Using MODFLOW for Groundwater Flow Modeling
(From MODFLOW Reference and User Manuals)

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INTRODUCTION

A groundwater flow model comprises of the following components: (1) An equation governing the groundwater flow (2) An algorithm to numerically solve the flow equation to compute the time and space distribution of the head (3) A set of algorithms to compute the problem-specific state variables (such as nodal depths to water table) from the pre-computed head distributions, and (4) A computer program to implement the selected algorithms. Amongst the several computer programs available, the MODFLOW code developed by US Geological Survey is one of the widely used programs by groundwater professionals.

MODFLOW is basically a computer program that simulates three-dimensional groundwater flow through a porous medium by using the finite-difference method. It was originally documented by McDonald and Harbaugh of US Geological Survey in 1984. As with most computer programs that are used over a long time period, MODFLOW has undergone several overall updates. The program uses a modular structure wherein similar program functions are grouped together, and specific computational and hydrologic options are constructed in such a manner that each option is independent of other options. The modular structure consists of a Main Program and a series of highly independent subroutines called "modules." The modules are grouped into "packages." Each package deals with a specific feature of the hydrologic system which is to be simulated, such as flow from rivers or flow into drains, or with a specific method of solving linear equations which describe the flow system, such as the Strongly Implicit Procedure or Slice-Successive Overrelaxation. Applications of MODFLOW are numerous including estimation of recharge from rainfall, effect of artificial recharge on water table, stream-aquifer interaction, pumpage and drainage problems etc.

MATHEMATICAL BACKGROUND

The three-dimensional partial-differential equation of groundwater flow used in MODFLOW is (McDonald and Harbaugh, 1988)

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)+W=S_s\frac{\partial h}{\partial t} \qquad (1)$$

where K_{xx}, K_{yy}, and K_{zz} are values of hydraulic conductivity along the x, y, and z coordinate axes, which are assumed to be parallel to the major axes of hydraulic conductivity (L/T); h is the potentiometric head (L); W is a volumetric flux per unit volume representing sources and/or sinks of water, with $W<0.0$ for flow out of the ground-water system, and $W>0.0$ for flow in (T^{-1}); S_S is the specific storage of the porous material (L^{-1}); and t is time (T). Equation (1), when

combined with boundary and initial conditions, describes transient three-dimensional groundwater flow in a heterogeneous and anisotropic medium, provided that the principal axes of hydraulic conductivity are aligned with the coordinate directions. The program solves Eq. (1) using the finite-difference method in which the groundwater flow system is divided into a grid of cells (Fig. 1).

