800-2890 If ILZ2 = 0, calculate and print the elevation of the top of the uppermost grid element layer.

2910-3440 Determine the quantities DD, BB, and ZZ.

3470-4240 Add variable density contributions to YQ, put into YQ1.

4260-4370 If SIP is being used (ISOR = 0), determine XY and the iteration parameters WS(I). Write the various SIP convergence parameters, and also the iteration parameters WS(I).

4400-4410 If SOR is being used (ISOR = 1), write the various SOR convergence parameters.

4430-4440 If PCG is being used (ISOR ≥ 2), write ITMAX, ERR, and XX10.

4460-4480 Enter DO loop for pumping intervals. Write pumping interval number IPINT. Read data for this pumping interval.

4510-4700 Read and write recharge rates YQ for this pumping interval. Add YQ1 to YQ, put into YQ. Calculated budgets.

4740-4780 Set TOTIME = 0. Enter DO loop for time intervals INT = 1, NINT. Write INT, DELT, and TOTIME.

4830-4880 Write NU1, NU2, and NU3, when IWR1 = 1.

4900-4920 Begin SIP, SOR, or PCG iterations. Write data for watching the convergence of SIP, SOR, or PCG, when IWR1 = 1.

4930 Write ICNT, ER5, SRZ, SUMRZ.

4950-4960 Save XX in XXS for use during the next time statement.

4970-6460 If LFLOW = 1, determine and possibly print the four types of flow rate data.

6480-6640 Determine hydraulic head from XX = h' = pressure head h) + z. Write out hydraulic head. Write XX = h', if IWRTXX = 1.

6680-6820 If IPDD = 1 print drawdowns for this pumping interval.

6840-7080 Formats.

7690 Stop.

Subroutine RDWRT

This subroutine performs the reading and writing of group II array data (see Attachment B.) IT15 is 1 for data sets 1-9, and 2 for data set 10. ICRO is always 0 except ICRO = 1 when LLRO = 1, in which case values for LRO are computed from water pressure, molality, and temperature. NK1115 is equal to NK11 or NK15 corresponding to the data set having values for grid elements only (NK1115 = NK11), or for both grid elements and confining bed grid elements (NK1115 = NK15). NT is used as a temporary storage location for data being read in. After returning to the main program the array data in NT is usually placed into another variable.

The dimension size of the array variables should be the same as in the main program and should be adjusted by the computer program user.

Subroutine SOR

This subroutine performs the successive over-relaxation method SOR.

The dimension size of the array variables should be the same as in the main program and should be adjusted by the computer program user.

Subroutine SIP

This subroutine performs the strongly implicit procedure SIP.

The dimension size of the array variables should be the same as in the main program and should be adjusted by the computer program user.

Subroutine PCG

This subroutine performs the preconditioned conjugate gradient (PCG) methods.

The dimension size of the array variables should be the same as in the main program and should be adjusted by the computer program user.

In addition, D2S and E22 need to be dimensioned, unless SIPCG and SFPCG are not going to be used, in which case the indicated deletions in the subroutine should be made.

ATTACHMENT B

DATA DECK INSTRUCTIONS

Group I: Model dimensions and options, parameters related to the use of SIP, SOR, or PCG

<u>CARD</u>	<u>COLUMN(S)</u>	<u>FORMAT</u>	<u>VARIABLE</u>	<u>DEFINITION</u>
0	1-10	G10.0	ISOR	ISOR = 0, 1, and 2 through 9 correspond to the use of SIP, SOR, and the 8 PCG methods, ICCG(1), ICCG(2), ICCG(3), RFCG, Pt. J. CG, Blk. J. CG, SIPCG, and SFPCG; and the use of cards 1a, 1b, and 1c, respectively. ISOR = 2-4, and 8-9 are usually preferred choices.
1 a	1-10	G10.0	L9	1, 2, and 3 for J, J and K, and K only direction reversal in SIP.
11-20		G10.0	LENGTH	Number of SIP iteration parameters. LENGTH = 5 is a common choice.
21-30		G10.0	HMAX	SIP parameter β' . Increasing β' usually causes faster convergence unless instability arises. Values of .5 - 1.3 are usually used.

<u>CARD</u>	<u>COLUMNS</u>	<u>FORMAT</u>	<u>VARIABLE</u>	<u>DEFINITION</u>
31-40		G10.0	XYFC	This factor is multiplied by XY before it is used for $(1 - \alpha_{\max})$ in SIP. First choice for XYFC is 1.0. Decreasing XYFC usually tends to cause faster convergence unless instability arises.
41-50		G10.0	WMAX	When not zero, WMAX is used for $(1 - \alpha_{\max})$. When zero, it is not used and $(1 - \alpha_{\max})$ is set equal to (XYFC) X (XY). Usually $0.000001 < \text{WMAX} < 0.1$, if used. Decreasing WMAX usually tends to cause faster convergence unless instability arises. Non-zero values of WMAX are not usually used, thus allowing the computer program to select XY.
51-60	1-10	G10.0	ITMAX	
61-70	11-20	G10.0	ERR	
71-80	71-80	G10.0	XX10	
1b		G10.0	NSKP1	See the successive over-relaxation section of the text
		G10.0	NSKP2	NSKP1, NSKP2, RELX1, RELX2, and
		G10.0	RELX1	COEF.
		G10.0	RELX2	
		G10.0	COEF	
51-60	1-10	G10.0	ITMAX	
61-70	11-20	G10.0	ERR	
71-80	71-80	G10.0	XX10	

CARD COLUMNS FORMAT VARIABLE DEFINITION

1c	1-10 11-20 21-30	G10.0 G10.0 G10.0	ITMAX ERR XX10
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For cards 1a, 1b, and 1c, ITMAX is the maximum allowed number of iterations for SIP, SOR, and the 8 PCG methods. Iteration terminates at iteration count n when the sum of the maximum change in fresh-water head h' between iterations $n-1$ and n , plus the change between iterations $n-2$ and $n-1$, is less than ERR. Iteration also terminates when the maximum residual error is less than XX10.

<u>CARD</u>	<u>COLUMNS</u>	<u>FORMAT</u>	<u>VARIABLE</u>	<u>DEFINITION</u>
2	1-10 11-20 21-30 31-40	I10 I10 I10 I10	N110 NJ10 NK10 NK4	Number of columns in modeled area. Number of rows in modeled area. Number of layers in modeled area. Number of intervening confining beds.
3	1-40	I4 314 314 314	IWRT NU1(I), I=1,3 NU2(I), I=1,3 NU3(I), I=1,3	Set IWRT to 1 if you want to watch the convergence of fresh-water head h' = XX, at the three locations: $I = NU1(1), J = NU1(2), K = NU1(3);$ $I = NU2(1), J = NU2(2), K = NU2(3);$ and $I = NU3(1), J = NU3(2), K = NU3(3).$

DEFINITION

<u>CARD</u>	<u>COLUMNS</u>	<u>FORMAT</u>	<u>VARIABLE</u>	<u>DEFINITION</u>
4	1-10	I10	NPINT	Number of pumping intervals.
	11-20	I10	IPDD	If IPDD = 1, the drawdown (decrease in hydraulic head H) during a pumping interval is printed.
	21-30	I10	LLRO	If LLRO = 0, read-in values for LRO are used. If LLRO = 1, read-in values for LRO are replaced by values for LRO calculated from water pressure, molality, and temperature, when such calculated values are available. Calculated values are made available only for those IJ or IJLB for which the pressure is specified to be greater than zero.
	31-40	I10	IWRXXX	If IWRXXX = 1, freshwater head $h' = (\text{pressure head } h) + z$ is printed along with the hydraulic head. If IWRXXX = 0, it is not printed. If IWRXXX = 2, only h' is printed.
	41-50	I10	IPRNT	Setting IPRNT = 0 causes IWRT and LFLOW to be set to zero, and the printing of hydraulic and freshwater head deleted, for all time intervals except the last.

CARD

COLUMN

FORMAT

VARIABLE

DEFINITION

51-60 I10 ILZ2

If ILZ2 = 0, the elevation of the top of the uppermost grid element layer is printed.

61-70 I10 IEVP

If IEVP ≠ 1, data sets 5 and 6 are not read. If IEVP = 1 these data sets are read, and the head dependant discharge option is available.

71-80 I10 IKZZ

If IKZZ ≠ 1, data set 9 is not read. If IKZZ = 1, data set 9, XKZZ = Kzz is read. In this case Kzz is specified by XKZZ rather than by NT from data set 10.

<u>CARD</u>	<u>COLUMN</u>	<u>FORMAT</u>	<u>VARIABLE</u>
5	1-10	I10	LFFLOW
	11-20	I10	LFL0(1)
	21-30	I10	LFL0(2)
	31-40	I10	LFL0(3)
	41-50	I10	LFL0(4)

Four types of flow rate data are available: 1) the flow rate out of each grid element in the negative I, J, and K directions, 2) the flow rate out of fixed head (MHD = 0) grid elements, 3) head dependant discharge flow rates from grid elements having such discharge, 4) total flow rate budgets for sets of grid elements having the same I, the same J, and the same K. All flow rates are in units of mass divided by $\rho_0 = 1 \text{ gm/cm}^3$ per unit time (L^3/T). See the Units section of the text. Set LFFLOW = 1 if you want any flow rate data, set LFL0 = 0 if no flow rate data is desired. Set LFL0(i) = 0 if you do not want type i flow rate data. For i = 1, set LFL0(1) = 1, 2, 3, for type 1 flow rate data in the negative I, J, and K directions respectively. If LFL0(1) = 4 all directions are given. Set LFL0(2) = 1 if you want type 2 flow rate data. Set LFL0(3) = 1 if you want type 3 flow rate data. Set LFL0(4) = 1, 2, 3, for the budgets of sets of grid elements having the same I, J, and K respectively. IF LFL0(4) = 4 budgets are given for I, J, and K. Corresponding to the integers 1, 2, and 3 in the first column of output the second column gives I, J, and K respectively.

DEFINITION

DEFINITION

VARIABLE

FORMAT

COLUMN

<u>CARD</u>	<u>COLUMN</u>	<u>FORMAT</u>	<u>VARIABLE</u>	<u>DEFINITION</u>
6,7...	1-80	2014	IPH(K) K=2,NK11	Set IPH(K) = 1 if you want: hydraulic head or freshwater head, flow rate data, or drawdown for layer K. Set IPH(K) = 0 if you do not want these quantities for layer K. The layers are numbered K = 2 through K = NK11 = NK10+1.

Group II: Array data

Each of the following data sets consists of a format card, one or more parameter cards and, if the data set contains variable data, a set of data cards. A single parameter card and corresponding set of data cards (for layers with variable data), are required for each layer.

CARD

DEFINITION

VARIABLE

FORMAT

COLUMN

Format card	1-4 5-40 41-80	I4 9A4 10A4	FCNT IVAR	Place the desired Fortran read format in columns 5-40, and the write format in lines 41-80. When writing with an I format, place a zero in column 4. When writing with a non-integer type format, place a 1 in column 4.
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Parameter cards.	1-10 11-10	G10.0 G10.0	FCNT IVAR	If IVAR = 0, values of the array are given the value FCNT, and no data cards are read. If IVAR = 1, values for the array are set equal to FCNT multiplied by the values read from the data cards following this card.
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CARD COLUMNS FORMAT VARIABLE DEFINITION

21-30	G10.0	IPRN	If IPRN = 0, the input data for this layer are printed. If IPRN = 1, the input data for this layer are not printed. If IPRN = 2, only parameter card data for the layer is printed.
31-40	G10.0	DDK	Multiplication factor for hydraulic conductivity in the I direction (data set 10 only).
41-50	G10.0	BBK	Multiplication factor for hydraulic conductivity in the J direction (data set 10 only).

When data cards are used for a layer, start each row on a new card. First, row J = 2, the first row of the layer, is read from as many cards as is necessary. Then, starting with a new card, row J = 3 is read, then row J = 4, and so forth, until the last row of the layer, J = NJ11 = NJ10+1, is read.

DATA CARDS:

DATA_SET COLUMNS FORMAT VARIABLE DEFINITION

1	1-80	Variable	MHD	When MHD(IJ) ≠ 0 the hydraulic head for grid element IJ is fixed at the value specified. When MHD(IJ) = 0, the head for grid element IJ is not fixed. There are NK10 layers of MHD values. Values given are truncated after the first decimal place.
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DATA_SET COLUMNSFORMATDEFINITION

2 1- 80 Variable LRO

$LRO(IJ) = (\rho' / \rho_0)$. $\rho = \rho' + \rho_0$ is the water density for grid element IJ.
 $LRO(IJLB) = (\rho' / \rho_0)$, where $\rho = \rho' + \rho_0$ is the water density for confining bed grid element IJLB. Values given are truncated after the fifth decimal place.

3 1- 80 Variable LBB

LBB is the elevation of the base of the lowermost K = 2 layer. LBB values exist only for this layer.

4 1- 80 Variable LB

LB(IJ) is the vertical dimension of grid element IJ. LB(IJLB) is the vertical dimension of confining bed grid element IJLB. There are NK10 layers of LB(IJ) values followed by NK4 layers of LB(IJLB) values.

5 1- 80 Variable XXE

The rate of water discharge (L^3/T) from a grid element is given by $Aa(H-H_e)$ when $H>H_e$ and is zero when $H < H_e$. H is the hydraulic head in the grid element and A is the area of the grid element, ((DXI(I)) X(DYJ(J)). XXE(IJ) of data set 5 is H_e , measured relative to the center of the grid element IJ. ALN(IJ) of data set 6 specifies the quantity a. When no discharge is desired, XXE(IJ) should be given a large value and the quantity a should be zero. If IEVP ≠ 1, data sets 5 and 6 are not read.

6 1- 80 Variable ALN

<u>DATA_SET</u>	<u>COLUMNS</u>	<u>FORMAT</u>	<u>VARIABLE</u>	<u>DEFINITION</u>
7	1- 80	Variable	Initial hydraulic head	Fixed hydraulic head values MHD ≠ 0 override values given for the initial hydraulic head.
8	1- 80	Variable	SV	SV(IJ) specifies specific storage S_s of grid element IJ.
9	1- 80	Variable	KKZZ	When this data set is read, IKZZ = 1, $K_{zz}(IJ) = XKZZ(IJ)$ rather than NT(IJ) in data set 10. Use of this data set allows one to vary the x, y, and z components of the hydraulic conductivity independently.
10	1- 80	Variable	NT	$K_{xx}(IJ) = NT(IJ)$ $X(DDK(K))$, $K_{yy}(IJ) = NT(IJ)$ $X(BBK(K))$, $K_{zz}(IJ) = NT(IJ)$ where $K_{xx}(IJ)$, $K_{yy}(IJ)$, and $K_{zz}(IJ)$ denote the x, y, and z components of K, the hydraulic conductivity for grid element IJ. There are values of NT(IJ), DDK(K), and BBK(K), for NK10 layers. These are followed by values of NT(IJLB) for NK4 confining bed layers. DDK and BBK are not needed for confining bed layers.

When LLR0 = 1, data sets 1a-c are required. If LLR0 = 0, they should be omitted. These data sets are used to calculate water density from the pressure, dissolved solids concentration, and temperature of the water. They are placed between data set 1 for MHD and data set 2 for LRO.

<u>DATA_SET_COLUMNS</u>	<u>FORMAT</u>	<u>VARIABLE</u>	<u>DEFINITION</u>
1a	1-80	Variable λ'	Water pressure, in feet, defined as the length of the column of water that would exist in a well bore extending to the center of the grid element. If pressure is zero, then LRO from data set 2 is used.
1b	1-80	Variable m	Dissolved solids concentration, expressed as molality. Values given are truncated after the second decimal point.
1c	1-80	Variable T	Temperature, in degrees Centigrade. Values given are truncated after the first decimal point.

There are values of λ' , m, and T for NK10 layers, followed by values for NK4 confining bed layers. See the WATER DENSITY CALCULATIONS section of the text for more detail.

Group_III: Additional array data

Except for LBB, the data sets of group II are 3-dimensional arrays corresponding to the three cartesian directions I, J, and K. The data sets of group III (except for Q2) are 1-dimensional arrays corresponding to only one of the cartesian directions I, J, or K.

<u>CARD</u>	<u>COLUMNS</u>	<u>FORMAT</u>	<u>VARIABLE</u>	<u>DEFINITION</u>
1	1-80	20I4	MAQ1	MAQ1(K) = 0 except when a confining bed lies between layers K-1 and K, in which case MAQ1(K) = 1. There are NK10 values for MAQ1(K) for K = 2, . . . , (NK10+1). If there are no confining beds (NK4 = 0), omit this data set. Values for MAQ1(K) are printed when NK4>0.
				If MDXII1 = 0, DXI(I) is set to FDXI and no data cards are read.
				If MDYJ1 = 0, DYJ(J) is set to FDYJ and no data cards are read.
2-parameter card	1-10	G10.0	FDXI	
	11-20	G10.0	FDYJ	
				If MDXII1 = 1, DXI(I) is read from data cards that follow the parameter card. If MDYJ1 = 1, DYJ(J) is read from data cards that follow the parameter card and also any data cards for DXI(K) when they are present.
				There are NI10 values of DXI(I) for I = 2, . . . , (NI10+1), and NJ10 values of DYJ(J) for J = 2, . . . , (NJ10+1). If MD2 = 0 the input data for this data set are printed. If MD2 = 1 the input data are not printed.
2-Data cards	1-80	8G10.0 8G10.0	DXI(I) DYJ(J)	

<u>CARD</u>	<u>COLUMNS</u>	<u>FORMAT</u>	<u>VARIABLE</u>	<u>DEFINITION</u>
3 - para - meter	1-10	I10	NWEL	Number of grid elements recharge.

3-data cards 1-80 4(313,
 E11.3)
 Q2
NI, NJ
NK, and
J = NJ, and K = NK.
Four values of
NJ, NK, and Q2 are read in per
card. If there is no recharge,
set NWEL to 1, choose any loca-
tion, and use Q2 = 0. Values for
NI, NJ, NK, and Q2 are always
printed. The recharge specified
with this data set is added to the
recharge YQ of data set 1 of
group IV. Either or both methods
for specifying recharge may be used.
However, Q2 is read only once, and
is the same for each pumping
interval, whereas YQ is different
for each pumping interval.

GROUP IV: Array data for pumping intervals

Many pumping intervals are allowed. Each pumping interval requires data related to the time intervals used, and the recharge. The total recharge (L_3/T) used in the computer model is $Q_2 + Y_Q$. Q_2 is read in only once, in group III data, but Y_Q is read in group IV data and changes with each pumping interval.

For each pumping interval a time interval card is followed by series of cards for YQ with exactly the same format as group II data. The format, parameter, and data cards used are the same as those for group II data sets (See Group II: Array data). When a layer has variable YQ, the usual case, data cards are needed (See Group II: Array data):

The time interval card has the following format:

<u>CARD</u>	<u>COLUMNS</u>	<u>FORMAT</u>	<u>VARIABLE</u>	<u>DEFINITION</u>
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Time interval	1-10	G10.0	NINT	Number of time intervals desired.
	11-20	G10.0	DTO	Duration of the first time interval.
	21-30	G10.0	TFAC	The ratio of the duration of a time interval divided by the duration of the preceding time interval.
	31-40	G10.0	TOT	If TOT \neq 0, DTO is calculated such that the duration of the pumping interval, the sum of the NINT time intervals, is TOT.

