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DOCUMENTATION OF FINITE—DIFFERENCE MODEL FOR SIMULATION OF THREE—DIMENSIONAL GROUND—WATER FLOW

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INTRODUCTION

User experience has indicated that the documentation of the model of three-dimensional ground-water flow (Trescott and Larson, 1975) should be expanded. This supplement is intended, in part, to fulfill that need. In addition, a few errors, both in the text and in the code, have been found and the appropriate corrections are noted. A reprint of the documentation was corrected as of the date of the printing but more recent changes should also be made.

Equations, figures and pages designated with Roman numerals refer to those in this supplement and equations, figures and pages with Arabic numerals are found in the documentation. The exceptions are the Roman and Arabic numerals which are used together for page numbers in appendices to the documentation. Symbols are either defined here or in the documentation. In the documentation an abbreviated subscript notation (in which subscripts except those with a +1 or -1 are eliminated) is used in eq. 9 and many subsequent equations. Herein the full subscript notation is used for all equations. Capitalized subscripts are used for arrays in the model.

BASIC THREE-DIMENSIONAL

FINITE-DIFFERENCE EQUATION

Another way of showing the development of the three-dimensional (3-D) finite-difference equation (as opposed to starting with eq. 3) is to look at the flow equation (assuming constant mass per unit volume) for block (i,j,k) (fig. I). The flow equation may be expressed in words as the sum of outflow minus the sum of inflow equals change in storage plus source terms; in more concise form, it is

$$\sum_{\alpha}[\emptyset_{\alpha(out)} - \emptyset_{\alpha(in)}] = S_{s(i,j,k)} \frac{\Delta h}{\Delta t} \Delta V_{i,j,k} + W_{i,j,k} \Delta V_{i,j,k} \qquad (I)$$

in which

α = x,y,z;

Δh = $h_{i,j,k} - \hat{h}_{i,j,k}$;

ΔV = $\Delta x_j \, \Delta y_i \, \Delta z_k$;

$\emptyset_{x(out)}$ = $K_{xx(i,j+\frac{1}{2},k)} \dfrac{\Delta h_{j+\frac{1}{2}}}{\Delta x_{j+\frac{1}{2}}} \Delta z_k \, \Delta y_i$ =

the volumetric flux out face $j+\frac{1}{2}$;
Five other similar terms are on the left-hand side of eq. I;

$K_{xx(i,j+\frac{1}{2},k)}$ = represents hydraulic conductivity in the x direction at face $j+\frac{1}{2}$ (fig. I);