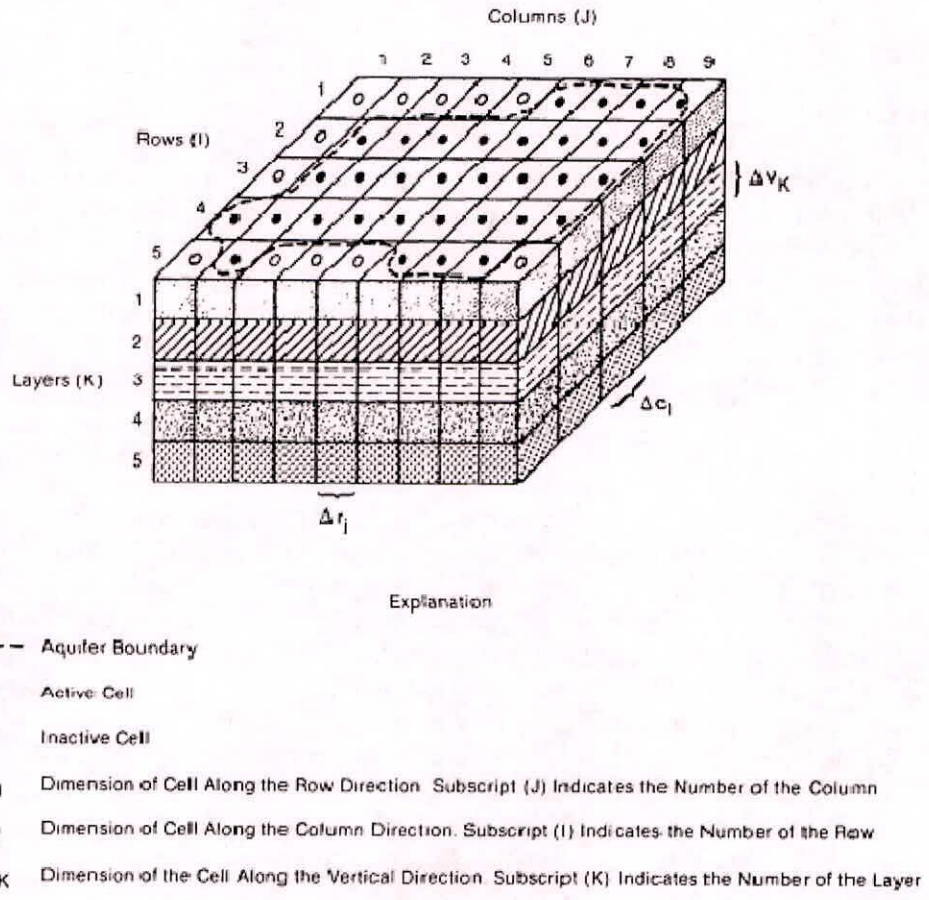

Fig. 1 A discretized hypothetical aquifer system (McDonald and Harbaugh, 1988)

For each cell, there is a single point, called a node, at which head is calculated. The finite-difference equation for a cell is (McDonald and Harbaugh, 1988)

$$\begin{aligned} &CR_{i,j-\frac{1}{2},k}\left(h^m_{i,j-1,k}-h^m_{i,j,k}\right) + CR_{i,j+\frac{1}{2},k}\left(h^m_{i,j+1,k}-h^m_{i,j,k}\right) \\ &+ CC_{i-\frac{1}{2},j,k}\left(h^m_{i-1,j,k}-h^m_{i,j,k}\right) + CC_{i+\frac{1}{2},j,k}\left(h^m_{i+1,j,k}-h^m_{i,j,k}\right) \\ &+ CV_{i,j,k-\frac{1}{2}}\left(h^m_{i,j,k-1}-h^m_{i,j,k}\right) + CV_{i,j,k+\frac{1}{2}}\left(h^m_{i,j,k+1}-h^m_{i,j,k}\right) \\ &+ P_{i,j,k}\,h^m_{i,j,k} + Q_{i,j,k} = SS_{i,j,k}\left(DELR_j \times DELC_i \times THICK_{i,j,k}\right)\frac{h^m_{i,j,k}-h^{m-1}_{i,j,k}}{t^m-t^{m-1}} \end{aligned} \qquad (2)$$

where $h^m_{i,j,k}$ is head at cell i,j,k at time step m (L); CV, CR, and CC are hydraulic conductances, or branch conductances, between node i,j,k and a neighboring node (L^2/T); $P_{i,j,k}$ is the sum of coefficients of head from source and sink terms (L^2/T); $Q_{i,j,k}$ is the sum of constants from source and sink terms, with $_{Qi,j,k} < 0.0$ for flow out of the ground-water system, and $Q_{i,j,k} > 0.0$ for flow in (L^3/T); $SS_{i,j,k}$ is the specific storage (L^{-1}); DELRj is the cell width of column j in all rows (L); $DELC_i$ is the cell width of row i in all columns (L); $THICK_{i,j,k}$ is the vertical thickness of cell i,j,k (L); and t^m is the time at time step m (T). To designate hydraulic conductance between nodes, as opposed to hydraulic conductance within a cell, the subscript notation '1/2' is used.

For steady-state stress periods, the storage term and, therefore, the right-hand side of Eq. (2) is set to zero. The application of Eq. (2) to all cells defines a set of simultaneous equations, and these equations are solved for head at each node. For solution by computer, Eq. (2) for a time step 'm' is modified into the form:

$$CV_{i,j,k-\frac{1}{2}}\,h_{i,j,k-1} + CC_{i-\frac{1}{2},j,k}\,h_{i-1,j,k} + CR_{i,j-\frac{1}{2},k}\,h_{i,j-1,k}$$

$$+ (-CV_{i,j,k-\frac{1}{2}} - CC_{i-\frac{1}{2},j,k} - CR_{i,j-\frac{1}{2},k} - CR_{i,j+\frac{1}{2},k} - CC_{i+\frac{1}{2},j,k} - CV_{i,j,k+\frac{1}{2}} + HCOF_{i,j,k})\,h_{i,j,k}$$

$$+ CR_{i,j+\frac{1}{2},k}\,h_{i,j+1,k} + CC_{i+\frac{1}{2},j,k}\,h_{i+1,j,k} + CV_{i,j,k+\frac{1}{2}}\,h_{i,j,k+1} = RHS_{i,j,k} \quad . \tag{3}$$

$HCOF_{i,j,k}$ contains $P_{i,j,k}$ and the negative of the part of the storage term that includes the head in the current time step m. RHS includes -Q and the part of the storage term that is multiplied by the head at time step m-1. The CV, CR, and CC coefficients and the storage-related parts of HCOF and RHS are all calculated by a single package, which is called an internal flow package. Each package that contributes a different source or sink term is called a source-term package. Sinks are viewed as negative sources. MODFLOW is designed so that any number of source-term packages can be in use in a simulation, but there can be only a single internal-flow package in use. However, there can be multiple internal-flow packages available from which to choose. The original MODFLOW included the Block-Centered Flow (BCF) Package; subsequently, the Generalized Finite-Difference (GFD) Package and Layer-Property Flow (LPF) Package have been developed.