DATA CARDS:

<u>DATA_SET</u>	<u>COLUMNS</u>	<u>FORMAT</u>	<u>VARIABLE</u>	<u>DEFINITION</u>
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1	1-80	Variable	YQ	YQ(IJ) along with Q2(I,J,K), specifies the recharge rate (L_3^3/T) into grid element IJ.
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ATTACHMENT C

EXAMPLE APPLICATION

This section presents an example steady state application of the computer program. The input data is shown on page C-3 and the resulting program output is shown on page C-6.

The hypothetical problem simulated has: 3 layers corresponding to $K = 2, 3, \text{ and } 4$; 5 rows corresponding to $J = 2, 3, 4, 5, \text{ and } 6$; and 25 columns corresponding to $I = 2, 3, 4, \dots, 26$. A confining bed appears in the output as layer five ($K_{LB} = 5$).

Proceeding through the computer program output on page C-6, we see that fixed hydraulic head MHD is fixed at: 645.6 ft (the length unit chosen is feet) at location $I = 2, J = 2, K = 2$; at 747.8 ft at location $I = 26, J = 2, K = 2$; at 748.8 ft at location $I = 2, J = 6, K = 2$; and at 750.3 ft at location $I = 26, J = 6, K = 2$. It is also fixed at 600.0 ft at all 125 locations in layer $K = 4$. We now proceed to the next data set, the water pressure as measured by the length λ' of water column that would exist in a well bore extending to the center of the grid element. Eighteen non-zero values for λ' are shown in layer $K = 3$, rows two and four. Values for LRO are calculated at these 18 locations. Values for molality $m = 1.0-6.0$, and temperature $T = 25-75^\circ\text{C}$ occur at these same 18 locations, on page C-7. The next data set shown is $LRO = [(\rho/\rho_0)-1]$. Eighteen of these LRO values were calculated from λ' , m , and t , at locations with $\lambda' > 0$. The remaining values for LRO , all but two of which are zero, are those read as the data set LRO . The next data set is base elevation, LBB , which has non-zero values in rows five and six. The next data set is the z dimension, LB , of the grid elements and confining bed grid elements. The grid elements have uniform values for LB of 200, 235, and 120 ft for $K = 2, 3, \text{ and } 4$. The confining bed grid elements all have $LB = 60$ ft. Following this are initial hydraulic head, and specific storage.

The next data set is K, the hydraulic conductivity. Shown also are K_{xx}/K_{zz} and K_{yy}/K_{zz} . In layer two: $K_{zz} = 5$ ft/d, $K_{xx}/K_{zz} = 1$, and $K_{yy}/K_{zz} = 1$. In layers three and four: $K_{zz} = 12$ and 20 ft/d, and $K_{xx}/K_{zz} = K_{yy}/K_{zz} = 1$. For the confining bed, $K_{LB} = 5$, $K_{zz} = 0.01$ ft/d. Zeros are shown for K_{xx}/K_{zz} and K_{yy}/K_{zz} , but are not used. The next data set is MAQ1(K). The 1, for layer four, indicates that layer four is underlain by a confining bed. The next data set shows the X (I direction) and Y (J direction) dimensions of the grid elements: $DXI(I) = 8000$ ft for $I = 2, 3, \dots, 26$ $DYJ(J) = 10000$ ft for $J = 2, 3, \dots, 6$. The next data set shows the recharge rates Q2 to grid elements: $I = 10, J = 4, K = 3$ and $I = 20, J = 4, K = 3$. The next data set shows the elevation of the top of the uppermost grid element layer, as calculated from values for LB and LBB. The next section lists the values that were chosen for the PCG(7) convergence parameters. The next section gives the pumping interval and YQ, data set 1 of group IV. The next section gives the time interval number, the duration of the time interval, and the total amount of time elapsed in the current pumping interval. It also follows the solution as it proceeds to convergence. Note the behavior of $XX(I = 5, J = 3, K = 2)$, $XX(I = 10, J = 3, K = 2)$ and $XX(I = 15, J = 3, K = 2)$ as they converge to their final values. Note that the maximum residual error decreases uniformly as iteration proceeds. The next output gives the water flow rate in the negative I, J, and K directions out of each grid element and shows that the dense water, which exists in some of the grid elements, is sinking. The flow of water adjacent to such elements is similar to that adjacent to a heavy object sinking in a fluid. The next two sections give: water flow rates out of fixed head ($MHD = 0$) grid elements total flow rate budgets for sets of grid elements having the same I, the same J, and the same K, respectively. The last data set printed is hydraulic head H. Because $IWRTXX = 1$, fresh-water head $XX = h' = (\text{pressure head } h) + z$ is also printed. H and XX are related by equation 4 in the text. Because $IPDD = 0$, no drawdown values are printed. Because $IPH(K)$ is equal to 0, 1, and 0, for $K = 2, 3$, and 4, water flow rates and head are given only for layer $K = 3$.

U(2064.0) (112, 2016, (12X, 2016))

Molality (m)	Osmotic Pressure (Π) at 20°C	Osmotic Pressure (Π) at 30°C	Osmotic Pressure (Π) at 40°C	Osmotic Pressure (Π) at 50°C
0	0	0	0	0
100	~100	~150	~200	~250
200	~200	~300	~400	~500
300	~300	~450	~600	~750
400	~400	~600	~800	~1000
500	~500	~750	~1000	~1250

0(20G4.0) 0 0 0 (112,2016/(112X,2016))

Temperature T	0	0	0	0	0	0	0	0
250	375	250	500	750	250	500	750	0
0	0	0	0	0	0	0	0	0
250	500	500	500	400	250	250	250	250

(112,1518)/(12X,1518))									
0(1366,0)			1			0			I, BB
0	0	0	0	0	0	0	0	0	
0	7	7	7	7	5	5	5	6	
6	7	7	4	3	0	3	4	5	
7	8	12	12	13	14	17	22	22	6
23	33	33	33	33	33	31	32	33	7
0	0	0	0	0	0	0	0	0	
200	0	0	0	0	0	0	0	0	
235	0	0	0	0	0	0	0	0	
120	0	0	0	0	0	0	0	0	
60	0	0	0	0	0	0	0	0	
0	0	0	0	0	0	0	0	0	
0	0	0	0	0	0	0	0	0	
0	0	0	0	0	0	0	0	0	
0	0	0	0	0	0	0	0	0	
1	0	0	0	0	0	0	0	0	
1	0	0	0	0	0	0	0	0	
1	0	0	0	0	0	0	0	0	
0	0	0	0	0	0	0	0	0	
5	0	0	0	0	1	1	1	1	
12	0	0	0	0	1	1	1	1	
20	0	0	0	0	1	1	1	1	
.01	0	0	0	0	0	0	0	0	
0	0	1	0	0	0	0	0	0	
8000	2	10000	0	0	0	0	0	0	
10	4	3	-1.D+5	20	4	3	-1.D+5	0	
1	1	1.D40	0	1.0	0	0	0	0	
0	0	0	0	0	0	0	0	0	
0	0	0	0	0	0	0	0	0	
0	0	0	0	0	0	0	0	0	

FIXED HYDRAULIC HEAD

LAYER	ROW	RDW
2	2	0.1000D+00
		6456
3	0	0
4	0	0
5	0	0
6	0	7488
7	0	0.0000D+00
8	0	0.6000D+03
9	0	0.0000D+00

LENGTH IN FEET OF WATER COLUMN IN WELL BORE

LAYER	RDW	0.0000D+00
2	0	1000D+01
3	2	4000
4	0	1000
5	0	0
6	0	0
7	0	0
8	0	0
9	0	0

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ROW	0 0000D+00	0 0000D+00	0 0000D+00	0 0000D+00
LAYER	2	3	4	5
2	0 1000D-01			
3	2 500 100	3 0 0	4 500 100	5 0 0
4		0 0 0	0 0 0	0 0 0
5		0 0 0	0 0 0	0 0 0

TEMPERATURE DEGREES CENTIGRADE

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BASE ELEVATION

Z DIMENSION OF GRID ELEMENTS

LAYER	ROW	COL
2	0	2000D+03
3	0	2350D+03
4	0	1200D+03
5	0	6000D+02

INITIAL HYDRAULIC HEAD

LAYER	ROW	2	3	4
		0 0000D+00	0 0000D+00	0 0000D+00

LAYER	ROW	2	3	4
		0. 1000D+01	0. 1000D+01	0. 1000D+01

SPECIFIC STORAGE

HYDRAULIC CONDUCTIVITY

LAYER	ROW	2	3	4	5
		0. 5000D+01	0. 1000D+01	0. 1000D+01	0. 1000D+01
		0. 1200D+02	0. 2000D+02	0. 1000D+02	0. 1000D+02
		0. 2000D+02	0. 1000D+01	0. 1000D+01	0. 1000D+01
		0. 1000D-01	0. 0000D+00	0. 0000D+00	0. 0000D+00

LAYERS UNDERLAIN BY A CONFINING BED HAVE 1. OTHER LAYERS 0

2	3	4
0	0	1

X AND Y DIMENSIONS OF GRID ELEMENTS

8000. 0	8000. 0	8000. 0	8000. 0	8000. 0	8000. 0	8000. 0	8000. 0
8000. 0	8000. 0	8000. 0	8000. 0	8000. 0	8000. 0	8000. 0	8000. 0
8000. 0	8000. 0	8000. 0	8000. 0	8000. 0	8000. 0	8000. 0	8000. 0
10000. 0	10000. 0	10000. 0	10000. 0	10000. 0	10000. 0	10000. 0	10000. 0

RECHARGE RATES Q2 (L*L*T/T)

10	4	3	-0. 1000D+06
----	---	---	--------------

20	4	3	-0. 1000D+06
----	---	---	--------------

ROW 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115

LAYER 4	ROW	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115
2	615	615	615	615	615	615	615	615	615	615	615	615	615	615	615	615	615
3	615	615	615	615	615	615	615	615	615	615	615	615	615	615	615	615	615
4	615	615	615	615	615	615	615	615	615	615	615	615	615	615	615	615	615
5	622	622	622	622	622	620	620	620	621	621	620	619	615	621	622	619	618
6	622	623	627	627	629	632	637	637	637	637	638	615	638	648	648	648	648
647	648	649	650	615													

ITMAX 100 0 000D+00 ERR XX10
100 0 000D+00 0 400D+02

PUMPING INTERVAL = 1

RECHARGE RATE YQ (L*L*T)

LAYER	ROW	COL
2	0.	0000D+00
3	0.	0000D+00
4	0.	0000D+00

TOTAL YQ RECHARGE RATE TO MODELED REGION= 0. 0000D+00
 TOTAL Q2 RECHARGE RATE TO MODELED REGION= -0. 2000D+06
 TOTAL RECHARGE RATE TO MODELED REGION= -0. 2000D+06

TIME INTERVAL NUMBER 1 DURATION = 0. 1000D+41 TOTAL ELAPSED TIME = 0. 1000D+41

WATCHING CONVERGENCE

I, J, K, IS THE LOCATION AT WHICH THE MAXIMUM CHANGE IN XX OCCURED.
 MAXIMUM RESIDUAL ERROR = THE MAXIMUM OVER ALL THE GRID ELEMENTS OF THE
 DIFFERENCE BETWEEN THE WATER FLOW RATE INTO AND OUT OF EACH GRID ELEMENT

	XX(I, J, K)	CHANGE IN XX(I, J, K)	MAX RESIDUAL	XX AT I= J= 3	XX AT I= J= 3	XX AT I= J= 3
1	0. 000000D+00	0. 000000D+00	0. 2022506D+10	0. 000000D+00	0. 000000D+00	0. 000000D+00
2	0. 7632667D+03	0. 7632667D+03	0. 4619078D+08	0. 378B751D+03	0. 3702612D+03	0. 36B25BD+03
3	0. 2164925D+03	0. 2164925D+03	0. 3049345D+07	0. 6043369D+03	0. 6001787D+03	0. 5967501D+03
4	0. 3688884D+02	0. 3688884D+02	0. 110719BD+07	0. 6027578D+03	0. 6042555D+03	0. 5997280D+03
5	0. 23297734D+01	0. 23297734D+01	0. 166597D+06	0. 6021166D+03	0. 6043710D+03	0. 6000251D+03
6	0. 8400994D+04	0. 8400994D+04	0. 6019397D+03	0. 6043595D+03	0. 6000190D+03	0. 600016BD+03
7	0. 4948052D+03	0. 4948052D+03	0. 6019073D+03	0. 6043411D+03	0. 600016BD+03	0. 6000167D+03
8	0. 1169914D+03	0. 1169914D+03	0. 6019047D+03	0. 604345D+03	0. 6000167D+03	0. 600016BD+03
9	0. 1903306D+02	0. 1903306D+02	0. 6019049D+03	0. 6043465D+03	0. 600016BD+03	0. 600016BD+03

ITERATIONS USED = 9 MAXIMUM CHANGE IN XX BETWEEN LAST 2 ITERATIONS = 0. 45BD-03
 MAXIMUM RESIDUAL ERROR FOR GRID ELEMENTS NOT HAVING FIXED HYDRAULIC HEAD = 0. 190D+02 TOTAL = -0. 288D+01

WATER FLOW RATE IN NEGATIVE I DIRECTION

LAYER	ROW	3	2	0	000D+00	-0	594D+05	-0	145D+05	-0	327D+04	0	677D+04	0	317D+05	0	669D+04	-0	505D+04	-0	145D+05	-0	100D+05	
	-0	200D+05	-0	628D+04	-0	131D+04	-0	276D+03	-0	611D+02	-0	213D+02	-0	301D+02	-0	693D+02	-0	693D+02	-0	883D+02	-0	883D+02	-0	254D+03
0	742D+03	0	331D+04	0	163D+05	0	818D+05	0	415D+06	0	352D+02	-0	227D+04	0	793D+04	0	393D+04	-0	267D+03	-0	530D+04	-0	254D+04	
1	0	000D+00	-0	131D+05	-0	452D+04	-0	204D+03	-0	336D+02	-0	380D+02	-0	113D+03	-0	402D+03	-0	104D+04	-0	104D+04	-0	113D+04		
2	-0	862D+04	-0	303D+03	-0	825D+05	0	180D+05	0	480D+03	0	317D+04	0	180D+05	0	129D+05	0	302D+04	-0	181D+03	0	467D+04		
3	0	725D+03	0	143D+04	0	517D+04	0	180D+05	0	480D+04	0	366D+04	0	380D+04	0	100D+05	0	302D+04	-0	181D+03	0	467D+04		
4	0	000D+00	-0	272D+05	-0	824D+04	0	699D+02	-0	285D+03	-0	699D+02	-0	777D+02	-0	335D+03	-0	194D+04	-0	109D+05	-0	110D+05		
5	-0	239D+05	-0	769D+04	-0	145D+04	0	103D+04	0	227D+04	0	606D+04	0	112D+05	0	297D+03	0	182D+04	0	416D+03	-0	252D+04		
6	0	000D+00	-0	516D+05	-0	187D+05	-0	408D+04	-0	297D+03	-0	408D+04	-0	334D+02	-0	112D+03	-0	402D+03	-0	104D+04	-0	113D+04		
7	-0	473D+04	-0	171D+03	-0	467D+03	-0	117D+03	-0	324D+02	-0	334D+02	-0	334D+02	-0	112D+03	-0	402D+03	-0	104D+04	-0	113D+04		
8	0	730D+03	0	145D+04	0	525D+04	0	488D+05	0	162D+05	0	308D+04	0	307D+03	0	251D+03	0	380D+02	-0	330D+03	-0	235D+03		
9	-0	666D+03	-0	417D+06	-0	823D+05	-0	162D+05	-0	308D+04	-0	308D+04	-0	308D+04	-0	116D+02	-0	280D+02	-0	687D+02	-0	256D+03		
10	0	753D+03	0	347D+03	-0	126D+03	-0	395D+02	-0	134D+02	-0	134D+02	-0	134D+02	-0	116D+02	-0	280D+02	-0	687D+02	-0	256D+03		
11	0	166D+05	0	336D+04	0	166D+05	0	831D+05	0	422D+06														

WATER FLOW RATE IN NEGATIVE J DIRECTION

LAYER	ROW	3	2	0	000D+00																			
	0	000D+00	0	000D+00	0	000D+00	0	000D+00	0	000D+00	0	000D+00	0	000D+00	0	000D+00	0	000D+00	0	000D+00	0	000D+00	0	000D+00
1	-0	417D+03	-0	120D+05	-0	364D+04	-0	357D+04	-0	646D+04	-0	217D+03	-0	233D+03	-0	204D+05	-0	145D+05	-0	974D+04	-0	328D+03		
2	0	244D+04	-0	364D+03	-0	555D+02	-0	933D+01	-0	451D+01	-0	152D+02	-0	685D+02	-0	281D+03	-0	888D+03	-0	328D+03				
3	-0	339D+03	-0	154D+04	-0	866D+04	-0	494D+03	-0	284D+06	-0	756D+04	0	891D+04	0	146D+05	0	838D+04	0	132D+05				
4	0	156D+03	0	659D+04	0	422D+04	0	658D+04	0	441D+01	-0	298D+02	-0	189D+03	-0	117D+04	-0	748D+04	-0	119D+04				
5	0	344D+04	0	458D+03	0	569D+02	0	538D+02	0	101D+05	-0	336D+05	-0	101D+05	-0	336D+05	-0	101D+05	-0	336D+05	-0	101D+05		
6	-0	291D+03	-0	547D+03	-0	240D+04	-0	147D+05	-0	210D+05	-0	224D+05	-0	126D+05										
7	0	212D+03	0	444D+04	-0	227D+04	-0	693D+04	-0	693D+04	-0	693D+04	-0	693D+04	-0	147D+05	-0	210D+05	-0	224D+05	-0	126D+05		
8	-0	459D+04	-0	760D+03	-0	129D+03	-0	220D+02	-0	726D+00	-0	290D+02	-0	185D+03	-0	117D+04	-0	748D+04	-0	119D+04				
9	0	295D+03	0	564D+03	0	247D+04	0	103D+05	0	344D+03	0	212D+04	-0	348D+04	-0	492D+04	-0	528D+04	-0	388D+04	-0	375D+04		
10	0	282D+06	0	481D+05	0	743D+04	-0	335D+03	-0	212D+04	-0	619D+02	-0	125D+02	-0	378D+00	-0	683D+02	-0	281D+03	-0	329D+03		
11	-0	115D+04	-0	280D+03	-0	619D+02	-0	503D+04	-0	289D+06	-0	683D+02	-0	281D+03										
12	0	344D+03	0	157D+04	0	881D+04																		