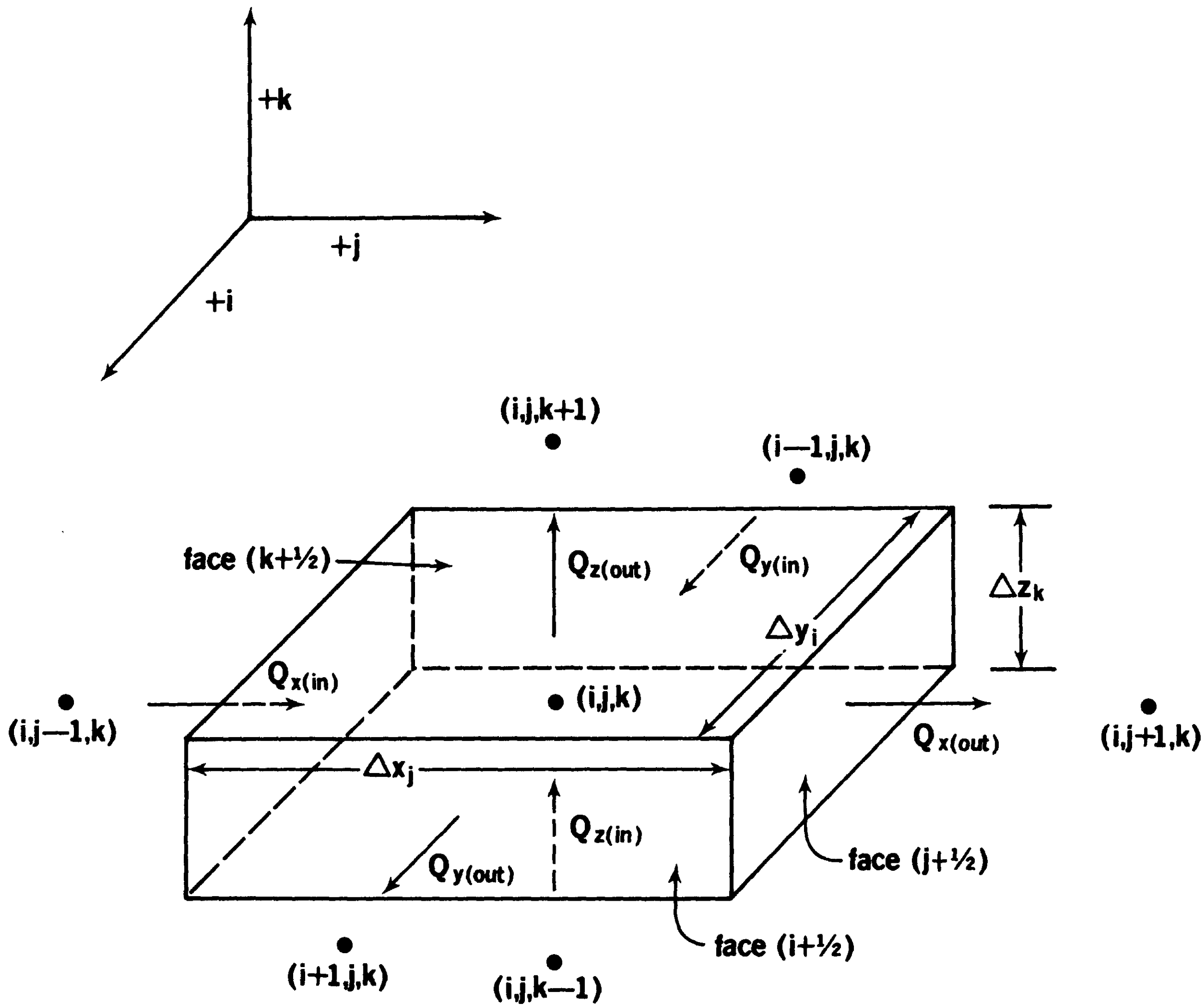


Figure I--Finite-difference block for three-dimensional ground-water flow.

$\frac{\Delta h_{j+\frac{1}{2}}}{\Delta x_{j+\frac{1}{2}}}$ is the hydraulic gradient in the x direction at face $j+\frac{1}{2}$;

$\Delta h_{j+\frac{1}{2}} = h_{i,j+1,k} - h_{i,j,k}$ and

$\Delta h_{j-\frac{1}{2}} = h_{i,j,k} - h_{i,j-1,k}$.

With the definitions given above, eq. I can be expanded as

$$K_{xx(i,j+\frac{1}{2},k)}\Delta z_k \Delta y_i \frac{\Delta h_{j+\frac{1}{2}}}{\Delta x_{j+\frac{1}{2}}} - K_{xx(i,j-\frac{1}{2},k)}\Delta z_k \Delta y_i \frac{\Delta h_{j-\frac{1}{2}}}{\Delta x_{j-\frac{1}{2}}}$$

$$+ \quad K_{yy(i+\frac{1}{2},j,k)}\Delta z_k \Delta x_j \frac{\Delta h_{i+\frac{1}{2}}}{\Delta y_{i+\frac{1}{2}}} - K_{yy(i-\frac{1}{2},j,k)}\Delta z_k \Delta x_j \frac{\Delta h_{i-\frac{1}{2}}}{\Delta y_{i-\frac{1}{2}}}$$

$$+ \quad K_{zz(i,j,k+\frac{1}{2})}\Delta x_j \Delta y_i \frac{\Delta h_{k+\frac{1}{2}}}{\Delta z_{k+\frac{1}{2}}} - K_{zz(i,j,k-\frac{1}{2})}\Delta x_j \Delta y_i \frac{\Delta h_{k-\frac{1}{2}}}{\Delta z_{k-\frac{1}{2}}}$$

$$= \quad S_{s(i,j,k)} \frac{\Delta h}{\Delta t} \Delta x_j \Delta y_i \Delta z_k + W_{i,j,k} \Delta x_j \Delta y_i \Delta z_k \qquad (II)$$