WATER FLOW RATE OUT GRID ELEMENT BOTTOM

LAYER	ROW	3	2	-0	172D+06	-0	295D+05	0	345D+04	-0	561D+03	-0	338D+05	0	630D+05	0	294D+05	0	344D+05	0	302D+04	0	310D+05
	-0	187D+05	-0	164D+04	-0	346D+03	-0	730D+02	-0	126D+02	0	848D+01	0	382D+02	0	107D+03	0	194D+03	-0	569D+02			
1	-0	791D+03	-0	406D+04	-0	202D+05	-0	102D+06	-0	265D+07	-0	128D+01	-0	371D+05	-0	448D+05	-0	436D+05	-0	318D+05			
2	-0	477D+05	-0	153D+05	-0	111D+05	-0	128D+05	-0	142D+05	-0	371D+05	-0	448D+05	-0	448D+05	-0	341D+03	-0	156D+04			
3	-0	409D+04	-0	108D+04	-0	261D+03	-0	589D+02	-0	246D+02	-0	726D+05	-0	317D+02	-0	144D+03	-0	341D+03	-0	450D+03			
4	-0	267D+03	-0	168D+04	-0	679D+04	-0	222D+05	0	104D+05	0	225D+05	0	541D+05	0	708D+05	0	141D+05	0	814D+05			
5	0	612D+05	-0	217D+05	-0	203D+04	0	671D+02	0	102D+01	0	778D+02	0	430D+03	0	234D+04	0	130D+05	0	228D+04			
6	-0	277D+05	-0	179D+04	-0	349D+03	-0	907D+04	-0	202D+05	-0	955D+04	-0	140D+05	-0	213D+05	-0	338D+05	-0	190D+05			
7	0	183D+03	-0	835D+03	-0	308D+04	-0	113D+05	-0	984D+04	-0	955D+04	-0	140D+05	-0	144D+03	-0	541D+03	-0	156D+04			
8	-0	231D+04	-0	611D+03	-0	149D+03	-0	332D+02	-0	140D+00	0	329D+02	0	144D+03	0	541D+03	0	156D+04	0	449D+03			
9	-0	273D+03	-0	171D+04	-0	690D+04	-0	250D+05	-0	738D+05	-0	174D+04	-0	144D+04	-0	168D+04	-0	141D+04	-0	118D+04			
10	-0	266D+07	-0	103D+06	-0	208D+05	-0	478D+04	-0	174D+04	-0	748D+00	-0	140D+02	-0	748D+00	-0	106D+03	-0	193D+03			
11	-0	522D+03	-0	178D+03	-0	531D+02	-0	140D+02	-0	748D+00	-0	103D+05	-0	205D+05	-0	270D+07	-0	600D+02					
12	-0	805D+03	-0	413D+04	-0	205D+05	-0	103D+06															

WATER FLOW RATES (ft/s) FROM GRID ELEMENTS											
2	2	0	244D+06	26	2	0	290D+07	2	6	2	0
3	2	4	-0	624D+05	4	2	4	-0	212D+04	5	2
6	2	4	0	646D+05	7	2	4	0	642D+05	10	2
13	2	4	-0	625D+04	14	2	4	-0	132D+04	15	2
18	2	4	0	146D+03	17	2	4	0	408D+03	20	2
23	2	4	-0	155D+03	24	2	4	-0	770D+03	25	2
3	3	4	-0	425D+03	4	3	4	-0	254D+03	5	3
8	3	4	-0	787D+03	9	3	4	-0	777D+03	10	3
13	3	4	-0	411D+04	14	3	4	-0	993D+03	15	3
18	3	4	0	550D+03	17	3	4	0	207D+04	20	3
23	3	4	-0	641D+04	24	3	4	-0	259D+03	25	3
3	4	4	-0	385D+03	4	4	4	-0	743D+04	5	4
8	4	4	0	997D+03	9	4	4	0	131D+06	10	4
13	4	4	-0	681D+04	14	4	4	-0	133D+04	15	4
18	4	4	0	164D+04	19	4	4	0	897D+04	20	4
23	4	4	-0	318D+04	24	4	4	-0	117D+03	25	4
3	5	4	-0	106D+06	4	5	4	-0	356D+03	5	4
8	5	4	-0	355D+03	9	5	4	-0	378D+03	10	5
13	5	4	-0	233D+04	14	5	4	-0	566D+03	15	5
18	5	4	0	551D+03	19	5	4	0	207D+04	20	5
23	5	4	-0	651D+04	24	5	4	-0	263D+05	25	4
3	6	4	-0	390D+06	4	6	4	-0	794D+03	5	6
8	6	4	-0	642D+04	7	6	4	-0	663D+04	10	6
13	6	4	-0	678D+03	14	6	4	-0	201D+03	15	6
18	6	4	0	148D+03	17	6	4	0	407D+03	20	6
23	6	4	-0	158D+05	24	6	4	-0	783D+03	25	6

FLOW RATE UNITS,

TOTAL RECHARGE TO MODIFIED REGION= -0.2000D+06
 TOTAL FLOW FROM FIXED HEAD GRID ELEMENTS INTO MODELED REGION= 0.2001D+06
 TOTAL HEAD DEPENDANT DISCHARGE FROM MODELED REGION 0.0000D+00

		RECHARGE	FLOW FROM HEAD FIXED HEADS	DEPENDANT DISCHARGE	FLOW IN BOTTOM	FLOW IN TOP	FLOW OUT BOTTOM	FLOW OUT TOP
1	2	0.000D+00	0.813D+06	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.813D+06
1	3	0.000D+00	-0.640D+06	0.000D+00	0.813D+06	0.000D+00	0.000D+00	0.173D+06
1	4	0.000D+00	-0.150D+06	0.000D+00	0.173D+06	0.103D+05	0.000D+00	0.335D+05
1	5	0.000D+00	-0.341D+05	0.000D+00	0.335D+05	0.155D+05	0.103D+05	0.457D+04
1	6	0.000D+00	-0.906D+05	0.000D+00	0.457D+04	0.102D+06	0.155D+05	0.415D+03
1	7	0.000D+00	0.578D+05	0.000D+00	0.413D+03	0.437D+05	0.102D+06	0.000D+00
1	8	0.000D+00	0.437D+05	0.000D+00	0.000D+00	0.901D+04	0.437D+05	0.903D+04
1	9	0.000D+00	0.732D+05	0.000D+00	0.903D+04	0.000D+00	0.901D+04	0.732D+05
1	10	-0.100D+06	0.343D+05	0.000D+00	0.732D+05	0.104D+05	0.000D+00	0.179D+05
1	11	0.000D+00	0.110D+06	0.000D+00	0.179D+05	0.000D+00	0.104D+05	0.180D+05
1	12	0.000D+00	-0.921D+05	0.000D+00	0.118D+06	0.000D+00	0.000D+00	0.258D+05
1	13	0.000D+00	-0.202D+05	0.000D+00	0.258D+05	0.000D+00	0.000D+00	0.566D+04
1	14	0.000D+00	0.441D+04	0.000D+00	0.566D+04	0.000D+00	0.000D+00	0.125D+04
1	15	0.000D+00	-0.934D+03	0.000D+00	0.125D+04	0.000D+00	0.000D+00	0.312D+03
1	16	0.000D+00	-0.644D+02	0.000D+00	0.312D+03	0.000D+00	0.000D+00	0.246D+03
1	17	0.000D+00	0.622D+03	0.000D+00	0.246D+03	0.000D+00	0.000D+00	0.867D+03
1	18	0.000D+00	0.304D+04	0.000D+00	0.867D+03	0.000D+00	0.000D+00	0.390D+04
1	19	0.000D+00	0.139D+05	0.000D+00	0.390D+04	0.000D+00	0.000D+00	0.178D+05
1	20	-0.100D+06	0.636D+05	0.000B+00	0.178D+05	0.186D+05	0.000D+00	0.000D+00
1	21	0.000D+00	0.117D+05	0.000D+00	0.000D+00	0.68BD+04	0.186D+05	0.000D+00
1	22	0.000D+00	-0.745D+04	0.000D+00	0.000D+00	0.143D+05	0.68BD+04	0.000D+00
1	23	0.000D+00	-0.474D+05	0.000D+00	0.000D+00	0.617D+05	0.143D+05	0.000D+00
1	24	0.000D+00	-0.219D+06	0.000D+00	0.000D+00	0.281D+06	0.617D+05	0.000D+00
1	25	0.000D+00	-0.100D+07	0.000D+00	0.000D+00	0.128D+07	0.281D+06	0.000D+00
1	26	0.000D+00	0.128D+07	0.000D+00	0.000D+00	0.000D+00	0.128D+07	0.000D+00
2	2	0.000D+00	0.785D+06	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.785D+06
2	3	0.000D+00	-0.958D+06	0.000D+00	0.785D+06	0.251D+06	0.000D+00	0.772D+05
2	4	-0.200D+06	0.519D+06	0.000D+00	0.772D+05	0.104D+06	0.251D+06	0.250D+06
2	5	0.000D+00	-0.105D+07	0.000D+00	0.250D+06	0.936D+06	0.104D+06	0.343D+05
2	6	0.000D+00	0.901D+06	0.000D+00	0.343D+05	0.000D+00	0.936D+06	0.000D+00
3	2	0.000D+00	0.901D+07	0.000D+00	0.000D+00	0.513D+06	0.000D+00	0.952D+07
3	3	-0.200D+06	0.000D+00	0.952D+07	0.106D+07	0.513D+06	0.987D+07	0.000D+00
3	4	0.000D+00	-0.881D+07	0.000D+00	0.987D+07	0.000D+00	0.106D+07	0.000D+00

Heldwell 1c - H (A)

LAYER	ROW	3	2	580 5	599 3	594 4	596 3	601 8	566 4	570 7	572 2	581 1	584 1	581 5	602 3	600 5	600 1	600 0	600 0
		600 0	600 0	600 0	599 9	600 0	600 0	601 2	605 8	629 0	746 7	607 9	602 3	600 5	600 1	600 0	600 0	600 0	
2	625 4	608 5	604 4	603 5	605 4	614 4	616 3	614 9	610 8	607 9	602 3	600 5	600 1	600 0	600 0	600 0	600 0	600 0	
3	600 0	600 0	600 0	599 9	600 0	600 0	601 2	605 8	629 0	746 7	603 6	601 2	600 3	600 1	600 0	600 0	600 0	600 0	
3	606 7	603 2	601 9	601 9	602 5	604 8	605 9	605 8	604 3	604 3	603 6	601 7	607 1	620 7	603 7	600 3	600 1	600 0	600 0
3	606 9	603 2	601 9	601 9	599 8	594 5	599 9	600 1	600 5	601 9	605 9	604 3	603 7	601 2	600 3	600 1	600 0	600 0	600 0
4	570 6	598 4	596 1	587 6	588 6	581 8	569 7	564 7	572 2	567 2	602 7	600 5	600 1	600 0	600 0	600 0	600 0	600 0	600 0
4	600 0	589 9	596 2	599 3	599 3	599 3	599 3	599 3	600 2	600 9	602 6	605 8	609 5	602 7	600 5	600 1	600 0	600 0	600 0
4	613 8	606 1	603 8	604 8	605 9	608 7	612 4	613 3	608 1	609 1	607 5	602 7	600 5	600 1	600 0	600 0	600 0	600 0	600 0
5	600 0	599 9	599 3	596 2	599 3	599 3	599 9	600 2	600 9	602 6	605 8	602 6	602 1	602 0	600 7	600 2	600 0	600 0	600 0
5	622 6	608 0	602 7	601 9	601 4	602 0	602 7	602 0	602 7	602 8	602 1	602 0	602 1	602 0	600 7	600 2	600 0	600 0	600 0
5	600 0	600 0	599 8	599 6	599 6	599 9	600 1	600 5	602 0	607 2	621 0	602 1	602 0	602 1	600 7	600 2	600 0	600 0	600 0
5	622 6	608 0	602 7	601 9	601 4	602 0	602 7	602 0	602 7	602 8	602 1	602 0	602 1	602 0	600 7	600 2	600 0	600 0	600 0
6	600 0	600 0	599 8	599 8	599 6	599 6	599 9	600 1	600 5	602 0	607 2	621 0	600 4	600 3	600 1	600 1	600 0	600 0	600 0
6	747 7	629 3	606 0	601 4	600 5	600 5	600 5	600 0	600 4	600 5	600 4	600 3	603 9	749 2	629 3	600 4	600 3	600 1	600 0
6	600 0	600 0	600 0	599 9	600 0	600 2	601 2	601 2	600 5	600 5	600 5	600 4	600 4	600 3	600 1	600 1	600 0	600 0	600 0
6	747 7	629 3	606 0	601 4	600 5	600 5	600 5	600 0	600 2	601 2	600 5	600 4	600 3	600 2	600 1	600 1	600 0	600 0	600 0

ATTACHMENT D

DEFINITION OF PROGRAM VARIABLES

ALN, XXE The rate of water discharge (L^3/T) from a grid element is given by $Aa(H-H_e)$ when $H>H_e$ and is zero when $H<H_e$. H is the hydraulic head in the grid element and A is the area of the grid element, ($DXI(I) \times DYJ(J)$). $XXE(IJ)$ of data set 5 is H_e , measured relative to the center of the grid element. $ALN(IJ)$ of data set 6 specifies the quantity a .

BBK See FCNT

DDK See FCNT

DTO Duration of the first time interval.

DXI,DYJ $DXI(I)$ is the I direction horizontal dimension of the grid elements in column I. $DYJ(J)$ is the J direction horizontal dimension of the grid elements in row J.

ERR, Iteration terminates when
XX10

$$\max_{(over IJ)} \left| XX^{ICNT} - XX^{(ICNT-1)} \right| +$$

$$\max_{(over IJ)} \left| XX^{(ICNT-1)} - XX^{(ICNT-2)} \right| < ERR,$$
 the maximum residual error

$$\max_{(over IJ)} \left| [M] XX^{ICNT} - YQ \right| < XX10, \text{ or } ICNT \geq ITMAX.$$

FCNT,NT, $K_{xx}(IJ) = (NT(IJ) \times (DDK(K)),$
DDK,BBK $K_{yy}(IJ) = (NT(IJ) \times (BBK(K)),$
 $K_{zz}(IJ) = (NT(IJ),$
 where $K_{xx}(IJ)$, $K_{yy}(IJ)$, and $K_{zz}(IJ)$ denote the x, y, and z components of K , the hydraulic conductivity for grid element IJ. $NT = 0$ is used as a flag to the computer program that the grid element lies outside the modeled region. NT is also used as a dummy variable for reading various data sets.

HMAX SIP parameter β' (Trescott and Larson, 1977).
 I Positional locator along a row, also column number.
 ICNT Iteration counter in the solution procedure.
 ICT In SIP, a repeating counter for iteration parameter number.
 IEVP If IEVP \neq 1, data sets 5 and 6 are not read.
 If IEVP = 1, these data sets are read, and the head dependant discharge option is available.
 IJ Single subscript replacement for I,J,K corresponding to grid element I,J,K.
 IJKM1 Replacement for I,J,K-1, or for I,J,K+1 when the K direction is reversed in SIP.
 IJKP1 Replacement for I,J,K+1, or for I,J,K-1 when the K direction is reversed in SIP.
 IJLB IJ for confining bed grid elements.
 IJM1K Replacement for I,J-1,K, or for I,J+1,K when the J direction is reversed in SIP.
 IJP1K Replacement for I,J+1,K, or for I,J-1,K when the J direction is reversed in SIP.
 ILZ2 If ILZ2 = 0, the elevation of the top of the uppermost grid element layer is printed.
 IKZZ If IKZZ \neq 1, data set 9 is not read. If IKZZ = 1, data set 9, XKZZ = K_{zz} is read. In this case K_{zz} is specified by XKZZ rather than by NT from data set 10.
 IM1JK Single subscript replacement for I-1,J,K
 IP1JK Single subscript replacement for I+1,J,K
 IPDD If IPDD = 1, the drawdown (decrease in hydraulic head H) during a pumping interval is printed.

IPH(K), K=2, NK11 Set IPH(K) = 1 if you want: hydraulic head or
 fresh-water head, flow rate data, or drawdown, for
 layer K. Set IPH(K) = 0 if you do not want these
 quantities for layer K. The layers are numbered K=2
 through K = NK11 = NK10+1.

IPRNT Setting IPRNT = 0 causes IWRT and LFLOW to be set to
 zero, and the printing of hydraulic and fresh-water
 head deleted, for all time intervals except the
 last.

ITMAX Maximum number of iterations allowed.

IWRT
NU1(I), I=1,3 Set IWRT to 1 if you want to watch the convergence
 of fresh-water head $h' - XX$, at the three locations:
 $I = NU1(1)$, $J = NU1(2)$, $K = NU1(3)$ $I = NU2(1)$,
 $J = NU2(2)$, $K = NU2(3)$ and $I = NU3(1)$, $J = NU3(2)$,
 $K = NU3(3)$.

NU3(I), I=1,3

IWRXXX If IWRXXX = 1, fresh-water head $h' = (\text{pressure head } h) + z$ is printed along with the hydraulic head.
 If IWRXXX = 0, it is not printed. If IWRXXX = 2, only h' is printed.

J Positional locator along a column, also row number.

K Layer number.

KOUT The total number of confining beds between layer 2
 and layer K. Only one effective confining bed is
 allowed between any two layers. If there are
 more than two confining beds, they are combined into
 one effective confining bed in accordance with
 equation 5 in the text.

L9 In SIP, L9 is: 1 for J direction reversal, 2 for J
 and K direction reversal, and 3 for K direction
 reversal.

LB LB(IJ) is the vertical dimension of grid element IJ.

LBB Elevation of the base of the lowermost layer, K = 2.

LENGTH Number of iteration parameters in SIP.
LFFLOW Four types of flow rate data are available: 1) the
LFLO(1) flow rate out of each grid element in the negative
LFLO(2) I, J, and K directions, 2) the flow rate out of
LFLO(3) fixed head ($MHD = 0$) grid elements, 3) head depen-
LFLO(4) dant discharge flow rates from grid elements having
such discharge, 4) total flow rate budgets for sets
of grid elements having the same I, the same J, and
the same K. All flow rates are in units of mass
divided by $\rho_0 = 1 \text{ gm/cm}^3$ per unit time (L^3/T). See
the Units section of the text. Set LFFLOW = 1 if you
want any flow rate data, set LFFLOW = 0 if no flow
rate data is desired. Set LFLO(i) = 0 if you do not
want type i flow rate data. For i = 1, set
LFLO(1) = 1, 2, 3, for type 1 flow rate data in the
negative I, J, and K directions respectively. If
LFLO(1) = 4 all directions are given. Set
LFLO(2) = 1 if you want type 2 flow rate data. Set
LFLO(3) = 1 if you want type 3 flow rate data. Set
LFLO(4) = 1, 2, 3, for the budgets of sets of grid
elements having the same I, J, and K respectively.
If LFLO(4) = 4 budgets are given for I, J, and K.
Corresponding to the integers 1, 2, and 3 in the
first column of output the second column gives I, J,
and K respectively.

LLRO If LLRO = 0, read-in values for LRO are used.
If LLRO = 1, read-in values for LRO are replaced by
values for LRO calculated from water pressure,
molality, and temperature, when such calculated
values are available. Calculated values are made
available only for those IJ or IJLB for which the
pressure is specified to be greater than zero.

LRO $LRO(IJ) = (\rho'/\rho_0)$. $\rho = \rho' + \rho_0$ is the water density
for grid element IJ. $LRO(IJLB) = (\rho'/\rho_0)$, where
 $\rho = \rho' + \rho_0$ is the water density for confining bed
grid element IJLB. Values given are truncated after
the fifth decimal place.

LZ2 $LZ2(IJ) = M$, where the integer M divided by 10 is
the elevation of node point IJ located at the center
of grid element IJ.

MAQ1	MAQ1(K) = 0 except when a confining bed lies between layers K-1 and K, in which case MAQ1(K) = 1.
MHD	When MHD(IJ) ≠ 0 the hydraulic head for grid element IJ is fixed at the value specified. When MHD(IJ) = 0, the head for grid element IJ is not fixed. There are NK10 layers of MHD values. Values given are truncated after the first decimal place.
NI10	Number of columns in the modeled area.
NJ10	Number of rows in the modeled area.
NK10	Number of layers in the modeled area.
NK4	Number of intervening confining beds.
NI	See Q2.
NINT	Number of time intervals desired in the current pumping interval.
NJ	See Q2.
NK	See Q2.
NNN	Total number of grid elements plus 2: [(NI10) X (NJ10) X (NK10)] + 2.
NPINT	Number of pumping intervals.
NSKP1, NSKP2, RELX1, RELX2, COEF	See the Successive over-relaxation section of the text for these.
NT	See FCNT.
NU1	See IWRT.
NU2	See IWRT.
NU3	See IWRT.

NWEL	Number of grid elements with pumping wells.
Q2,NI, NJ,NK,YQ	YQ(IJ) + Q2(NI,NJ,NK) is the recharge rate (L^3/T) into the grid element located at I=NI, J=NJ, and K=NK.
SRZ	SRZ is the maximum residual error $\max_{(over IJ)} [M]XXICNT-YQ $ with units (L^3/T). For each grid element in the modeled region that does not have fixed hydraulic head, the computer program seeks to satisfy the conservation of mass, i.e. mass in equals mass out. The maximum residual error is the maximum over these grid elements, of the difference between mass in and mass out.
SUMRZ	SUMRZ is the sum, over all the grid elements in the modeled region not having fixed hydraulic head, of the members of residual vector $[M]XICNT-YQ$. In the computer output, SUMRZ is printed following the value printed for maximum residual error SRZ, and is denoted by "total." Both SRZ and SUMRZ are a measure of the accuracy of the solution found.
SV	SV specifies specific storage S_s .
TFAC	The ratio of the duration of a time interval divided by the duration of the preceding time interval.
TOT	If TGT = 0, DTO is calculated such that the duration of the pumping, the sum of the NINT time intervals, is TOT.
WMAX	In SIP, (XYFC) X (XY) is used for $(1 - \alpha_{max})$ (Weinstein and others, 1969) when WMAX = 0. When WMAX = 0, $(1 - \alpha_{max}) = WMAX$ is used.
XX	Fresh-water head $h' = (\text{pressure head } h) + z$.
XXS	The value of XX for the previous time step.
XY	See equation (8) in text.
XYFC	See WMAX.
YQ	See Q2.

ATTACHMENT E

PROGRAM LISTING

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IMPLICIT REAL*8 (A-H, O-Z) MAN00010
COMMON WS, HMAX, RELX1, RELX2, COEF, ERR, XX10, DELT, ER5, SRZ, SUMRZ MAN00020
1, XX, DT, VV, E2, F2, G2, YQ, NIJ10, NI11, NJ11, NK11, NNN, NSKP1 MAN00030
2, NSKP2, ITMAX, ICNT, IEVP, IWR1, NW1, NW2, NW3, N320, NUM4 MAN00040
3, L9, LENGTH, NK1115, IT01, IT15, ICRO, DDK, BBK MAN00050
4, NT, DD, BB, ZZ, XXE, XXS, ALN, SV MAN00060
5, NI10, NJ10, NK10, NI12, NJ12, NK12, LB, MHD MAN00070
REAL*4 DD(377), BB(377), ZZ(377), SV(377), YQ(377), XXS(377) MAN00080
1, G2(300), DDK(50), BBK(50), NT(502) MAN00090
2, DXI(250), DYJ(250), ALN(377), XXE(377), XXSTR(377), YQ1(377) MAN00100
3, XKZZ(377) MAN00110
INTEGER*2 LRD(502), IPH(50), LFLO(4), I7(5), J7(5), K7(5) MAN00120
1, NI(300), NJ(300), NK(300), MAG1(50), NU1(3), NU2(3), NU3(3) MAN00130
DIMENSION DT(377), E2(377), F2(377), G2(377), VV(377), XX(377) MAN00140
1, WS(10), MHD(377), LZ2(377), LB(502), LBB(127) MAN00150
2, AOC(4), BOC(4), COC(4), DOC(4) MAN00160
3, SUMF(3, 250), SUNF(3, 250), SG2(3, 250), SG2(3, 250), SYG(3, 250) MAN00170
4, SVV(3, 250) MAN00180
PI=3. 1415926 MAN00190
DATA AOC/12. 43, 4. 19, -1. 405, . 268333/, BOC/3. 07, -1. 297, . 592, MAN00200
1-. 256833/, COC/-, 02, . 118, -. 107, . 0713333/, DOC/1. 000117, -. 0030861, -. 0029377, MAN00210
3. 0002689/ MAN00220
DO 10 I=1, 50 MAN00230
10 MAG1(I)=0 MAN00240
C READ IN GROUP I DATA MAN00250
READ(5, 2000) ISOR MAN00260
IF(ISOR.EQ.0) READ(5, 2000) L9, LENGTH, HMAX, XYFC, WMAX, ITMAX, ERR, XX10 MAN00280
IF(ISOR.EQ.1) READ(5, 2000) NSKP1, NSKP2, RELX1, RELX2, COEF, ITMAX, ERR, XX10 MAN00290
IF(ISOR.GE.2) READ(5, 2000) ITMAX, ERR, XX10 MAN00310
READ(5, 2020) NI10, NJ10, NK10, NK4 MAN00320
READ(5, 2003) IWRT, (NU1(I), I=1, 3), (NU2(I), I=1, 3), (NU3(I), I=1, 3) MAN00330
READ(5, 2020) NPINT, IPDD, LLRO, IWRTXX, IPRNT, ILZ2, IEVP, IKZZ MAN00340
READ(5, 2020) LFLOW, (LFLO(I), I=1, 4) MAN00350
NK11=NK10+1 MAN00360
READ(5, 2003) (IPH(K), K=2, NK11) MAN00370
NUM4=ISOR-1 MAN00380
NI11=NI10+1 MAN00390
NJ11=NJ10+1 MAN00400
NK15=NK11+NK4 MAN00410
NI12=NI10+2 MAN00420
NJ12=NJ10+2 MAN00430
NK12=NK10+2 MAN00440
NIJ10=NI10*NJ10 MAN00450
NIJK10=NIJ10*NK10 MAN00460
NNN=NIJK10+2 MAN00470
N315=NIJ10+1 MAN00480
N320=NIJK10+1 MAN00490
N325=NIJ10*(NK10+NK4)+1 MAN00500
NW1=NU1(1)+NI10*(NU1(2)-2)+NIJ10*(NU1(3)-2) MAN00510
NW2=NU2(1)+NI10*(NU2(2)-2)+NIJ10*(NU2(3)-2) MAN00520
NW3=NU3(1)+NI10*(NU3(2)-2)+NIJ10*(NU3(3)-2) MAN00530
C READ IN AND PRINT ARRAYS MHD, LRD, LBB, LB, XXE, ALN, XX, SV, FCNT, MAN00540
DDK, BBK, NT, MAG1, DXI, DYJ, G2, NI, NJ, NK MAN00550
C GROUP II MAN00560
WRITE(6, 5000) MAN00570
NK1115=NK11 MAN00580
IT15=1 MAN00590
ICRO=0 MAN00600

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      CALL RDWRT          MAN00610
      DO 20 IJ=2,N320    MAN00620
20     MHD(IJ)=NT(IJ)*10 MAN00630
         IF(LLR0.EQ.0) GO TO 80 MAN00640
C   DETERMINE WATER DENSITIES FROM PRESSURE, MOLALITY, AND TEMPERATURE
      C624=.0298912D0      MAN00650
      WRITE(6,4997)          MAN00660
      NK1115=NK15            MAN00670
      CALL RDWRT            MAN00680
      DO 30 IJ=2,N325      MAN00690
30     LB(IJ)=NT(IJ)       MAN00700
      WRITE(6,4998)          MAN00710
      CALL RDWRT            MAN00720
      DO 40 IJ=2,N325      MAN00730
40     LRO(IJ)=NT(IJ)*100 MAN00740
      WRITE(6,4999)          MAN00750
      CALL RDWRT            MAN00760
      DO 70 IJ=2,N325      MAN00770
50     XM=LRO(IJ)/100. DO MAN00780
         X=NT(IJ)/25. DO MAN00790
         X3=X*(X-1)        MAN00800
         X4=X3*(X-2)        MAN00810
         AO=AOC(1)+AOC(2)*X+AOC(3)*X3+AOC(4)*X4 MAN00820
         BO=BOC(1)+BOC(2)*X+BOC(3)*X3+BOC(4)*X4 MAN00830
         CO=COC(1)+COC(2)*X+COC(3)*X3+COC(4)*X4 MAN00840
         DO=DOC(1)+DOC(2)*X+DOC(3)*X3+DOC(4)*X4 MAN00850
         XM32=XM*DSQRT(XM) MAN00860
         DE=1000+58.448D0*XM MAN00870
         DG=DE/(1000/DO+AO*X+BO*XM32+CO*XM*XM) MAN00880
         AMB=(-(X-1)*.75+.25)*XM+((X-1)*3.5+2) MAN00890
         RHO=1                MAN00900
         RB4=1.0D-5*(.84*(X-1)+3.75) MAN00910
         DO 60 L3=1,3          MAN00920
         P=PO*RHO              MAN00930
         DLT=AMB*1.0D-5*P      MAN00940
         IF(P.GT.100) DLT=AMB*1.0D-3+RB4*(P-100) MAN00950
60     RHO=DG+DLT          MAN00960
         LB(IJ)=(RHO-1)*1.0D5 MAN00970
70     CONTINUE             MAN00980
C   WATER DENSITIES ARE NOW DETERMINED
80     CONTINUE             MAN00990
         WRITE(6,5002)          MAN01000
         NK1115=NK15            MAN01010
         ICRO=LLR0              MAN01020
         CALL RDWRT            MAN01030
         DO 90 IJ=2,N325      MAN01040
90     LRO(IJ)=NT(IJ)*1.0D5 MAN01050
         WRITE(6,5003)          MAN01060
         NK1115=2                MAN01070
         ICRO=0                  MAN01080
         CALL RDWRT            MAN01090
         DO 100 IJ=2,N315      MAN01100
100    LBB(IJ)=NT(IJ)       MAN01110
         WRITE(6,5004)          MAN01120
         NK1115=NK15            MAN01130
         CALL RDWRT            MAN01140
         DO 110 IJ=2,N325      MAN01150

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110 LB(IJ)=NT(IJ) MAN01220
LB(1)=1 MAN01230
IF(IEVP, NE, 1) GO TO 140 MAN01240
WRITE(6,8000) MAN01250
NK1115=NK11 MAN01260
CALL RDWRT MAN01270
DO 120 IJ=2,N320 MAN01280
120 XXE(IJ)=NT(IJ)*10 MAN01290
WRITE(6,8001) MAN01300
CALL RDWRT MAN01310
DO 130 IJ=2,N320 MAN01320
130 ALN(IJ)=NT(IJ) MAN01330
140 CONTINUE MAN01340
        WRITE(6,5052) MAN01350
NK1115=NK11 MAN01360
CALL RDWRT MAN01370
DO 150 IJ=2,N320 MAN01380
150 XX(IJ)=NT(IJ)*10 MAN01390
XX(1)=0 MAN01400
XX(NNN)=0 MAN01410
WRITE(6,5054) MAN01420
CALL RDWRT MAN01430
DO 160 IJ=2,N320 MAN01440
160 SV(IJ)=NT(IJ) MAN01450
IF(IKZZ, EQ, 0) GO TO 167 MAN01460
WRITE(6,5060) MAN01470
CALL RDWRT MAN01480
DO 166 IJ=2,N320 MAN01490
166 XKZZ(IJ)=NT(IJ) MAN01500
167 CONTINUE MAN01510
        WRITE(6,5005) MAN01520
NK1115=NK15 MAN01530
IT15=2 MAN01540
CALL RDWRT MAN01550
C ***** REMOVE PINCHED OUT NODES WHEN APPROPRIATE *****
DO 165 I=2,NI11 MAN01570
DO 165 J=2,NJ11 MAN01580
IJIJ=I+NI10*(J-2) MAN01590
DO 165 K=2,NK11 MAN01600
IJ=IJIJ+NIJ10*(K-2) MAN01610
IF(LB(IJ), NE, 0) GO TO 165 MAN01620
IF((K, EQ, 2), OR, (K, EQ, NK11)) GO TO 164 MAN01630
IT5=0 MAN01640
KM1=K-1 MAN01650
DO 161 K1=2,KM1 MAN01660
IJ1=IJIJ+NIJ10*(K1-2) MAN01670
161 IF(LB(IJ1), NE, 0) IT5=IT5+1 MAN01680
IT6=0 MAN01690
KP1=K+1 MAN01700
DO 162 K2=KP1,NK11 MAN01710
IJ2=IJIJ+NIJ10*(K2-2) MAN01720
162 IF(LB(IJ2), NE, 0) IT6=IT6+1 MAN01730
IF((IT5*IT6), GT, 0) GO TO 165 MAN01740
164 NT(IJ)=0 MAN01750
165 CONTINUE MAN01760
C ***** DONE *****
C GROUP III
IF(NK4, EQ, 0) GO TO 170 MAN01770
READ(5,2003) (MAQ1(K),K=2,NK11) MAN01780
WRITE(6,5010) MAN01800
WRITE(6,4002) (K,MAQ1(K),K=2,NK11) MAN01810
MAN01820

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170  CONTINUE                                           MAN01830
      READ(5,2000) FDXI,FDYJ,MDXI1,MDYJ1,MD2          MAN01840
      IF(MDXI1.EQ.1) READ(5,2000) (DXI(I),I=2,NI11)   MAN01850
      IF(MDYJ1.EQ.1) READ(5,2000) (DYJ(J),J=2,NJ11)   MAN01860
      IF(MDXI1.EQ.1) GO TO 190                         MAN01870
      DO 180 I=2,NI11                                  MAN01880
180  DXI(I)=FDXI                                     MAN01890
190  IF(MDYJ1.EQ.1) GO TO 210                         MAN01900
      DO 200 J=2,NJ11                                  MAN01910
200  DYJ(J)=FDYJ                                     MAN01920
210  IF(MD2.NE.0) GO TO 220                          MAN01930
      WRITE(6,5001)
      WRITE(6,3010) (DXI(I),I=2,NI11)                MAN01940
      WRITE(6,3010) (DYJ(I),I=2,NJ11)                MAN01950
220  CONTINUE                                           MAN01960
      DXI(1)=1                                         MAN01970
      DYJ(1)=1                                         MAN01980
      DXI(NI12)=1                                      MAN01990
      DYJ(NJ12)=1                                      MAN02000
      WRITE(6,5055)
      READ(5,2020) NWEL                            MAN02010
      NWEL=NWEL+1                                     MAN02020
      READ(5,2007) (NI(N),NJ(N),NK(N),G2(N),N=2,NWEL) MAN02030
      WRITE(6,3007) (NI(N),NJ(N),NK(N),G2(N),N=2,NWEL) MAN02040
C  READ IN AND PRINTING OF ARRAYS NOW COMPLETE        MAN02050
C  INITIALIZE VARIOUS ARRAYS TO ZERO                 MAN02060
      DO 230 IJ=1,NNN                                MAN02070
      DD(IJ)=0                                         MAN02080
      BB(IJ)=0                                         MAN02090
      ZZ(IJ)=0                                         MAN02100
      DT(IJ)=0                                         MAN02110
      E2(IJ)=0                                         MAN02120
      F2(IJ)=0                                         MAN02130
      G2(IJ)=0                                         MAN02140
      YQ(IJ)=0                                         MAN02150
      VV(IJ)=0                                         MAN02160
230  VV(IJ)=0                                         MAN02170
C  DETERMINE LZ2 AND INITIAL OR FIXED XX. PUT RECHARGE RATES G2 INTO YQ. MAN02190
C  IF IEVP=1, MODIFY XXE AND ALN.                   MAN02200
      SUMG2=0                                         MAN02210
      DO 231 IDBZ=1,3                               MAN02220
      DO 231 N=1,250                                MAN02230
231  SQ2(IDBZ,N)=0                                 MAN02240
      KOUT=0                                         MAN02250
      DO 280 K=2,NK11                                MAN02260
      KOUT=KOUT+MAG1(K)                            MAN02270
      DO 280 J=2,NJ11                                MAN02280
      DO 280 I=2,NI11                                MAN02290
      DXY=DXI(I)*DYJ(J)                            MAN02300
      IJF=I+NI10*(J-2)                            MAN02310
      IJ=IJF+NIJ10*(K-2)                            MAN02320
      LBIJ=LBB(IJ)                                 MAN02330
      KLB=NK11+KOUT                                MAN02340
      IJLB=IJF+NIJ10*(KLB-2)                        MAN02350
      DTIJ=LRO(IJ)*1.0D-5                           MAN02360
      SV(IJ)=SV(IJ)*DXY*LBIJ                         MAN02370
C  DETERMINE LZ2                                     MAN02380
      IJKM1=IJ-NIJ10                                MAN02390
      IF(K.EQ.2) GO TO 240                           MAN02400
      LZ2(IJ)=LZ2(IJKM1)+5*(LBIJ+LB(IJKM1))+10*MAG1(K)*LB(IJLB) MAN02410
      GO TO 250                                     MAN02420
240  LZ2(IJ)=LBIJ*5+10*(LBB(IJ)+MAG1(K)*LB(IJLB)) MAN02430

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250  CONTINUE
C DETERMINE INITIAL OR FIXED XX
  XXMHD=XX(IJ)
  MHDIJ=MHD(IJ)
  IF(MHDIJ.NE.0) XXMHD=MHDIJ
  LZ2IJ=LZ2(IJ)
  X=((XXMHD-LZ2IJ)*(DTIJ+1)+LZ2IJ)*.1D0
  IF(NT(IJ).EQ.0.0) X=0.0
  XX(IJ)=X
  XXSTR(IJ)=X
  XXS(IJ)=X
  IX=0
  IF(MHDIJ.NE.0) IX=1
  IF(NT(IJ).EQ.0.0) IX=2
  MHD(IJ)=IX
C IF IEVP=1, MODIFY XXE AND ALN
  IF(IEVP.NE.1) GO TO 260
  XXE(IJ)=(XXE(IJ)*(DTIJ+1)+LZ2IJ)*.1D0
  ALN(IJ)=ALN(IJ)*DXY/(DTIJ+1)
260  CONTINUE
C PUT PUMPING RATES Q2 INTO YQ
  YQIJ=0
  DO 270 N=2,NWEL
  IF(.NOT.((I.EQ.NI(N)).AND.((J.EQ.NJ(N)).AND.(K.EQ.NK(N)))))1GO TO 270
  YQIJ=Q2(N)
270  CONTINUE
  YQ(IJ)=YQIJ
  SQ2(1,I)=SQ2(1,I)+YQIJ
  SQ2(2,J)=SQ2(2,J)+YQIJ
  SQ2(3,K)=SQ2(3,K)+YQIJ
  SUMQ2=SUMQ2+YQIJ
280  CONTINUE
C LZ2, XX, AND YQ=Q2 ARE NOW DETERMINED.
C IF ILZ2=0, CALCULATE AND PRINT THE ELEVATION OF THE TOP OF THE
C UPPERMOST GRID ELEMENT LAYER.
  IF(ILZ2.NE.0) GO TO 310
  WRITE(6,8002)
  WRITE(6,6000)
  WRITE(6,4002) NK11
  DO 300 J=2,NJ11
  DO 290 I=2,NI11
  IJ=I+NI10*(J-2)+NIJ10*(NK11-2)
290  LBB(I)=LZ2(IJ)*.1D0+LB(IJ)*.5D0+.1
300  WRITE(6,3004) J,(LBB(I),I=2,NI11)
310  CONTINUE
C DETERMINE THE QUANTITIES DD, BB, AND ZZ
  KOUT=0
  DO 320 K=2,NK11
  MAG1K=MAG1(K)
  KOUT=KOUT+MAG1K
  KLB=NK11+KOUT
  DO 320 J=2,NJ11
  DO 320 I=2,NI11
  IJF=I+NI10*(J-2)
  IJ=IJF+NIJ10*(K-2)
  IJLB=IJF+NIJ10*(KLB-2)
  IM1JK=IJ-1
  IJM1K=IJ-NI10
  IJKM1=IJ-NIJ10
  IF(IJM1K.LT.1) IJM1K=1