The next step is to divide eq. II by $\Delta x_j \; \Delta y_i \; \Delta z_k$ to obtain

$$\frac{K_{xx(i,j+\frac{1}{2},k)}}{\Delta x_j} \frac{\Delta h_{j+\frac{1}{2}}}{\Delta x_{j+\frac{1}{2}}} - \frac{K_{xx(i,j-\frac{1}{2},k)}}{\Delta x_j} \frac{\Delta h_{j-\frac{1}{2}}}{\Delta x_{j-\frac{1}{2}}}$$

$$+ \frac{K_{yy(i+\frac{1}{2},j,k)}}{\Delta y_i} \frac{\Delta h_{i+\frac{1}{2}}}{\Delta y_{i+\frac{1}{2}}} - \frac{K_{yy(i-\frac{1}{2},j,k)}}{\Delta y_i} \frac{\Delta h_{i-\frac{1}{2}}}{\Delta y_{i-\frac{1}{2}}}$$

$$+ \frac{K_{zz(i,j,k+\frac{1}{2})}}{\Delta z_k} \frac{\Delta h_{k+\frac{1}{2}}}{\Delta z_{k+\frac{1}{2}}} - \frac{K_{zz(i,j,k-\frac{1}{2})}}{\Delta z_k} \frac{\Delta h_{k-\frac{1}{2}}}{\Delta z_{k-\frac{1}{2}}}$$

$$= S_{s(i,j,k)} \frac{\Delta h}{\Delta t} + W_{i,j,k} \; . \qquad \text{(III)}$$

In order to simplify the finite-difference equation, it is convenient to use the harmonic mean to compute part of the coefficients in eq. 9. Using the basic equation approach this is done by modifying eq. 8a to eq. 8f.

In equations 8a to 8d insert hydraulic conductivity for transmissivity. Referring to eq. III and 8c as an example,

$$F_{i,j,k} = \frac{K_{xx(i,j+\frac{1}{2},k)}}{\Delta x_j \Delta x_{j+\frac{1}{2}}} = \left[\frac{2K_{xx(i,j+1,k)}K_{xx(i,j,k)}}{K_{xx(i,j,k)}\Delta x_{j+1} + K_{xx(i,j+1,k)}\Delta x_j}\right] / \Delta x_j$$

Equations 8e and 8f (as corrected in this supplement) are modified by dividing by Δz_k. As an example,

$$S_{i,j,k} = \left[\frac{2K_{zz(i,j,k+1)}K_{zz(i,j,k)}}{K_{zz(i,j,k)}\Delta z_{k+1} + K_{zz(i,j,k+1)}\Delta z_k}\right] / \Delta z_k \qquad \text{(IV)}$$

After making the computations described above, eq. III can be rearranged to have the same form as eq. 9.