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IF(IJKM1.LT.1) IJKM1=1 MAN03050
DXII=DXI(I) MAN03060
DYJJ=DYJ(J) MAN03070
DXIM1=DXI(I-1) MAN03080
DYJM1=DYJ(J-1) MAN03090
BO=LB(IJ) MAN03100
LBIM1=LB(IM1JK) MAN03110
LBIJM=LB(IJM1K) MAN03120
BDD=(LBIM1*DXII+BO*DXIM1)/(DXII+DXIM1) MAN03130
BBB=(LBIJM*DYJJ+BO*DYM1)/(DYJJ+DYM1) MAN03140
WDD=LBIM1*BO MAN03150
WBB=LBIJM*BO MAN03160
IF(WDD.EQ.0.0D00) BDD=0 MAN03170
IF(WBB.EQ.0.0) BBB=0 MAN03180
B4=LB(IJKM1) MAN03190
CO=NT(IJ) MAN03200
CD=NT(IM1JK) MAN03210
CB=NT(IJM1K) MAN03220
CZ=NT(IJKM1) MAN03230
CO1=CO MAN03240
CZ1=CZ MAN03250
IF(IKZZ.EQ.0) GO TO 319 MAN03260
CO1=XKZZ(IJ) MAN03270
CZ1=XKZZ(IJKM1) MAN03280
319 CONTINUE MAN03290
IF(I.EQ.2) CD=0 MAN03300
IF(J.EQ.2) CB=0 MAN03310
IF(K.EQ.2) CZ=0 MAN03320
IF(K.EQ.2) CZ1=0 MAN03330
DD(IJ)=-DYJJ*2*DDK(K)*BDD*CD*CO/(DXII*CD+DXIM1*CO+1.D-30) MAN03340
BB(IJ)=-DXII*2*BBK(K)*BBB*CB*CO/(DYJJ*CB+DYM1*CO+1.D-30) MAN03350
CC=NT(IJLB) MAN03360
IF(MAG1K.EQ.0) CC=1 MAN03370
ALP=.5D0*(BO*CC*CZ1+B4*CC*CO1)+MAG1K*LB(IJLB)*CO1*CZ1 MAN03380
CCC=CO1*CC*CZ1 MAN03390
ZZIJ=1.D0 MAN03400
IF(ALP.NE.0.0) ZZIJ=CCC/ALP MAN03410
IF(CCC.EQ.0.0) ZZIJ=0 MAN03420
ZZ(IJ)=-DXI(I)*DYJ(J)*ZZIJ MAN03430
320 CONTINUE MAN03440
C THE QUANTITIES DD, BB, AND ZZ, ARE NOW DETERMINED. MAN03450
C ADD VARIABLE DENSITY CONTRIBUTIONS TO YQ, PUT INTO YQ1. MAN03460
SUX=0 MAN03470
NCNT=0 MAN03480
NI2=NI10*NI10 MAN03490
NJ2=NJ10*NJ10 MAN03500
NK2=NK10*NK10 MAN03510
KOUT=0 MAN03520
DO 350 K=2,NK11 MAN03530
KOUT=KOUT+MAG1(K) MAN03540
KLB=NK11+KOUT MAN03550
DO 350 J=2,NJ11 MAN03560
DO 340 I=2,NI11 MAN03570
IJF=I+NI10*(J-2) MAN03580
IJ=IJF+NIJ10*(K-2) MAN03590
IF(MHD(IJ).GE.1) GO TO 340 MAN03600
NCNT=NCNT+1 MAN03610
IJLB=IJF+NIJ10*(KLB-2) MAN03620
IJLB1=IJLB+NIJ10 MAN03630
IP1JK=IJ+1 MAN03640
IM1JK=IJ-1 MAN03650

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IJP1K=IJ+NI10          MAN03660
IJM1K=IJ-NI10          MAN03670
IJKP1=IJ+NIJ10          MAN03680
IJKM1=IJ-NIJ10          MAN03690
IF(IJM1K, LT, 1) IJM1K=1 MAN03700
IF(IJKM1, LT, 1) IJKM1=1 MAN03710
IF(IJP1K, GT, NNN) IJP1K=NNN MAN03720
IF(IJKP1, GT, NNN) IJKP1=NNN MAN03730
IF(IJLB1, GT, N325) IJLB1=N325 MAN03740
DD1=DD(IJ)              MAN03750
DD2=DD(IP1JK)           MAN03760
BB1=BB(IJ)              MAN03770
BB2=BB(IJP1K)           MAN03780
ZZ1=ZZ(IJ)              MAN03790
ZZ2=ZZ(IJKP1)           MAN03800
IF((WMAX, NE, 0, 0), OR, (ISOR, NE, 0, 0)) GO TO 330
D1=(BB1+BB2+ZZ1+ZZ2)/(DD1+DD2-1, D-30) MAN03820
B1=(DD1+DD2+ZZ1+ZZ2)/(BB1+BB2-1, D-30) MAN03830
Z1=(DD1+DD2+BB1+BB2)/(ZZ1+ZZ2-1, D-30) MAN03840
IF(D1, GT, 1, D+9) D1=0 MAN03850
IF(B1, GT, 1, D+9) B1=0 MAN03860
IF(Z1, GT, 1, D+9) Z1=0 MAN03870
D1=1/(NI2*(1+D1))      MAN03880
B1=1/(NJ2*(1+B1))      MAN03890
Z1=1/(NK2*(1+Z1))      MAN03900
X=D1                     MAN03910
IF(B1, LT, X) X=B1       MAN03920
IF(Z1, LT, X) X=Z1       MAN03930
SUX=SUX+X                MAN03940
330  CONTINUE             MAN03950
B0=LB(IJ)                MAN03960
B4=LB(IJKM1)             MAN03970
B5=LB(IJKP1)             MAN03980
BT0=LRO(IJ)*1, D-5       MAN03990
BT4=LRO(IJKM1)*1, D-5    MAN04000
BT5=LRO(IJKP1)*1, D-5    MAN04010
BTDD=LRO(IM1JK)*1, D-5   MAN04020
BTFF=LRO(IP1JK)*1, D-5   MAN04030
BTBB=LRO(IJM1K)*1, D-5   MAN04040
BTHH=LRO(IJP1K)*1, D-5   MAN04050
X=(.5D0*(BT0*B0+BT4*B4)+MAG1(K)*(LRO(IJLB)*1, 0D-5)*LB(IJLB))*ZZ1
1-(.5D0*(BT0*B0+BT5*B5)+MAG1(K+1)*(LRO(IJLB1)*1, 0D-5)*LB(IJLB1)) MAN04070
2*ZZ2+YG(IJ)             MAN04080
LZ0=LZ2(IJ)               MAN04090
DXII=DXI(I)               MAN04100
DXIM1=DXI(I-1)            MAN04110
DXIP1=DXI(I+1)            MAN04120
DYJJ=DYJ(J)               MAN04130
DYJM1=DYJ(J-1)            MAN04140
DYJP1=DYJ(J+1)            MAN04150
BTOX=BT0*DXII             MAN04160
BTOY=BT0*DYJJ             MAN04170
YQ1(IJ)=X-(((BTDD*DXIM1+BTOX)/(DXIM1+DXII))*DD1*(LZ2(IM1JK)-LZ0)
1           +((BTFF*DXIP1+BTOX)/(DXIP1+DXII))*DD2*(LZ2(IP1JK)-LZ0) MAN04190
2           +((BTBB*DYJM1+BTOY)/(DYJM1+DYJJ))*BB1*(LZ2(IJM1K)-LZ0) MAN04200
3           +((BTHH*DYJP1+BTOY)/(DYJP1+DYJJ))*BB2*(LZ2(IJP1K)-LZ0) MAN04210
4)*.1D0                  MAN04220
340  CONTINUE             MAN04230
350  CONTINUE             MAN04240
C  YQ1 NOW DETERMINED     MAN04250
IF(ISOR, NE, 0) GO TO 370

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XY= 5DO*PI*PI*SUX/NCNT          MAN04270
C XY IS NOW DETERMINED          MAN04280
XY=XYFC*XY                      MAN04290
IF(WMAX.NE.0.0) XY=WMAX          MAN04300
C DETERMINE ITERATION PARAMETERS WS(I)      MAN04310
DO 360 I=1,LENGTH               MAN04320
360  WS(I)=1-XY**((I-1.)/(LENGTH-1))        MAN04330
      WRITE(6,5056)                  MAN04340
      WRITE(6,1003) L9, ITMAX, LENGTH, HMAX, XYFC, ERR, WMAX, XX10
      WRITE(6,5006)
      WRITE(6,3555) (WS(I), I=1,LENGTH)       MAN04350
      GO TO 390                      MAN04360
370  IF(ISOR.NE.1) GO TO 380          MAN04370
      WRITE(6,5057)                  MAN04380
      WRITE(6,1003) NSKP1, NSKP2, ITMAX, RELX1, RELX2, COEF, ERR, XX10
      GO TO 390                      MAN04390
380  WRITE(6,5058) NUM4             MAN04400
      WRITE(6,4501) ITMAX, ERR, XX10       MAN04410
390  CONTINUE
      DO 640 IPINT=1,NPINT           MAN04420
      WRITE(6,8003) IPINT            MAN04430
      READ(5,2000) NINT, DTO, TFAC, TOT
      IF(TOT.NE.0.0) DTO=TOT*(TFAC-1)/(TFAC**NINT-1)    MAN04440
C READ IN AND PRINT YQ FOR THIS PUMPING INTERVAL
      WRITE(6,5053)                  MAN04450
      NK1115=NK11                   MAN04460
      IT15=1                        MAN04470
      ICRO=0                        MAN04480
      CALL RDWRD
      SUMYQ=SUMQ2                   MAN04490
      DO 391 IDBZ=1,3              MAN04500
      DO 391 N=1,250                MAN04510
391  SYQ(IDBZ,N)=SQ2(IDBZ,N)       MAN04520
      DO 400 K=2,NK11                MAN04530
      DO 400 J=2,NJ11                MAN04540
      DO 400 I=2,NI11                MAN04550
      IJ=I+NI10*(J-2)+NIJ10*(K-2)  MAN04560
      YQIJ=NT(IJ)                  MAN04570
      YQ(IJ)=YQIJ+YQ1(IJ)          MAN04580
      SYQ(1,I)=SYQ(1,I)+YQIJ      MAN04590
      SYQ(2,J)=SYQ(2,J)+YQIJ      MAN04600
      SYQ(3,K)=SYQ(3,K)+YQIJ      MAN04610
      SUMYQ=SUMYQ+YQIJ            MAN04620
      400  CONTINUE
      X=SUMYQ-SUMQ2                MAN04630
      WRITE(6,9011) X, SUMQ2, SUMYQ   MAN04640
C ADD YQ1 TO YQ, PUT INTO YQ.
      TOTIME=0                      MAN04650
      DO 600 INT=1,NINT             MAN04660
      DELT=DTO*(TFAC***(INT-1))    MAN04670
      TOTIME=DELT+TOTIME           MAN04680
      WRITE(6,7000) INT, DELT, TOTIME
      IO1=1
      IF((IPRNT.EQ.0).AND.(INT.LT.NINT)) IO1=0
      IWR1=IWR1*IO1
      LFL01=LFL01*IO1
      IF(IWR1.NE.1) GO TO 420
      WRITE(6,5007)
      WRITE(6,5072) NU1(1),NU2(1),NU3(1)
      WRITE(6,5073) NU1(2),NU2(2),NU3(2)
      WRITE(6,5074) NU1(3),NU2(3),NU3(3)

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420  CONTINUE
C BEGIN SIP, SOR, OR PCG ITERATIONS.
  IF(ISOR.EQ.0) CALL SIP
  IF(ISOR.EQ.1) CALL SOR
  IF(ISOR.GE.2) CALL PCG
  WRITE(6,5075) ICNT, ERS, SRZ, SUMRZ
MAN04880
MAN04890
MAN04900
MAN04910
MAN04920
MAN04930
MAN04940
MAN04950
MAN04960
MAN04970
MAN04980
MAN04990
MAN05000
MAN05010
MAN05020
MAN05030
MAN05040
MAN05050
MAN05060
MAN05070
MAN05080
MAN05090
MAN05100
MAN05110
MAN05120
MAN05130
MAN05140
MAN05150
MAN05160
MAN05170
MAN05180
MAN05190
MAN05200
MAN05210
MAN05220
MAN05230
MAN05240
MAN05250
MAN05260
MAN05270
MAN05280
MAN05290
MAN05300
MAN05310
MAN05320
MAN05330
MAN05340
MAN05350
MAN05360
MAN05370
MAN05380
MAN05390
MAN05400
MAN05410
MAN05420
MAN05430
MAN05440
MAN05450
MAN05460
MAN05470
MAN05480

C SAVE XX, FOR USE DURING THE NEXT TIME STEP, IN XXS
  DO 430 IJ=2,N320
  XXS(IJ)=XX(IJ)
  IF(LFL01.EQ.0) GO TO 560
C DETERMINE WATER FLOW RATES
  DO 440 IJ=1,NNN
  G2(IJ)=0
  DO 510 IDBZ=1,3
  DO 450 N=1,250
  SUNF(IDBZ,N)=0
  450 SUMF(IDBZ,N)=0
  IRITE=0
  L1=LFL0(1)
  IF((L1.EQ.IDBZ).OR.(L1.EQ.4)) IRITE=1
  IF(IRITE.NE.1) GO TO 460
  IF(IDBZ.EQ.1) WRITE(6,5101)
  IF(IDBZ.EQ.2) WRITE(6,5102)
  IF(IDBZ.EQ.3) WRITE(6,5103)
  WRITE(6,6000)
  460 CONTINUE
  KOUT=0
  DO 510 K=2,NK11
  KOUT=KOUT+MAQ1(K)
  KLB=NK11+KOUT
  IF((IRITE.EQ.1).AND.(IPH(K).EQ.1)) WRITE(6,4002) K
  DO 510 J=2,NJ11
  IJMI=NI10*(J-2)+NIJ10*(K-2)
  IJLBMI=NI10*(J-2)+NIJ10*(KLB-2)
  DO 500 I=2,NI11
  IJ=IJMI+I
  IJLB=IJLBMI+I
  XX0=XX(IJ)
  BTO=LRO(IJ)*1.0D-5
  LZ0=LZ2(IJ)
  IF(IDBZ.NE.1) GO TO 470
  DBZ=DD(IJ)
  IF(I.EQ.2) GO TO 490
  IM1JK=IJ-1
  XI=XX(IM1JK)
  BTDD=LRO(IM1JK)*1.0D-5
  DXII=DXI(I)
  DXIM1=DXI(I-1)
  BTOX=BTO*DXII
  FLOW=((BTDD*DXIM1+BTOX)/(DXIM1+DXII))*(LZ2(IM1JK)-LZ0)*.1D0
  GO TO 490
  470 IF(IDBZ.NE.2) GO TO 480
  DBZ=BB(IJ)
  IF(J.EQ.2) GO TO 490
  IJM1K=IJ-NI10
  XI=XX(IJM1K)
  BTBB=LRO(IJM1K)*1.0D-5
  DYJJ=DYJ(J)
  DYJM1=DYJ(J-1)
  BTOY=BTO*DYJJ
  FLOW=((BTBB*DYJM1+BTOY)/(DYJM1+DYJJ))*(LZ2(IJM1K)-LZ0)*.1D0

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GO TO 490                                MAN05490
480  DBZ=ZZ(IJ)                            MAN05500
     IF(K.EQ.2) GO TO 490                  MAN05510
     IJKM1=IJ-NIJ10                         MAN05520
     XXI=XX(IJKM1)                          MAN05530
     BO=LB(IJ)                             MAN05540
     B4=LB(IJKM1)                          MAN05550
     BT4=LRO(IJKM1)*1.OD-5                 MAN05560
     FLOW=-(.5D0*(BT0*BO+BT4*B4)+MAQ1(K)*(LRO(IJLB)*1.OD-5)*LB(IJLB))  MAN05570
490  X=DBZ*(XXI-XX0+FLOW)                  MAN05580
     DT(I)=X                               MAN05590
     IJK=I                                MAN05600
     IF(IDBZ.EQ.2) IJK=J                  MAN05610
     IF(IDBZ.EQ.3) IJK=K                  MAN05620
     IF(X.GT.0) SUMF(IDBZ,IJK)=SUMF(IDBZ,IJK)+X  MAN05630
     IF(X.LT.0) SUNF(IDBZ,IJK)=SUNF(IDBZ,IJK)-X  MAN05640
     G2(IJ)=G2(IJ)+X                      MAN05650
     IM=1                                 MAN05660
     IF(IDBZ.EQ.2) IM=NI10                MAN05670
     IF(IDBZ.EQ.3) IM=NIJ10                MAN05680
     IJM=IJ-IM                           MAN05690
     IF(IJM.LT.1) IJM=1                  MAN05700
     G2(IJM)=G2(IJM)-X                  MAN05710
500  CONTINUE                                MAN05720
510  IF((IRITE.EQ.1).AND.(IPH(K).EQ.1)) WRITE(6,4500) J,(DT(I),I=2
      1,NI11)
     IF(LFLO(2).EQ.1) WRITE(6,B010)
     I5=0
     SUMG2=0
     DO 549 IDBZ=1,3
     DO 549 N=1,250
549  SG2(IDBZ,N)=0
     DO 550 K=2,NK11
     DO 550 J=2,NJ11
     DO 550 I=2,NI11
     IJ=I+NI10*(J-2)+NIJ10*(K-2)
     IF(MHD(IJ).NE.1) GO TO 540
     G2IJ=G2(IJ)
     I5=I5+1
     DT(I5)=G2IJ
     I7(I5)=I
     J7(I5)=J
     K7(I5)=K
     SG2(1,I)=SG2(1,I)+G2IJ
     SG2(2,J)=SG2(2,J)+G2IJ
     SG2(3,K)=SG2(3,K)+G2IJ
     SUMG2=SUMG2+G2IJ
540  IF(I5.NE.5) GO TO 550
     I5=0
     IF(LFLO(2).EQ.1) WRITE(6,3560) (I7(L),J7(L),K7(L),DT(L),L=1,5)  MAN05980
550  CONTINUE                                MAN05990
     IF((LFLO(2).EQ.1).AND.(I5.GE.1))
1WRITE(6,3560) (I7(L),J7(L),K7(L),DT(L),L=1,I5)  MAN06000
     IF(LFLO(3).EQ.1) WRITE(6,9010)
     I5=0
     SUMVV=0
     DO 649 IDBZ=1,3
     DO 649 N=1,250
649  SVV(IDBZ,N)=0
     DO 650 K=2,NK11
     DO 650 J=2,NJ11