USE OF THE MODEL WITH THE BASIC 3-D EQUATION

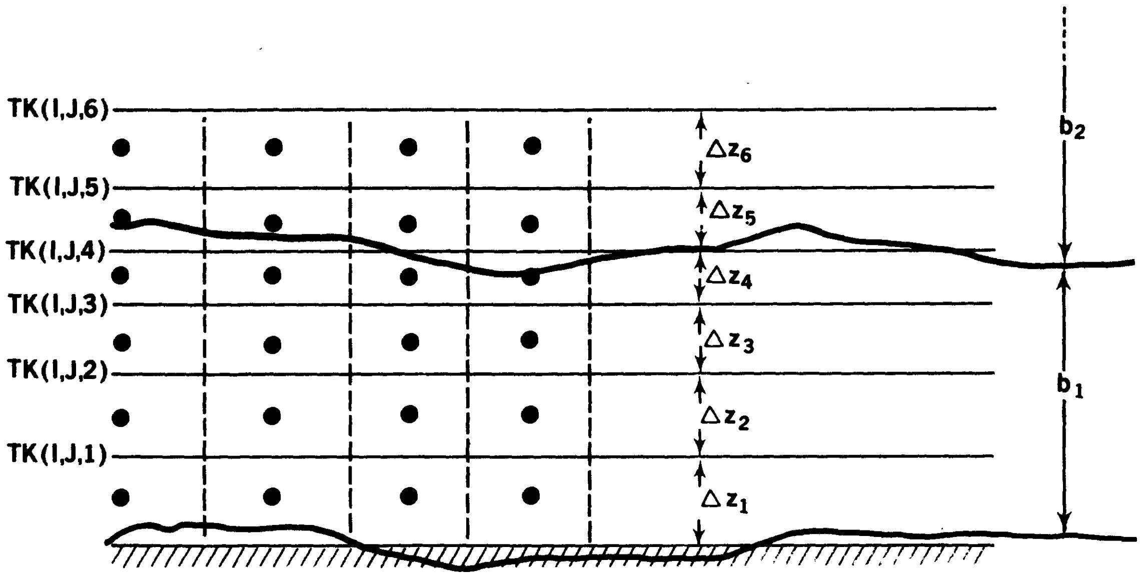
A cross section showing two hydrogeologic units represented by several layers is shown in figure II. The lowest layer has an impermeable base and is normally treated this way unless modifications are made to the code. Source terms and construction of finite-difference grids are described in the documentation. Be sure to note that the change in Δz (as well as with Δx and Δy) should not be greater than 1½ in either direction to minimize truncation errors.

The model has been coded to solve the modified equation described in the next section. Consequently note the form of data input (pages 4 and 10) required for using the model to solve the 3-D equation in basic form.

The model will compute the coefficients for each node based on the hydraulic conductivity for the node and anisotropy (if any) for a layer. More flexibility in varying vertical hydraulic conductivity is available in the code by reading in part of the vertical coefficients as

$$TK(I,J,K) = \frac{2K_{zz(i,j,k+1)}K_{zz(i,j,k)}}{K_{zz(i,j,k)}\Delta z_{k+1}+K_{zz(i,j,k+1)}\Delta z_k} \qquad (V)$$

Observe that eq. V is nearly identical to eq. IV, but the final division by Δz_k is done in the code in SOLVE.



EXPLANATION

//////////	Impermeable base of aquifer system
TK	Defined by equation V
Δz	Thickness of a finite-difference layer
b	Thickness of a hydrogeologic unit

Figure II--Two hydrogeologic units, each represented by several finite-difference layers.

Although it is possible to treat the upper layer as having a free surface using the basic 3-D equation, in general it is better to use the modified 3-D equation for this type of simulation. Therefore, most of the discussion will be deferred to a later section except to note that PERM (I,J) is read twice for the upper layer; once into the T matrix and once into the PERM matrix. In effect the hydraulic conductivity for flow in the horizontal directions will be reduced as the water-table blocks desaturate.

MODIFIED 3-D FINITE-DIFFERENCE EQUATION

The model is coded to solve a modified 3-D finite-difference equation that is developed in eq. 6 to eq. 9. These equations have the thickness of a hydrogeologic unit, b, incorporated in every term (see eq. 4 and note corrections to equations 5, 6, 8e and 8f given in this supplement) whereas the basic 3-D finite-difference equation does not. This is the only difference in the two approaches.

The value of Δz_k for each layer is obtained by averaging (in some manner) its thickness over the area of the model. Significant truncation errors in the discretization of the vertical space dimension may result if the change in Δz from layer to layer is greater than suggested for use with the basic 3-D equation. However, a series of experiments with small-scale models of your problem may justify greater changes in Δz between layers and thus reduce the total number of layers required to obtain reasonable results.

USE OF THE MODEL WITH THE MODIFIED 3-D EQUATION

Commonly, either because of insufficient data for definition of a 3-D aquifer system in which all hydrogeologic units are represented or because the stratigraphy is complex and storage and run cost in the computer may be excessive, use of the modified 3-D equation is suggested. This results in a model such as illustrated in figure III. For example, Jorgensen (1975) designed an analog model in which numerous hydrogeologic units in the Houston aquifer system are combined into a few layers of nodes in his model. A method of combining many confining beds into one with equivalent storage properties is given in Helm (1975, p. 474). The references cited above can aid in chosing appropriate thickness (or Δz_k) values.

Because the model was designed to use the modified 3-D equations, it should be relatively easy to follow the data input instructions. If additional flexibility in vertical coefficients is needed, they may be computed by eq. 26c (identical to eq. V) and read with data input. This is analogous to the same feature available for solving the basic finite-difference equation. (See eq. V.)

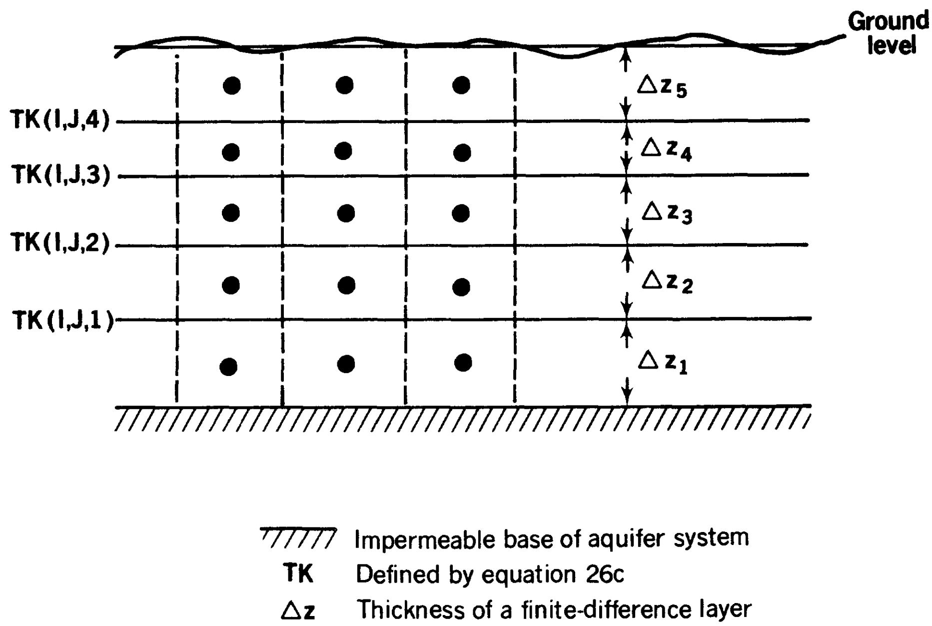


Figure III--A finite-difference grid in which one or more layers may have a combination of hydrogeologic units.

If the upper layer in the simulation model has a free surface, the transmissivity in the areal plane is a function of saturated thickness (see p. 9). By examining eq. 26c, however, it can be seen that a change in saturated thickness of the water-table layer has no effect on the conductivity at the lower boundary of this layer. Therefore, TK(I,J,K) at the boundary between the water-table layer and the one underlying it is constant until the water-table block desaturates. Then TK(I,J,K) at the lower boundary is set to zero.

REFERENCES CITED

Bredehoeft, J.D., and Pinder, G.F., 1970, Digital analysis of areal flow in multiaquifer groundwater systems: A quasi three-dimensional model: Water Resources Research, v. 6, no. 3, p. 883-888.

Helm, D.C., 1975, One dimensional simulation of aquifer system compaction near Pixley, California 1: Constant parameters: Water Resources Research, v. 11, no. 3, p. 465-478.

Jorgensen, D.G., 1975, Analog-model studies of ground-water hydrology in the Houston District, Texas: Water Development Board, Rept. 190, 84 p.

Trescott, P.C., 1975, Documentation of finite-difference model for simulation of three-dimensional ground-water flow: U.S. Geological Survey Open File Report 75-438, 32 p.