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DO 650 I=2,NI11
IJ=I+NI10*(J-2)+NIJ10*(K-2) MAN06100
X=XX(IJ)-XXE(IJ) MAN06110
VVIJ=X*ALN(IJ) MAN06120
IF(. NOT. ((IEVP.EQ.1).AND.(VVIJ.GT.0))) GO TO 641 MAN06130
I5=I5+1 MAN06140
DT(I5)=VVIJ MAN06150
I7(I5)=I MAN06160
J7(I5)=J MAN06170
K7(I5)=K MAN06180
SVV(1,I)=SVV(1,I)+VVIJ MAN06200
SVV(2,J)=SVV(2,J)+VVIJ MAN06210
SVV(3,K)=SVV(3,K)+VVIJ MAN06220
SUMVV=SUMVV+VVIJ MAN06230
641 IF(I5.NE.5) GO TO 650 MAN06240
I5=0 MAN06250
IF(LFL0(3).EQ.1) WRITE(6,3560) (I7(L),J7(L),K7(L),DT(L),L=1,5) MAN06260
650 CONTINUE MAN06270
IF((LFL0(3).EQ.1).AND.(I5.GE.1)) MAN06280
1WRITE(6,3560) (I7(L),J7(L),K7(L),DT(L),L=1,I5)
WRITE(6,8011) SUMYQ,SUMQ2,SUMVV
IF(LFL0(4).EQ.0) GO TO 530 MAN06310
WRITE(6,7001)
IDBZ1=LFL0(4) MAN06320
IDBZ3=IDBZ1 MAN06330
MAN06340
IF(IDBZ1.GE.4) IDBZ1=1 MAN06350
IF(IDBZ3.GE.4) IDBZ3=3 MAN06360
DO 520 IDBZ=IDBZ1, IDBZ3
N20=NI11 MAN06370
IF(IDBZ.EQ.2) N20=NJ11 MAN06380
IF(IDBZ.EQ.3) N20=NK11 MAN06390
DO 519 N=2,N20
NP1=N+1
519 WRITE(6,8012) IDBZ,N,SYG(IDBZ,N),S02(IDBZ,N),SVV(IDBZ,N) MAN06430
1,SUNF(IDBZ,N),SUMF(IDBZ,NP1),SUMF(IDBZ,N),SUNF(IDBZ,NP1)
520 CONTINUE MAN06440
530 CONTINUE MAN06450
540 IF(I01.EQ.0) GO TO 590 MAN06460
WRITE(6,5008)
WRITE(6,6000)
C DETERMINE HYDRAULIC HEAD FROM XX = H PRIME = (PRESSURE HEAD H) + Z MAN06500
DO 580 K=2,NK11
IF(IPH(K).NE.1) GO TO 580 MAN06510
WRITE(6,4002) K MAN06520
MAN06530
DO 580 J=2,NJ11
IJMI=NI10*(J-2)+NIJ10*(K-2) MAN06540
DO 570 I=2,NI11
IJ=IJMI+I
XZ210=LZ2(IJ)*.1DO
DTI=(1/(LR0(IJ)*1.0D-5+1))*(XX(IJ)-XZ210)+XZ210 MAN06550
IF(MHD(IJ).EQ.2) DTI=0 MAN06560
570 DT(I)=DTI
IF(IWRXXX.LE.1) WRITE(6,1001) J,(DT(I),I=2,NI11) MAN06610
IF(IWRXXX.GE.1) WRITE(6,1001) J,(XX(IJMI+I),I=2,NI11)
580 CONTINUE MAN06620
590 CONTINUE MAN06630
600 CONTINUE MAN06640
MAN06650
C IF IPDD=1, DETERMINE DRAWDOWNS FOR THIS PUMPING INTERVAL
IF(IPDD.NE.1) GO TO 630 MAN06660
WRITE(6,8004)
WRITE(6,6000)

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DO 620 K=2,NK11 MAN06710
IF(IPH(K).NE.1) GO TO 620 MAN06720
WRITE(6,4002) K MAN06730
DO 620 J=2,NJ11 MAN06740
IJMI=NI10*(J-2)+NIJ10*(K-2) MAN06750
DO 610 I=2,NI11 MAN06760
IJ=IJMI+I MAN06770
DT(I)=(XXSTR(IJ)-XX(IJ))/(LRO(IJ)*1.D-5+1) MAN06780
610 XXSTR(IJ)=XX(IJ) MAN06790
WRITE(6,1001) J,(DT(I),I=2,NI11) MAN06800
620 CONTINUE MAN06810
630 CONTINUE MAN06820
640 CONTINUE MAN06830
1001 FORMAT(I12,15F8.1/(12X,15F8.1)) MAN06840
1003 FORMAT(3I10,6D18.4) MAN06850
1004 FORMAT(12X,15F8.1) MAN06860
2000 FORMAT(8G10.0) MAN06870
2003 FORMAT(20I4) MAN06880
2007 FORMAT(4(3I3,D11.3)) MAN06890
2020 FORMAT(8I10) MAN06900
3004 FORMAT(I12,20I6/(12X,20I6)) MAN06910
3007 FORMAT(4(I12,2I4,D11.3)) MAN06920
3010 FORMAT(' ',12F10.1) MAN06930
3555 FORMAT(BD15.7) MAN06940
3560 FORMAT(' ',5(3I4,D12.3)) MAN06950
4002 FORMAT(I6,I12) MAN06960
4500 FORMAT(I12,10D12.3/(12X,10D12.3)) MAN06970
4501 FORMAT(I12,9D12.3) MAN06980
4997 FORMAT('1',44X,'LENGTH IN FEET OF WATER COLUMN IN WELL BORE') MAN06990
4998 FORMAT('1',64X,'MOLALITY') MAN07000
4999 FORMAT('1',53X,'TEMPERATURE DEGREES CENTIGRADE') MAN07010
5000 FORMAT('1',52X,'FIXED HYDRAULIC HEAD ') MAN07020
5001 FORMAT('1',49X,'X AND Y DIMENSIONS OF GRID ELEMENTS') MAN07030
5002 FORMAT('1',41X,'(DENSITY OF WATER RHO, IN GRAMS PER CUBIC CENTIMETER)') MAN07040
1ER)-1.0') MAN07050
5003 FORMAT('1',59X,'BASE ELEVATION') MAN07060
5004 FORMAT('1',52X,'Z DIMENSION OF GRID ELEMENTS') MAN07070
5005 FORMAT('1',54X,'HYDRAULIC CONDUCTIVITY') MAN07080
5052 FORMAT('1',56X,'INITIAL HYDRAULIC HEAD') MAN07090
5053 FORMAT('0',53X,'RECHARGE RATE QG (L*L*L/T)') MAN07100
5054 FORMAT('1',57X,'SPECIFIC STORAGE') MAN07110
5055 FORMAT('1',53X,'RECHARGE RATES Q2 (L*L*L/T)') MAN07120
5056 FORMAT('1',51X,'SIP CONVERGENCE PARAMETERS CHOSEN'// 18X,'L9',5X,'ITMAX',4X,'LENGTH',14X,'HMAX',14X,'XYFC', 215X,'ERR',14X,'WMAX',14X,'XX10') MAN07130
5057 FORMAT('1',51X,'SOR CONVERGENCE PARAMETERS CHOSEN'// 15X,'NSKP1',5X,'NSKP2',5X,'ITMAX',13X,'RELX1',13X,'RELX2', 214X,'COEF',15X,'ERR',14X,'XX10') MAN07140
5058 FORMAT('1',51X,'PCG(,I1,) CONVERGENCE PARAMETERS CHOSEN'// 17X,'ITMAX',9X,'ERR',8X,'XX10') MAN07150
5060 FORMAT('1',50X,'Z COMPONENT OF HYDRAULIC CONDUCTIVITY') MAN07160
5006 FORMAT('0',58X,'SIP COEFFICIENTS') MAN07170
5007 FORMAT('0',56X,'WATCHING CONVERGENCE'//25X,'I,J,K, IS THE LOCATION'// 1 AT WHICH THE MAXIMUM CHANGE IN XX OCCURED.'//25X,'MAXIMUM RESIDUAL') MAN07180
2 ERROR = THE MAXIMUM OVER ALL THE GRID ELEMENTS OF THE'//25X,'DIFFERENCE BETWEEN THE WATER FLOW RATE INTO AND OUT OF EACH GRID ELEMENT'// 4NT.') MAN07190
5074 FORMAT(7X,' I      J      K',9X,'XX(I,J,K)',9X,'XX(I,J,K)',13X,'ERROR'// 1,3(12X,'K=',I4)) MAN07200
5072 FORMAT('0',72X,3(6X,'XX AT I=',I4)) MAN07250
5073 FORMAT(46X,'CHANGE IN',6X,'MAX RESIDUAL',3(12X,'J=',I4)) MAN07260
                                         MAN07270
                                         MAN07280
                                         MAN07290
                                         MAN07300
                                         MAN07310

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5075 FORMAT('O', 'ITERATIONS USED =', I3, MAN07320
1'      MAXIMUM CHANGE IN XX BETWEEN LAST 2 ITERATIONS =', D11. 3/ MAN07330
2'      MAXIMUM RESIDUAL ERROR FOR GRID ELEMENTS NOT HAVING FIXED HYDRAUMAN07340
3'LIC HEAD =', D11. 3, '      TOTAL =', D11. 3) MAN07350
5008 FORMAT('1', 59X, 'HYDRAULIC HEAD') MAN07360
5010 FORMAT('1', 37X, MAN07370
1'LAYERS UNDERLAIN BY A CONFINING BED HAVE 1, OTHER LAYERS 0') MAN07380
5101 FORMAT('1', 46X, 'WATER FLOW RATE IN NEGATIVE I DIRECTION') MAN07390
5102 FORMAT('1', 46X, 'WATER FLOW RATE IN NEGATIVE J DIRECTION') MAN07400
5103 FORMAT('1', 46X, 'WATER FLOW RATE OUT GRID ELEMENT BOTTOM') MAN07410
6000 FORMAT('O', 'LAYER ROW') MAN07420
7000 FORMAT('1', 'TIME INTERVAL NUMBER', I3, '      DURATION =', D11. 4, ' MAN07430
1      TOTAL ELAPSED TIME =', D11. 4) MAN07440
7001 FORMAT('O', 31X, 'FLOW FROM', 1X, 'HEAD DEPENDANT', 8X, 'FLOW IN' MAN07450
1, 8X, 'FLOW IN', 7X, 'FLOW OUT', 7X, 'FLOW OUT' MAN07460
2/18X, 'RECHARGE', 4X, 'FIXED HEADS', 6X, 'DISCHARGE', 9X, 'BOTTOM' MAN07470
3, 12X, 'TOP', 9X, 'BOTTOM', 12X, 'TOP')//') MAN07480
8000 FORMAT('1', 25X, 'THE ELEVATION OF THE HYDRAULIC HEAD (MEASURED RELAMAN07490
1TIVE TO THE CENTER OF')//26X, 'THE GRID ELEMENT) AT WHICH HEAD DEPENDMAN07500
2ANT DISCHARGE BEGINS') MAN07510
8001 FORMAT('1', 20X, '(RATE OF LOSS (L/T))/(((HYDRAULIC HEAD)-(ELEVATIONMAN07520
1 AT WHICH DISCHARGE BEGINS)) (L)))') MAN07530
8002 FORMAT('1', 36X, 'THE ELEVATION OF THE TOP OF THE UPPERMOST GRID ELMAN07540
1ELEMENT LAYER') MAN07550
8003 FORMAT('1', 'PUMPING INTERVAL=', I5) MAN07560
8004 FORMAT('1', 45X, 'DRAWDOWN DURING THIS PUMPING INTERVAL') MAN07570
8010 FORMAT('1', 30X, 'WATER FLOW RATES OUT OF FIXED HEAD GRID ELEMENTS') MAN07580
8011 FORMAT('1', 50X, 'FLOW RATE BUDGETS')//5X MAN07590
1, 'TOTAL RECHARGE TO MODELED REGION=', D13. 4/5X MAN07600
2, 'TOTAL FLOW FROM FIXED HEAD GRID ELEMENTS INTO MODELED REGION=' MAN07610
3, D13. 4/5X, 'TOTAL HEAD DEPENDANT DISCHARGE FROM MODELED REGION' MAN07620
4, D13. 4) MAN07630
8012 FORMAT(' ', 2I5, 7D15. 3) MAN07640
9010 FORMAT('1', 50X, 'HEAD DEPENDANT DISCHARGE RATES') MAN07650
9011 FORMAT('O', 4X, 'TOTAL YQ RECHARGE RATE TO MODELED REGION=', D13. 4/ MAN07660
15X, 'TOTAL Q2 RECHARGE RATE TO MODELED REGION=', D13. 4/ MAN07670
25X, 'TOTAL RECHARGE RATE TO MODELED REGION=', D13. 4) MAN07680
STOP MAN07690
END MAN07700
SUBROUTINE RDWRT RDW00010
IMPLICIT REAL*8 (A-H, O-Z) RDW00020
COMMON WS, HMAX, RELX1, RELX2, COEF, ERR, XX10, DELT, ER5, SRZ, SUMRZ RDW00030
1, XX, DT, VV, E2, F2, Q2, YQ, NIJ10, NI11, NJ11, NK11, NNN, NSKP1 RDW00040
2, NSKP2, ITMAX, ICNT, IEVP, IWR1, NW1, NW2, NW3, N320, NUM4 RDW00050
3, L9, LENGTH, NK1115, IT01, IT15, ICRO, DDK, BBK RDW00060
4, NT, DD, BB, ZZ, XXE, XXS, ALN, SV RDW00070
5, NI10, NJ10, NK10, NI12, NJ12, NK12, LB, MHD RDW00080
REAL*4 DD(377), BB(377), ZZ(377), XXE(377), XXS(377), ALN(377), RDW00090
1SV(377), YQ(377), DDK(50), BBK(50), NT(502) RDW00100
DIMENSION XX(377), DT(377), VV(377), E2(377), F2(377) RDW00110
1, WS(10), MHD(377), Q2(377), LB(502) RDW00120
2, IF1(10), IF2(10), NNT(250) RDW00130
READ(5, 1000) II, (IF1(I1), I1=1, 9), (IF2(I2), I2=1, 10) RDW00140
WRITE(6, 6000) RDW00150
DO 161 K=2, NK1115 RDW00160
READ(5, 2000) FCNTK, IVAR, IPRN, DDK(K), BBK(K) RDW00170
IF(IPRN.EQ.1) GO TO 158 RDW00180
IF(IT15.EQ.1) WRITE(6, 1002) K, FCNTK RDW00190
IF(IT15.EQ.2) WRITE(6, 1002) K, FCNTK, DDK(K), BBK(K) RDW00200
158 DO 161 J=2, NJ11 RDW00210
IJMI=NI10*(J-2)+NIJ10*(K-2) RDW00220

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IF(IVAR.EQ.1) READ(5, IF1) (NT(IJMI+I), I=2, NI11) RDW00230
DO 159 I=2, NI11 RDW00240
IJ=IJMI+I RDW00250
X=1 RDW00260
IF(IVAR.EQ.1) X=NT(IJ) RDW00270
159 NT(IJ)=X RDW00280
IF(ICRO.EQ.0) GO TO 1605 RDW00290
DO 13 I=2, NI11 RDW00300
IJ=IJMI+I RDW00310
LBIJ=LBIJ(IJ) RDW00320
IF(LBIJ.NE.-30000) NT(IJ)=LBIJ*1.D-5/FCNTK RDW00330
13 CONTINUE RDW00340
1605 IF(.NOT.((IPRN.EQ.0).AND.(IVAR.EQ.1))) GO TO 41 RDW00350
DO 40 I=2, NI11 RDW00360
40 NNT(I)=NT(IJMI+I) RDW00370
IF(II.EQ.0) WRITE(6, IF2) J, (NNT(I), I=2, NI11) RDW00380
IF(II.EQ.1) WRITE(6, IF2) J, (NT(IJMI+I), I=2, NI11) RDW00390
41 CONTINUE RDW00400
DO 42 I=2, NI11 RDW00410
IJ=IJMI+I RDW00420
42 NT(IJ)=NT(IJ)*FCNTK RDW00430
161 CONTINUE RDW00440
1000 FORMAT(I4, 19A4) RDW00450
1002 FORMAT(I6, 6D18.4) RDW00460
2000 FORMAT(BG10.0) RDW00470
4000 FORMAT(I6, I10) RDW00480
6000 FORMAT('0', 'LAYER      ROW')
RETURN RDW00490
END RDW00500
SUBROUTINE SOR SOR00010
IMPLICIT REAL*8 (A-H, O-Z) SOR00020
COMMON WS, HMAX, RELX1, RELX2, COEF, ERR, XX10, DELT, ER5, SRZ, SUMRZ SOR00030
1, XX, DT, VV, E2, F2, G2, YG, NIJ10, NI11, NJ11, NK11, NNN, NSKP1 SOR00040
2, NSKP2, ITMAX, ICNT, IEVP, IWR1, NW1, NW2, NW3, N320, NUM4 SOR00050
3, L9, LENGTH, NK1115, IT01, IT15, ICRO, DDK, BBK SOR00060
4, NT, DD, BB, ZZ, XXE, XXS, ALN, SV SOR00070
5, NI10, NJ10, NK10, NI12, NJ12, NK12, LB, MHD SOR00080
REAL*4 DD(377), BB(377), ZZ(377), XXE(377), XXS(377), ALN(377), SOR00090
15V(377), YG(377), DDK(50), BBK(50), NT(502) SOR00100
DIMENSION XX(377), DT(377), VV(377), E2(377), F2(377) SOR00110
1, WS(10), MHD(377), G2(377), LB(502) SOR00120
ICNT=0 SOR00130
ER5S=100 SOR00140
DO 200 ITER=1, 100 SOR00150
ICNT=ICNT+1 SOR00160
IF(ICNT.EQ. ITMAX) GO TO 202 SOR00170
RELX3=1 SOR00180
IF(ICNT.GE. 6) RELX3=RELX2 SOR00190
IF(ICNT.GE. 21) RELX3=RELX2*(1-(ICNT-20)*COEF) SOR00200
IF(RELX3.LT..2) RELX3=.2 SOR00210
DO 101 I3=1, 3 SOR00220
IF((I3.EQ. NSKP1).OR. (I3.EQ. NSKP2)) GO TO 101 SOR00230
GO TO (1, 2, 3), I3 SOR00240
1 MI11=NI11 SOR00250
MJ11=NJ11 SOR00260
MK11=NK11 SOR00270
GO TO 4 SOR00280
2 MI11=NJ11 SOR00290
MJ11=NK11 SOR00300
MK11=NI11 SOR00310
GO TO 4 SOR00320