USE AS A QUASI-THREE DIMENSIONAL MODEL

The equation solved in the model can be made to have the form of a quasi-3-D model (Bredehoeft and Pinder, 1970). (See pages 28 and 29 of the documentation.) This is accomplished by using the modified 3-D equation and eliminating the layers of nodes representing the confining beds (fig. 9). The resistance to vertical flow in the confining beds is incorporated in the finite-difference equations for aquifers by reading

$$TK(I,J,K) = \frac{K_{zz}}{b} \qquad (VI)$$

in which (for equation VI)

K_{zz} = vertical hydraulic conductivity for the confining bed;

b = thickness of the confining bed.

Location subscripts of K_{zz} and b in eq. VI are left off because confining bed layers are not explicitly represented in the model. With the use of eq. VI for the coefficients, terms 5 and 6 of eq. 6 are identical to leakage terms (for confining beds in which storage can be considered insignificant) which appear as source terms in the quasi-3-D model written by Bredehoeft and Pinder (1970). If a confining bed is intermittent, the TK values will be computed by eq. VI where the confining bed exists, and by eq. 26c (eq. V) where the confining bed is absent between aquifers.

CORRECTIONS TO DOCUMENTATION

p. 1, ℓ. 12 replace "hydraulic" with "hydrogeologic"

p. 4, ℓ. 3 should read, "plied by b, the thickness of the hydrogeologic unit giving approximately"

p. 4, eq. 4 should read

$$\frac{\partial}{\partial x}\left(T_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(T_{yy}\frac{\partial h}{\partial y}\right) + b\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right) = S'\frac{\partial h}{\partial t} + bW(x,y,z,t)$$

p. 6, ℓ. 3 of eq. 5 should read

$$\left(\frac{b}{\Delta z}\right)_k \left[\left(K_{zz}\frac{\partial h}{\partial z}\right)_{i,j,k+\frac{1}{2}} - \left(K_{zz}\frac{\partial h}{\partial z}\right)_{i,j,k-\frac{1}{2}}\right] =$$

p. 6 after the last line, add "The multiplier $(b/\Delta z)_k$ for terms 5 and 6 is 1 because $b_k = \Delta z_k$ and therefore drops out."

p. 7, ℓ. 3 of eq. 6 should read

$$\left[(K_{zz})_{i,j,k+\frac{1}{2}}\frac{(h_{i,j,k+1}-h_{i,j,k})}{\Delta z_{k+\frac{1}{2}}}\right] - \left[(K_{zz})_{i,j,k-\frac{1}{2}}\frac{(h_{i,j,k}-h_{i,j,k-1})}{\Delta z_{k-\frac{1}{2}}}\right]$$

p. 8, eq. 8e should read

$$S_{i,j,k} = \frac{2K_{zz(i,j,k+1)}K_{zz(i,j,k)}}{K_{zz(i,j,k)}\,\Delta z_{k+1} + K_{zz(i,j,k+1)}\,\Delta z_k}$$

p. 8, eq. 8f should read

$$Z_{i,j,k} = \frac{2K_{zz(i,j,k-1)}K_{zz(i,j,k)}}{K_{zz(i,j,k)}\Delta z_{k-1} + K_{zz(i,j,k-1)}\,\Delta z_k}$$

p. 9, ℓ. 1 and ℓ. 7 replace "hydrologic" with "hydrogeologic"

p. 10, ℓ. 7 replace "hydraulic" with "hydrogeologic"

p. 12, ℓ. 8 should be revised to read, "matrix $\bar{\bar{B}}\bar{h}$ can be added to both sides of eq. 10 such that $(\overline{\overline{A+B}})$ factors into $\bar{\bar{L}}$ and $\bar{\bar{U}}$ as shown in"

p. 17, ℓ. 3 from bottom should read, "second-order correct approximation for $\xi_{i-1,j+1}$ if uniform grid spacing is used; otherwise, it is first-order correct"

p. 25 eq. 24 should read

$$\omega_{\ell+1} = 1 + (1 - \omega_{max})^{\ell/(L-1)}, \quad \ell = 0,1,\ldots, L-1$$

p. 27, ℓ. 5 replace "hydraulic" with "hydrogeologic"

p. 28, ℓ. 8 from bottom should read, "to the ratio K_{zz}/b for each confining bed."

p. 30, ℓ. 16 delete the last two sentences of paragraph 2. starting with, "If one layer of nodes . . ."

Documentation, Appendix II

p. II-5, ℓ. 20 the second word should be "if" not "of"

p. II-6, ℓ. 10 to ℓ. 12 should read,

"The T coefficients TR, TC and TK may be computed once and saved for artesian units; for water-table units, TR and TC are re-computed every iteration and TK stays constant until block K+1 desaturates, then TK (I,J,K) = 0.0. They are defined as"

p. II-6, eq. 26c should read

$$TK(I,J,K) = \frac{2K_{zz(k+1)}K_{zz}}{K_{zz}\ \Delta z_{k+1} + K_{zz(k+1)}\ \Delta z}$$

Documentation, Appendix III

p. III-2 add to the definition of ITK, "(See Supplement also.)"

p. III-2 add another variable:

COLUMNS	FORMAT	VARIABLE	DEFINITION
51-54	A4	IEQN	EQN3 if eq. 3 is being solved; otherwise it is assumed that eq. 4 is being solved.

p. III-3, ℓ. 16 in the definition of ERR, change "criteria" to "criterion"

p. III-5, ℓ. 4 the first part that now reads, "data cards for each layer in the model." should read, "data cards. If the data set requires data for each layer, a parameter card and data cards (for layers with variable data) are required for each layer".

p. III-6 add to the note under data set 3, "If equation 3 is to be solved, read specific storage instead of storage coefficient." Add note 4) to data set 4 "4) If equation 3 is to be solved, read hydraulic conductivity instead of transmissivity."

p. III-8, ℓ. 5 add the following sentence, "If NUMT is greater than 50 change the dimension of ITTØ in subroutine STEP to the appropriate size."

p. III-8, ℓ. 8 change "100" to "50".