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3   MI11=NK11          SOR00330
    MJ11=NI11          SOR00340
    MK11=NJ11          SOR00350
4   CONTINUE          SOR00360
    SUMRZ=0            SOR00370
    SRZ=0              SOR00380
    DO 100 K1=2,MK11   SOR00390
    DO 100 J1=2,MJ11   SOR00400
    GO TO (8,9,10),I3  SOR00410
8   J=J1              SOR00420
    K=K1              SOR00430
    GO TO 11           SOR00440
9   K=J1              SOR00450
    I=K1              SOR00460
    GO TO 11           SOR00470
10  I=J1              SOR00480
    J=K1              SOR00490
11  CONTINUE          SOR00500
    MI12=MI11+1        SOR00510
    DO 12 IJ=1,MI12   SOR00520
    DT(IJ)=0            SOR00530
12  UV(IJ)=0          SOR00540
    DO 90 I1=2,MI11   SOR00550
    IF(I3.EQ.1) I=I1   SOR00560
    IF(I3.EQ.2) J=I1   SOR00570
    IF(I3.EQ.3) K=I1   SOR00580
    IJ=I+NI10*(J-2)+NIJ10*(K-2)  SOR00590
    IF(MHD(IJ).GE.1) GO TO 90  SOR00600
    IJM1K=IJ-NI10        SOR00610
    IJP1K=IJ+NI10        SOR00620
    IJKM1=IJ-NIJ10       SOR00630
    IJKP1=IJ+NIJ10       SOR00640
    IF(IJM1K.LT.1) IJM1K=1  SOR00650
    IF(IJP1K.GT.NNN) IJP1K=NNN  SOR00660
    IF(IJKM1.LT.1) IJKM1=1  SOR00670
    IF(IJKP1.GT.NNN) IJKP1=NNN  SOR00680
    XXIJ=XX(IJ)          SOR00690
    D=DD(IJ)             SOR00700
    B=BB(IJ)             SOR00710
    Z=ZZ(IJ)             SOR00720
    F=DD(IJ+1)           SOR00730
    H=BB(IJP1K)          SOR00740
    S=ZZ(IJKP1)          SOR00750
    SVDT=SV(IJ)/DELT    SOR00760
    E=-(D+F+B+H+Z+S)+SVDT  SOR00770
    LEV=0                SOR00780
    IF((IEVP.EQ.1).AND.(XXIJ.GT.XXE(IJ))) LEV=1  SOR00790
    IF(LEV.NE.1) GO TO 44  SOR00800
    ALNI=ALN(IJ)          SOR00810
    E=E+ALNI             SOR00820
44  CONTINUE          SOR00830
    DF=D*XX(IJ-1)+F*XX(IJ+1)  SOR00840
    BH=B*XX(IJM1K)+H*XX(IJP1K)  SOR00850
    ZS=Z*XX(IJKM1)+S*XX(IJKP1)  SOR00860
    AFLW=DF+BH+ZS          SOR00870
    GO TO (18,19,20),I3  SOR00880
18  DI=D              SOR00890
    FI=F              SOR00900
    QP=BH+ZS          SOR00910
    GO TO 21           SOR00920
19  DI=B              SOR00930

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      FI=H                      SOR00940
      QP=DF+ZS                  SOR00950
      GO TO 21                  SOR00960
20     DI=2                      SOR00970
      FI=S                      SOR00980
      QP=DF+BH                  SOR00990
21     CONTINUE
      AI=DI                     SOR01000
      BI=E-AI*DT(I1-1)          SOR01010
      DT(I1)=FI/BI              SOR01020
      YQIJ=YQ(IJ)+SVDT*XXS(IJ) SOR01030
      IF(LEV.EQ.1) YQIJ=YQIJ+ALNI*XXE(IJ) SOR01040
      VV(I1)=(YQIJ-QP-AI*VV(I1-1))/BI SOR01050
      RZ=YQIJ-AFLW-XXIJ*E       SOR01060
      SUMRZ=SUMRZ+RZ            SOR01070
      DSR=DABS(RZ)              SOR01080
      IF(DSR.GT.SRZ) SRZ=DSR    SOR01090
90     CONTINUE
      DO 95 I1R=2,MI11           SOR01100
      I1=MI11+2-I1R             SOR01110
      IF(I3.EQ.1) I=I1           SOR01120
      IF(I3.EQ.2) J=I1           SOR01130
      IF(I3.EQ.3) K=I1           SOR01140
      IJ=I+NI10*(J-2)+NIJ10*(K-2) SOR01150
      IF(MHD(IJ).GE.1) GO TO 95 SOR01160
      F2(IJ)=XX(IJ)              SOR01170
      IP=IJ+1                   SOR01180
      IF(I3.EQ.2) IP=IJ+NI10    SOR01190
      IF(I3.EQ.3) IP=IJ+NIJ10   SOR01200
      IF(IP.GT.NNN) IP=NNN      SOR01210
      X=VV(I1)-DT(I1)*XX(IP)   SOR01220
      XX(IJ)=X                   SOR01230
      SOR01240
      SOR01250
      SOR01260
95     CONTINUE
      DO 96 I1=2,MI11           SOR01270
      IF(I3.EQ.1) I=I1           SOR01280
      IF(I3.EQ.2) J=I1           SOR01290
      IF(I3.EQ.3) K=I1           SOR01300
      IJ=I+NI10*(J-2)+NIJ10*(K-2) SOR01310
      IF(MHD(IJ).GE.1) GO TO 96 SOR01320
      XX(IJ)=RELX1*XX(IJ)+(1-RELX1)*F2(IJ) SOR01330
96     CONTINUE
100    CONTINUE
101    CONTINUE
      ER5=0                      SOR01340
      DO 150 K=2,NK11            SOR01350
      DO 150 J=2,NJ11            SOR01360
      DO 150 I=2,NI11            SOR01370
      IJ=I+NI10*(J-2)+NIJ10*(K-2) SOR01380
      E2IJ=E2(IJ)                SOR01390
      X=RELX3*XX(IJ)+(1-RELX3)*E2IJ SOR01400
      CHG=DABS(X-E2IJ)           SOR01410
      IF(CHG.LT.ER5) GO TO 111   SOR01420
      IMX=I                      SOR01430
      JMX=J                      SOR01440
      KMX=K                      SOR01450
      XXPMX=X                     SOR01460
      ER5=CHG                     SOR01470
      SOR01480
      SOR01490
      SOR01500
      SOR01510
      SOR01520
      SOR01530
      SOR01540
111    CONTINUE
      XX(IJ)=X
150    E2(IJ)=X
      IF(IWR1.EQ.1) WRITE(6,1000) ICNT,IMX,JMX,KMX,XXPMX,ER5,SRZ,

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1XX(NW1), XX(NW2), XX(NW3) SOR01550
IF((ER5+ER5S). LT. ERR) GO TO 202 SOR01560
IF(SRZ. LT. XX10) GO TO 202 SOR01570
ER5S=ER5 SOR01580
200 CONTINUE SOR01590
202 CONTINUE SOR01600
1000 FORMAT(' ', I3, 3I5, 6D18. 7) SOR01610
      RETURN SOR01620
      END SOR01630
      SUBROUTINE PCQ PCG00010
      IMPLICIT REAL*8 (A-H, O-Z) PCG00020
      COMMON WS, HMAX, RELX1, RELX2, COEF, ERR, XX10, DELT, ER5, SRZ, SUMRZ PCG00030
1, XX, DT, VV, E2, F2, G2, YQ, NIJ10, NI11, NJ11, NNN, NSKP1 PCG00040
2, NSKP2, ITMAX, ICNT, IEVP, IWR1, NW1, NW2, NW3, N320, NUM4 PCG00050
3, L9, LENGTH, NK1115, IT01, IT15, ICRO, DDK, BBK PCG00060
4, NT, DD, BB, ZZ, XXE, XXS, ALN, SV PCG00070
5, NI10, NJ10, NK10, NI12, NJ12, NK12, LB, MHD PCG00080
      REAL*4 DD(377), BB(377), ZZ(377), XXE(377), XXS(377), ALN(377), PCG00090
1SV(377), YQ(377), DDK(50), BBK(50), NT(502) PCG00100
2, D2S(377), E22(377) PCG00110
      DIMENSION XX(377), DT(377), VV(377), E2(377), F2(377) PCG00120
1, WS(10), MHD(377), G2(377), LB(502) PCG00130
C IF YOU WANT TO SAVE STORAGE, REMOVE D2S AND E22 FROM THE DIMENSION PCG00140
C STATEMENT AND CARDS "76 CONTINUE" THROUGH "56 CONTINUE", AND "86 PCG00150
C CONTINUE" THROUGH "662 CONTINUE". THIS REMOVES PCQ METHODS SIPCG PCG00160
C AND SFPCQ. PCG00170
      IG31=0 PCG00180
      IF(NUM4. EQ. 3) IG31=1 PCG00190
      DO 1 IJ=1, NNN PCG00200
      D2S(IJ)=0 PCG00210
      E22(IJ)=0 PCG00220
      DT(IJ)=0 PCG00230
      E2(IJ)=0 PCG00240
      F2(IJ)=0 PCG00250
      G2(IJ)=0 PCG00260
1      VV(IJ)=0 PCG00270
      DO 16 IJ=2, N320 PCG00280
      E2(IJ)=XX(IJ) PCG00290
      IF(MHD(IJ). GE. 1) GO TO 16 PCG00300
      DELY=(SV(IJ)/DELT)*XXS(IJ) PCG00310
      IF((IEVP. EQ. 1). AND. (XX(IJ). GT. XXE(IJ))) DELY=DELY+ALN(IJ)*XXE(IJ) PCG00320
      VV(IJ)=YQ(IJ)+DELY PCG00330
16    CONTINUE PCG00340
      DO 2 IJ=2, N320 PCG00350
      DELE=0 PCG00360
      IF(MHD(IJ). GE. 1) GO TO 19 PCG00370
      DELE=SV(IJ)/DELT PCG00380
      IF((IEVP. EQ. 1). AND. (XX(IJ). GT. XXE(IJ))) DELE=DELE+ALN(IJ) PCG00390
      XXS(IJ)=DELE PCG00400
19    CONTINUE PCG00410
2      CONTINUE PCG00420
      GO TO (71, 71, 71, 80, 74, 74, 76, 76), NUM4 PCG00430
71    CONTINUE PCG00440
      DO 51 IJ=2, N320 PCG00450
      IF(. NOT. (MHD(IJ). GE. 1)) GO TO 777 PCG00460
      Y1=0 PCG00470
      Z1=0 PCG00480
      GO TO 51 PCG00490
777   CONTINUE PCG00500
      IJP1K=IJ+NI10 PCG00510
      IJM1K=IJ-NI10 PCG00520
      IJKP1=IJ+NIJ10

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IJKM1=IJ-NIJ10          PCG00530
IF(IJP1K GT NNN) IJP1K=NNN
IF(IJKP1 GT NNN) IJKP1=NNN
IF(IJM1K LT 1) IJM1K=1
IF(IJKM1 LT 1) IJKM1=1
X=DD(IJ)
Y=BB(IJ)
Z=ZZ(IJ)
Y1Z1=0
XP=X
F2X=F2(IJ-1)
F2Y=F2(IJM1K)
F2Z=F2(IJKM1)
IF(NUM4 EQ 1) GO TO 20
JP1=IJM1K+1
KP1=IJKM1+1
IJMMN=IJ-(NIJ10-NI10)
IF(IJMMN LT 1) IJMMN=1
WY1=0
WZ1=0
IF(F2Y NE 0.0) WY1=Y/F2Y
IF(F2Z NE 0.0) WZ1=Z/F2Z
XP=X-(WY1*Y1+WZ1*Z1)
G2(IJ)=XP
Y1=-WY1*G2(JP1)
Z1=-WZ1*G2(KP1)
ZB=-WZ1*BB(IJMMN)*IG31
F21=F2(JP1)
F22=F2(KP1)
F23=F2(IJMMN)
P1=0
P2=0
P3=0
IF(F21 NE 0.0) P1=Y1*Y1/F21
IF(F22 NE 0.0) P2=Z1*Z1/F22
IF(F23 NE 0.0) P3=ZB*ZB/F23
Y1Z1=P1+P2+P3
20 CONTINUE
EEIJ=-(X+Y+Z+DD(IJ+1)+BB(IJP1K)+ZZ(IJKP1))+XXS(IJ)
XF=0
YF=0
ZF=0
IF(F2X NE 0.0) XF=XP*XP/F2X
IF(F2Y NE 0.0) YF=Y*Y/F2Y
IF(F2Z NE 0.0) ZF=Z*Z/F2Z
F2(IJ)=EEIJ-(XF+YF+ZF+Y1Z1)
51 CONTINUE
GO TO 80
74 CONTINUE
DO 54 IJ=2,N320
IF(MHD(IJ).GE.1) GO TO 54
IJP1K=IJ+NI10
IJKP1=IJ+NIJ10
IF(IJP1K GT NNN) IJP1K=NNN
IF(IJKP1 GT NNN) IJKP1=NNN
EEIJ=(-(DD(IJ)+BB(IJ)+ZZ(IJ)+DD(IJ+1))
1+BB(IJP1K)+ZZ(IJKP1))+XXS(IJ))
IF(NUM4 EQ 5) GO TO 539
X=DD(IJ)
F2X=F2(IJ-1)
XF=0

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IF(F2X, NE, 0, 0) XF=X*X/F2X          PCG01140
F2(IJ)=EEIJ-XF                      PCG01150
GO TO 54                            PCG01160
539 F2(IJ)=EEIJ                      PCG01170
54  CONTINUE                         PCG01180
GO TO 80                            PCG01190
76  CONTINUE                         PCG01200
W=. 95-(NUM4-7)*. 55                PCG01210
DO 56 IJ=2, N320                  PCG01220
IF(MHD(IJ), GE, 1) GO TO 56        PCG01230
IP1JK=IJ+1                          PCG01240
IJP1K=IJ+NI10                      PCG01250
IJKP1=IJ+NIJ10                     PCG01260
IM1JK=IJ-1                          PCG01270
IJM1K=IJ-NI10                      PCG01280
IJKM1=IJ-NIJ10                     PCG01290
IF(IJP1K, GT, NNN) IJP1K=NNN       PCG01300
IF(IJKP1, GT, NNN) IJKP1=NNN       PCG01310
IF(IJM1K, LT, 1) IJM1K=1           PCG01320
IF(IJKM1, LT, 1) IJKM1=1           PCG01330
Z=ZZ(IJ)                           PCG01340
B=BB(IJ)                           PCG01350
D=DD(IJ)                           PCG01360
F=DD(IP1JK)                        PCG01370
H=BB(IJP1K)                        PCG01380
S=ZZ(IJKP1)                        PCG01390
E=-(Z+B+D+F+H+S)+XXS(IJ)         PCG01400
E2I=E22(IM1JK)                    PCG01410
E2J=E22(IJM1K)                    PCG01420
E2K=E22(IJKM1)                    PCG01430
F2I=F2(IM1JK)                     PCG01440
F2J=F2(IJM1K)                     PCG01450
F2K=F2(IJKM1)                     PCG01460
G2I=G2(IM1JK)                     PCG01470
G2J=G2(IJM1K)                     PCG01480
G2K=G2(IJKM1)                     PCG01490
IF(NUM4, EQ, 8) GO TO 761          PCG01500
A2=Z/(1+W*(E2K+F2K))             PCG01510
B2=B/(1+W*(G2J+E2J))             PCG01520
C2=D/(1+W*(G2I+F2I))             PCG01530
GO TO 762                          PCG01540
761 A2=G2K*D2S(IJKM1)              PCG01550
B2=F2J*D2S(IJM1K)                PCG01560
C2=E2I*D2S(IM1JK)                PCG01570
762 CONTINUE                         PCG01580
AC=W*(A2+E2K+B2+E2J)              PCG01590
TG=W*(A2+F2K+C2+F2I)              PCG01600
WU=W*(C2+G2I+B2+G2J)              PCG01610
D2=E+(AC+TG+WU)-C2*E2I-B2*F2J-A2*G2K
D2S(IJ)=D2
D2=1/D2
E22(IJ)=D2*(F-AC)
F2(IJ)=D2*(H-TG)
G2(IJ)=D2*(S-WU)
56  CONTINUE                         PCG01670
80  CONTINUE                         PCG01680
CONTINUE                         PCG01690
SPR=1, D-50                         PCG01700
ICNT=0                             PCG01710
ER5S=100                           PCG01720
L78=2, 5*ER5S                       PCG01730
DO 100 ITER=1, L78                 PCG01740

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ICNT=ICNT+1 PCG01750
IF(ICNT.EQ.1TMAX) GO TO 202 PCG01760
SPP=0 PCG01770
DO 3 IJ=2,N320 PCG01780
IF(MHD(IJ).GE.1) GO TO 3 PCG01790
IP1JK=IJ+1 PCG01800
IJP1K=IJ+NI10 PCG01810
IJM1K=IJ-NI10 PCG01820
IJKP1=IJ+NIJ10 PCG01830
IJKM1=IJ-NIJ10 PCG01840
IF(IJP1K.GT.NNN) IJP1K=NNN PCG01850
IF(IJKP1.GT.NNN) IJKP1=NNN PCG01860
IF(IJM1K.LT.1) IJM1K=1 PCG01870
IF(IJKM1.LT.1) IJKM1=1 PCG01880
DDIJ=DD(IJ) PCG01890
DDIP1=DD(IP1JK) PCG01900
BBIJ=BB(IJ) PCG01910
BBIJP=BB(IJP1K) PCG01920
ZZIJ=ZZ(IJ) PCG01930
ZZIJK=ZZ(IJKP1) PCG01940
E2IJ=E2(IJ) PCG01950
DTIJ=(-(DDIJ+DDIP1+BBIJ+BBIJP+ZZIJ+ZZIJK)+XXS(IJ))*E2IJ PCG01960
1+DDIJ*E2(IJ-1)+DDIP1*E2(IP1JK) PCG01970
2+BBIJ*E2(IJM1K)+BBIJP*E2(IJP1K) PCG01980
3+ZZIJ*E2(IJKM1)+ZZIJK*E2(IJKP1) PCG01990
DT(IJ)=DTIJ PCG02000
SPP=SPP+E2IJ*DTIJ PCG02010
CONTINUE PCG02020
A1=SPR/(SPP+1.D-70) PCG02030
A2=A1 PCG02040
IF(ITER.GT.1) GO TO 35 PCG02050
A1=0 PCG02060
A2=1 PCG02070
SRZ=0 PCG02080
SUMRZ=0 PCG02090
ER5=0 PCG02100
DO 4 K=2,NK11 PCG02110
DO 4 J=2,NJ11 PCG02120
DO 4 I=2,NI11 PCG02130
IJ=I+NI10*(J-2)+NIJ10*(K-2) PCG02140
IF(MHD(IJ).GE.1) GO TO 4 PCG02150
DX=A1*E2(IJ) PCG02160
X=XX(IJ)+DX PCG02170
XX(IJ)=X PCG02180
ADX=DABS(DX) PCG02190
IF(ADX.LT.ER5) GO TO 111 PCG02200
IMX=I PCG02210
JMX=J PCG02220
KMX=K PCG02230
XXPMX=X PCG02240
ER5=ADX PCG02250
CONTINUE PCG02260
X=VV(IJ)-A2*DT(IJ) PCG02270
SUMRZ=SUMRZ+X PCG02280
DSR=DABS(X) PCG02290
IF(DSR.GT.SRZ) SRZ=DSR PCG02300
VV(IJ)=X PCG02310
CONTINUE PCG02320
IF(IWR1.EQ.1) WRITE(6,1000) ICNT, IMX, JMX, KMX, XXPMX, ER5, SRZ, PCG02330
1XX(NW1), XX(NW2), XX(NW3) PCG02340
IF((ER5+ER5S).LT.ERR) GO TO 202 PCG02350

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IF(SRZ.LT.XX10) GO TO 202          PCG02360
ER5S=ER5                          PCG02370
SPRS=SPR                          PCG02380
SPR=0                            PCG02390
GO TO (81,81,81,83,83,85,86,86),NUM4   PCG02400
81    CONTINUE                      PCG02410
DO 10 IJ=2,N320                  PCG02420
IF(MHD(IJ).GE.1) GO TO 10          PCG02430
IJM1K=IJ-NI10                     PCG02440
IJKM1=IJ-NIJ10                   PCG02450
IF(IJM1K.LT.1) IJM1K=1            PCG02460
IF(IJKM1.LT.1) IJKM1=1            PCG02470
B6=0                            PCG02480
Z6=0                            PCG02490
DDIJ=DD(IJ)                      PCG02500
IF(NUM4.EQ.1) GO TO 21            PCG02510
DDIJ=G2(IJ)                      PCG02520
JP1=IJM1K+1                      PCG02530
KP1=IJKM1+1                      PCG02540
IJMMN=IJ-(NIJ10-NI10)             PCG02550
IF(IJMMN.LT.1) IJMMN=1            PCG02560
B6=(DT(KP1)*G2(JP1)/(F2(IJM1K)+1.D-40)  PCG02570
Z6=(DT(KP1)*G2(KP1)+DT(IJMMN)*BB(IJMMN)*IG31)/(F2(IJKM1)+1.D-40)  PCG02580
21    CONTINUE                      PCG02590
DT(IJ)=(VV(IJ)-DDIJ*DT(IJ-1)-BB(IJ)*(DT(IJM1K)-B6)  PCG02600
1-ZZ(IJ)*(DT(IJKM1)-Z6))/F2(IJ)  PCG02610
10    CONTINUE                      PCG02620
DO 11 IJB=2,N320                PCG02630
IJ=N320+2-IJB                    PCG02640
IF(MHD(IJ).GE.1) GO TO 11          PCG02650
IP1JK=IJ+1                       PCG02660
IJP1K=IJ+NI10                     PCG02670
IJKP1=IJ+NIJ10                   PCG02680
JM1=IJP1K-1                      PCG02690
KM1=IJKP1-1                      PCG02700
IF(IJP1K.GT.NNN) IJP1K=NNN        PCG02710
IF(IJKP1.GT.NNN) IJKP1=NNN        PCG02720
XAD=0                            PCG02730
DDD=DD(IP1JK)                  PCG02740
IF(NUM4.EQ.1) GO TO 22            PCG02750
IF(JM1.GT.NNN) JM1=NNN            PCG02760
IF(KM1.GT.NNN) KM1=NNN            PCG02770
IJM1K=IJ-NI10                     PCG02780
IJPMN=IJ+(NIJ10-NI10)             PCG02790
IF(IJM1K.LT.1) IJM1K=1            PCG02800
IF(IJPMN.GT.NNN) IJPMN=NNN        PCG02810
DDD=G2(IP1JK)                  PCG02820
X=G2(IJ)/(F2(IJ-1)+1.D-40)       PCG02830
XAD=-(BB(JM1)*DT(JM1)+ZZ(KM1)*DT(KM1))*X  PCG02840
1-ZZ(IJPMN)*BB(IJ)*DT(IJPMN)*IG31/(F2(IJM1K)+1.D-40)  PCG02850
22    CONTINUE                      PCG02860
DTIJ=DT(IJ)-(DDD*DT(IP1JK)+BB(IJP1K)*DT(IJP1K)+ZZ(IJKP1))  PCG02870
1*DT(IJKP1)+XAD)/F2(IJ)          PCG02880
DT(IJ)=DTIJ                      PCG02890
SPR=SPR+DTIJ*VV(IJ)              PCG02900
11    CONTINUE                      PCG02910
GO TO 90                          PCG02920
83    CONTINUE                      PCG02930
DO 63 IJ=2,N320                  PCG02940
IF(MHD(IJ).GE.1) GO TO 63          PCG02950
F2IJ=1                          PCG02960

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IF(NUM4.EQ.5) F2IJ=F2(IJ) PCG02970
VVIJ=VV(IJ) PCG02980
DTIJ=VVIJ/F2IJ PCG02990
DT(IJ)=DTIJ PCG03000
SPR=SPR+DTIJ*VVIJ PCG03010
63 CONTINUE PCG03020
GO TO 90 PCG03030
85 CONTINUE PCG03040
DO 651 IJ=2,N320 PCG03050
IF(MHD(IJ).GE.1) GO TO 651 PCG03060
DT(IJ)=(VV(IJ)-DD(IJ)*DT(IJ-1))/F2(IJ) PCG03070
651 CONTINUE PCG03080
DO 652 IJB=2,N320 PCG03090
IJ=N320+2-IJB PCG03100
IF(MHD(IJ).GE.1) GO TO 652 PCG03110
IP1JK=IJ+1 PCG03120
DTIJ=DT(IJ)-DD(IP1JK)*DT(IP1JK)/F2(IJ) PCG03130
DT(IJ)=DTIJ PCG03140
SPR=SPR+DTIJ*VV(IJ) PCG03150
652 CONTINUE PCG03160
GO TO 90 PCG03170
86 CONTINUE PCG03180
DO 661 IJ=2,N320 PCG03190
IF(MHD(IJ).GE.1) GO TO 661 PCG03200
IM1JK=IJ-1 PCG03210
IJM1K=IJ-NI10 PCG03220
IJKM1=IJ-NIJ10 PCG03230
IF(IJM1K.LT.1) IJM1K=1 PCG03240
IF(IJKM1.LT.1) IJKM1=1 PCG03250
C2S=D2S(IM1JK)*E22(IM1JK) PCG03260
B2S=D2S(IJM1K)*F2(IJM1K) PCG03270
A2S=D2S(IJKM1)*G2(IJKM1) PCG03280
DT(IJ)=(VV(IJ)-C2S*DT(IJ-1)-B2S*DT(IJM1K) PCG03290
1-A2S*DT(IJKM1))/D2S(IJ) PCG03300
661 CONTINUE PCG03310
DO 662 IJB=2,N320 PCG03320
IJ=N320+2-IJB PCG03330
IF(MHD(IJ).GE.1) GO TO 662 PCG03340
IP1JK=IJ+1 PCG03350
IJP1K=IJ+NI10 PCG03360
IJKP1=IJ+NIJ10 PCG03370
IF(IJP1K.GT.NNN) IJP1K=NNN PCG03380
IF(IJKP1.GT.NNN) IJKP1=NNN PCG03390
DTIJ=DT(IJ)-(E22(IJ)*DT(IP1JK)+F2(IJ)*DT(IJP1K) PCG03400
1+G2(IJ)*DT(IJKP1)) PCG03410
DT(IJ)=DTIJ PCG03420
SPR=SPR+DTIJ*VV(IJ) PCG03430
662 CONTINUE PCG03440
90 CONTINUE PCG03450
B6=SPR/SPRS PCG03460
IF(ITER.EQ.1) B6=0 PCG03470
DO 5 IJ=2,N320 PCG03480
E2IJ=DT(IJ)+B6*E2(IJ) PCG03490
IF(MHD(IJ).GE.1) E2IJ=0 PCG03500
E2(IJ)=E2IJ PCG03510
5 CONTINUE PCG03520
100 CONTINUE PCG03530
202 CONTINUE PCG03540
1000 FORMAT(' ',I3,3I5,6D18.7) PCG03550
RETURN PCG03560
END PCG03570

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SUBROUTINE SIP SIP00010
IMPLICIT REAL*8 (A-H, O-Z) SIP00020
COMMON WS, HMAX, RELX1, RELX2, COEF, ERR, XX10, DELT, ER5, SRZ, SUMRZ SIP00030
1, XX, DT, VV, E2, F2, G2, YQ, NIJ10, NI11, NJ11, NK11, NNN, NSKP1 SIP00040
2, NSKP2, ITMAX, ICNT, IEVP, IWR1, NW1, NW2, NW3, N320, NUM4 SIP00050
3, L9, LENGTH, NK1115, IT01, IT15, ICRO, DDK, BBK SIP00060
4, NT, DD, BB, ZZ, XXE, XXS, ALN, SV SIP00070
5, NI10, NJ10, NK10, NI12, NJ12, NK12, LB, MHD SIP00080
REAL*4 DD(377), BB(377), ZZ(377), XXE(377), XXS(377), ALN(377), SIP00090
1SV(377), YQ(377), DDK(50), BBK(50), NT(502) SIP00100
DIMENSION XX(377), DT(377), VV(377), E2(377), F2(377) SIP00110
1, WS(10), MHD(377), G2(377), LB(502) SIP00120
DO 889 IJ=1, NNN SIP00130
E2(IJ)=0 SIP00140
DO 889 IJ=1, NNN SIP00150
E2(IJ)=0 SIP00160
F2(IJ)=0 SIP00170
G2(IJ)=0 SIP00180
VV(IJ)=0 SIP00190
889 DT(IJ)=0 SIP00200
ICNT=0 SIP00210
ICT=0 SIP00220
ER55=100 SIP00230
DO 501 ITER0=1, 60 SIP00240
DO 499 I33=1, 2 SIP00250
I3=I33 SIP00260
I4=1 SIP00270
IF(L9, EQ, 2) I4=I3 SIP00280
IF(L9, LT, 3) GO TO 195 SIP00290
I3=1 SIP00300
I4=I33 SIP00310
195 CONTINUE SIP00320
ICT=ICT+1 SIP00330
IF( ICT, EQ, (LENGTH+1)) ICT=1 SIP00340
ICNT=ICNT+1 SIP00350
IF( ICNT, EQ, ITMAX) GO TO 202 SIP00360
W=WS(ICT) SIP00370
JJM1=2*I3-3 SIP00380
JJP1=-JJM1 SIP00390
KKM1=2*I4-3 SIP00400
KKP1=-KKM1 SIP00410
C ACCOMPLISH EQUATIONS (10) AND (14) BY WEINSTEIN [1969] SIP00420
SRZ=0 SIP00430
SUMRZ=0 SIP00440
DO 100 KB=2, NK11 SIP00450
ISF1=0 SIP00460
IF((KB, GE, 3), AND, (KB, LE, NK10)) ISF1=1 SIP00470
DO 100 JB=2, NJ11 SIP00480
ISF2=0 SIP00490
IF((JB, GE, 3), AND, (JB, LE, NJ10)) ISF2=1 SIP00500
J=JB SIP00510
K=KB SIP00520
IF(I3, EQ, 2) J=NJ12+1-JB SIP00530
IF(I4, EQ, 2) K=NK12+1-KB SIP00540
DO 50 I=2, NI11 SIP00550
IJF=I+NI10*(J-2) SIP00560
IJ=IJF+NIJ10*(K-2) SIP00570
IF(MHD(IJ), GE, 1) GO TO 50 SIP00580
IM1JK=IJ-1 SIP00590
IP1JK=IJ+1 SIP00600
IJM1K=IJ+JJM1*NI10 SIP00610

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IJP1K=IJ+JJP1*NI10	SIP00620
IJP2K=IJ+NI10	SIP00630
IJKM1=IJ+KKM1*NIJ10	SIP00640
IJKP1=IJ+KKP1*NIJ10	SIP00650
IJKP2=IJ+NIJ10	SIP00660
IF(ISF1.EQ.1) GO TO 91	SIP00670
IF(IJKM1.LT.1) IJKM1=1	SIP00680
IF(IJKM1.GT.NNN) IJKM1=NNN	SIP00690
IF(IJKP1.LT.1) IJKP1=1	SIP00700
IF(IJKP1.GT.NNN) IJKP1=NNN	SIP00710
IF(IJKP2.GT.NNN) IJKP2=NNN	SIP00720
IF(ISF2.EQ.1) GO TO 91	SIP00730
IF(IJM1K.LT.1) IJM1K=1	SIP00740
IF(IJM1K.GT.NNN) IJM1K=NNN	SIP00750
IF(IJP1K.LT.1) IJP1K=1	SIP00760
IF(IJP1K.GT.NNN) IJP1K=NNN	SIP00770
IF(IJP2K.GT.NNN) IJP2K=NNN	SIP00780
91 CONTINUE	SIP00790
XXIJ=XX(IJ)	SIP00800
Z=ZZ(IJ)	SIP00810
B=BB(IJ)	SIP00820
D=DD(IJ)	SIP00830
F=DD(IP1JK)	SIP00840
H=BB(IJP2K)	SIP00850
S=ZZ(IJKP2)	SIP00860
IF(I3.EQ.1) GO TO 42	SIP00870
BS=B	SIP00880
B=H	SIP00890
H=BS	SIP00900
42 CONTINUE	SIP00910
IF(I4.EQ.1) GO TO 43	SIP00920
ZS=Z	SIP00930
Z=S	SIP00940
S=ZS	SIP00950
43 CONTINUE	SIP00960
SVDT=SV(IJ)/DELT	SIP00970
E=-(Z+B+D+F+H+S)+SVDT	SIP00980
LEV=0	SIP00990
IF((IEVP.EQ.1).AND.(XXIJ.GT.XXE(IJ))) LEV=1	SIP01000
IF(LEV.NE.1) GO TO 44	SIP01010
ALNI=ALN(IJ)	SIP01020
E=E+ALNI	SIP01030
44 CONTINUE	SIP01040
E2I=E2(IM1JK)	SIP01050
E2J=E2(IJM1K)	SIP01060
E2K=E2(IJKM1)	SIP01070
F2I=F2(IM1JK)	SIP01080
F2J=F2(IJM1K)	SIP01090
F2K=F2(IJKM1)	SIP01100
G2I=G2(IM1JK)	SIP01110
G2J=G2(IJM1K)	SIP01120
G2K=G2(IJKM1)	SIP01130
A2=Z/(1+W*(E2K+F2K))	SIP01140
B2=B/(1+W*(G2J+E2J))	SIP01150
C2=D/(1+W*(G2I+F2I))	SIP01160
AC=W*(A2*E2K+B2*E2J)	SIP01170
TG=W*(A2*F2K+C2*F2I)	SIP01180
WU=W*(C2*G2I+B2*G2J)	SIP01190
D2=E+(AC+TG+WU)-C2*E2I-B2*F2J-A2*G2K	SIP01200
D2=1/D2	SIP01210
E2(IJ)=D2*(F-AC)	SIP01220

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F2(IJ)=D2*(H-TQ)                      SIP01230
G2(IJ)=D2*(S-WU)                      SIP01240
RZ=YQ(IJ)-(XX(IM1JK)*D+XX(IP1JK)*F+XX(IJM1K)*B+XX(IJP1K)*H
1+XX(IJKM1)*Z+XX(IJKP1)*S+XXIJ*E)+SVDT*XXS(IJ)          SIP01250
IF(LEV, EQ, 1) RZ=RZ+ALNI*XXE(IJ)        SIP01260
SUMRZ=SUMRZ+RZ                          SIP01270
DSR=DABS(RZ)                           SIP01280
IF(DSR, GT, SRZ) SRZ=DSR              SIP01290
VV(IJ)=D2*(RZ-A2*VV(IJKM1)-B2*VV(IJM1K)-C2*VV(IM1JK))    SIP01300
50  CONTINUE                            SIP01320
100 CONTINUE                            SIP01330
C EQUATIONS (10) AND (14) ARE NOW ACCOMPLISHED      SIP01340
C ACCOMPLISH EQUATION (15) BY WEINSTEIN [1969]      SIP01350
ER5=0                                     SIP01360
DO 102 KB=2,NK11                         SIP01370
ISF1=0                                     SIP01380
IF((KB, GE, 3), AND, (KB, LE, NK10)) ISF1=1    SIP01390
DO 102 JB=2,NJ11                         SIP01400
ISF2=0                                     SIP01410
IF((JB, GE, 3), AND, (JB, LE, NJ10)) ISF2=1    SIP01420
J=NJ12+1-JB                            SIP01430
K=NK12+1-KB                            SIP01440
IF(I3, EQ, 2) J=JB                        SIP01450
IF(I4, EQ, 2) K=KB                        SIP01460
DO 62 IB=2,NI11                         SIP01470
I=NI12+1-IB                            SIP01480
IJ=I+NI10*(J-2)+NIJ10*(K-2)            SIP01490
IF(MHD(IJ), GE, 1) GO TO 62             SIP01500
IP1JK=IJ+1                             SIP01510
IJP1K=IJ+JJP1#NI10                     SIP01520
IJKP1=IJ+KJP1#NIJ10                     SIP01530
IF(ISF1, EQ, 1) GO TO 92                SIP01540
IF(IJKP1, LT, 1) IJKP1=1                 SIP01550
IF(IJKP1, GT, NNN) IJKP1=NNN           SIP01560
IF(ISF2, EQ, 1) GO TO 92                SIP01570
IF(IJP1K, LT, 1) IJP1K=1                 SIP01580
IF(IJP1K, GT, NNN) IJP1K=NNN           SIP01590
92  CONTINUE                            SIP01600
X=VV(IJ)-E2(IJ)*DT(IP1JK)-F2(IJ)*DT(IJP1K)-G2(IJ)*DT(IJKP1)    SIP01610
DT(IJ)=X                                SIP01620
X=X*HMAX                               SIP01630
XXP=XX(IJ)+X                           SIP01640
XX(IJ)=XXP                             SIP01650
X=DABS(X)                               SIP01660
IF(X, LE, ER5) GO TO 111                SIP01670
IMX=I                                   SIP01680
JMX=J                                   SIP01690
KMX=K                                   SIP01700
XXPMX=XXP                             SIP01710
ER5=X                                   SIP01720
111 CONTINUE                            SIP01730
62  CONTINUE                            SIP01740
102 CONTINUE                            SIP01750
C EQUATION (15) IS NOW ACCOMPLISHED      SIP01760
IF(IWR1, EQ, 1) WRITE(6, 1000)           SIP01770
1  ICNT, IMX, JMX, KMX, XXPMX, ER5, SRZ, XX(NW1), XX(NW2), XX(NW3)    SIP01780
IF((ER5+ER5S), LT, ERR) GO TO 202       SIP01790
IF(SRZ, LT, XX10) GO TO 202             SIP01800
ER5S=ER5                               SIP01810
499 CONTINUE                            SIP01820
501 CONTINUE                            SIP01830

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202  CONTINUE          S1P01840
1000 FORMAT(' ', I3, 3I5, 6D18. 7)    S1P01850
      RETURN           S1P01860
      END             S1P01870
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