DOCUMENTATION, APPENDIX VI

On the following three pages are corrections and additions to the code. The sequence number on the right-hand side of each printed line indicates its proper location in the code. Replace cards with the same sequence number as those in the list. In addition, remove SP31360, SP31370, SP32230, SP32240, CHK710, CHK1510, and CHK1530 from the card deck.

```
   2H,IDK1,IDK2,IWATER,IQRE,IP,JP,IQ,JQ,IK,JK,K5,IPU1,IPU2,ITK,IEQN     MAN0170


   1,IEQN                                                               MAN0395


   1,IEQN                                                               MAN0405


    K=K0                                                                MAN1595


   2H,IDK1,IDK2,IWATER,IQRE,IP,JP,IQ,JQ,IK,JK,K5,IPU1,IPU2,ITK,IEQN     DAT0180


    DO 245 K=1,K0                                                       DAT1761
    DO 245 I=1,I0                                                       DAT1762
    DO 245 J=1,J0                                                       DAT1763
245 WELL(I,J,K)=0.0                                                     DAT1764


   2H,IDK1,IDK2,IWATER,IQRE,IP,JP,IQ,JQ,IK,JK,K5,IPU1,IPU2,ITK,IEQN     STP 180


220 FORMAT (10F8.4)                                                     STP1350


   2H,IDK1,IDK2,IWATER,IQRE,IP,JP,IQ,JQ,IK,JK,K5,IPU1,IPU2,ITK,IEQN     SP3 180


    IF(K.EQ.1) GO TO 124                                                SP31361
    Z=TK(NKB)                                                           SP31362
    IF(IEQN.EQ.ICHK(11)) Z=Z/DELZ(K)                                    SP31363
124 IF(K.EQ.K0) GO TO 125                                               SP31371
    SU=TK(N)                                                            SP31372
    IF(IEQN.EQ.ICHK(11))SU=SU/DELZ(K)                                   SP31373
125 RHO=S(N)/DELT                                                       SP31380


    IF(K.EQ.1) GO TO 174                                                SP32231
    Z=TK(NKB)                                                           SP32232
    IF(IEQN.EQ.ICHK(11)) Z=Z/DELZ(K)                                    SP32233
174 IF(K.EQ.K0) GO TO 175                                               SP32241
    SU=TK(N)                                                            SP32242
    IF(IEQN.EQ.ICHK(11))SU=SU/DELZ(K)                                   SP32243
```

```
175 RHO=S(N)/DELT                                                  SP32250

  2H,IDK1,IDK2,IWATER,IQRE,IP,JP,IQ,JQ,IK,JK,K5,IPU1,IPU2,ITK,IEQN   COF 170

      DATA N3/1/                                                     COF 195

      IF (K0.EQ.1.OR.ITK.EQ.ICHK(10).OR.N3.EQ.0) RETURN              COF 660

  2H,IDK1,IDK2,IWATER,IQRE,IP,JP,IQ,JQ,IK,JK,K5,IPU1,IPU2,ITK,IEQN   CHK 170

      VOLUME=AREA*DELZ(K)                                            CHK 455

      IF(IEQN.EQ.ICHK(11)) X=X*DELZ(K)                               CHK 555

      IF(IEQN.EQ.ICHK(11)) X=X*DELZ(K)                               CHK 625

      X=(PHI(I,J,K)-PHI(I,J,K-1))*TK(I,J,K-1)*AREA                   CHK 700

      X=(PHI(I,J,K)-PHI(I,J,K+1))*TK(I,J,K)*AREA                     CHK 790

      IF(IEQN.EQ.ICHK(11)) X=X*DELZ(K)                               CHK 865

      IF(IEQN.EQ.ICHK(11)) X=X*DELZ(K)                               CHK 935

C      ---CHECK FOR EQUATION BEING SOLVED---                         CHK1001
  180 IF(IEQN.EQ.ICHK(11)) GO TO 211                                 CHK1002
C                                                                    CHK1003
C     ---EQUATION 4---                                               CHK1004
C     ---RECHARGE AND WELLS---                                       CHK1010
      IF (K.EQ.K0.AND.IGRE.EQ.ICHK(7)) QREFLX=QREFLX+QRE(I,J)*AREA   CHK1020
      IF (WELL(I,J,K)) 190,210,200                                   CHK1030
  190 PUMP=PUMP+WELL(I,J,K)*AREA                                     CHK1040
      GO TO 210                                                      CHK1050
  200 CFLUX=CFLUX+WELL(I,J,K)*AREA                                   CHK1060
C                                                                    CHK1070
C     ---COMPUTE VOLUME FROM STORAGE---                              CHK1080
```

```
  210 STOR=STOR+S(I,J,K)*(OLD(I,J,K)-PHI(I,J,K))*AREA                  CHK1090
      GO TO 220                                                        CHK1091
C                                                                      CHK1092
C     ---EQUATION 3---                                                 CHK1093
C     ---RECHARGE AND WELLS---                                         CHK1094
  211 IF (K.EQ.K0.AND.IQRE.EQ.ICHK(7)) QREFLX=QREFLX+QRE(I,J)*VOLUME   CHK1095
      IF (WELL(I,J,K)) 212,214,213                                     CHK1096
  212 PUMP=PUMP+WELL(I,J,K)*VOLUME                                     CHK1097
      GO TO 214                                                        CHK1098
  213 CFLUX=CFLUX+WELL(I,J,K)*VOLUME                                   CHK1099
C                                                                      CHK1100
C     ---COMPUTE VOLUME FROM STORAGE---                                CHK1101
  214 STOR=STOR+S(I,J,K)*(OLD(I,J,K)-PHI(I,J,K))*VOLUME                CHK1102
  220 CONTINUE                                                         CHK1103


      X=X+(PHI(I,J,1)-PHI(I,J,2))*TK(I,J,1)*DELX(J)*DELY(I)            CHK1500
  250 Y=Y+(PHI(I,J,K1)-PHI(I,J,K0))*TK(I,J,K1)*DELX(J)*DELY(I)         CHK1520


     2H,IDK1,IDK2,IWATER,IQRE,IP,JP,IQ,JQ,IK,JK,K5,IPU1,IPU2,ITK,IEQN  PRN 150


     1UN2','ITKR','EQN3',2*0/                                          BLK 140
//
```