Equation (3) is written only at cells for which head must be calculated. A variable named IBOUND is defined at each cell to indicate that the head in the cell should be calculated (called a variable-head cell); that water cannot flow through the cell (called a no-flow cell); or that the head should not change from a user-specified value (called a constant- or specified-head cell).

Space Discretization

The finite-difference grid is assumed to be rectangular horizontally, while the grid can be distorted vertically (Fig. 2). The program requires the definition of the complete geometry of the each cell including vertical cell geometry. The horizontal grid dimensions are specified in variables DELR and DELC (Fig. 2A). Columns are numbered starting from the left side of the grid. Rows are numbered starting from the upper edge (plan view) of the grid. DELRj is the width of the cells (from the left side to the right side) in column j. That is, all the cells in a

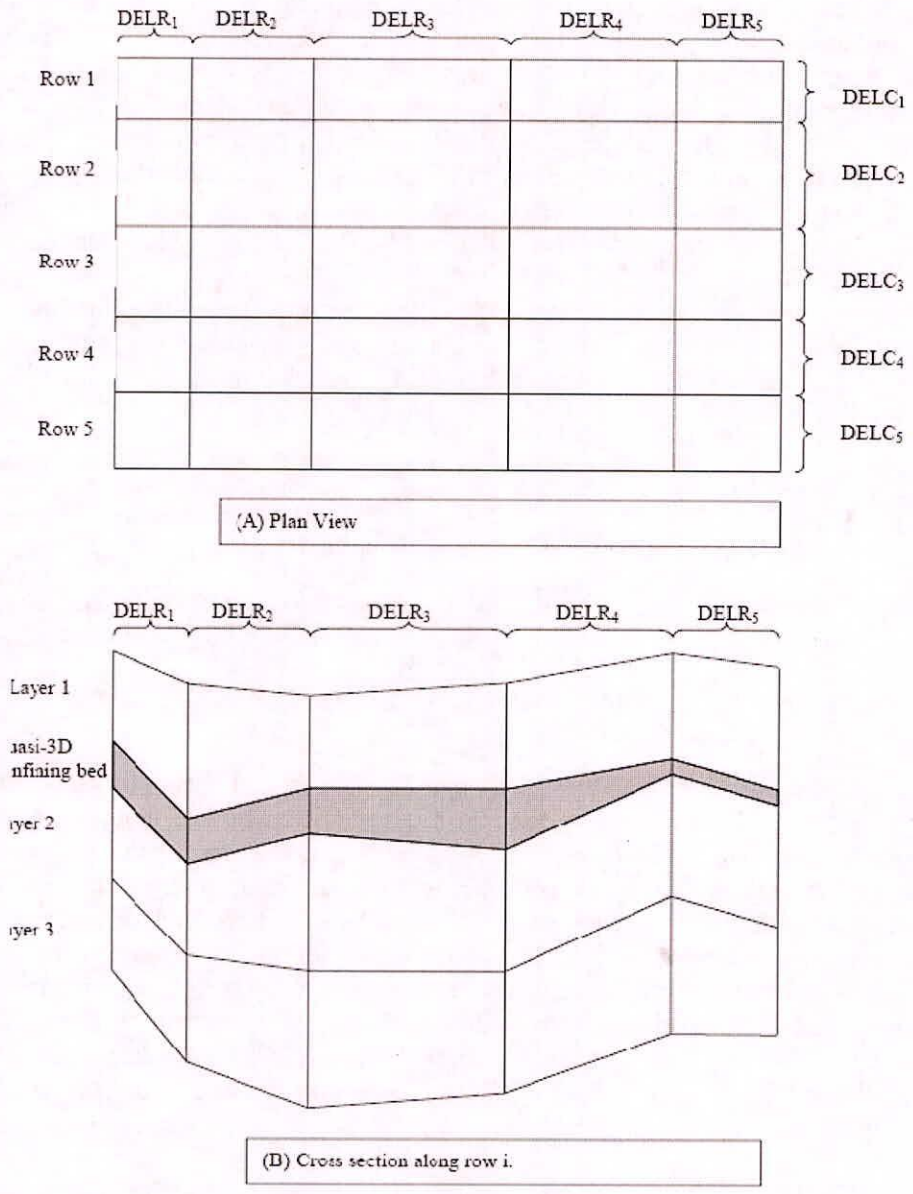

Fig. 2 Finite-difference grid with (A) plan view and (B) cross-section view (McDonald and Harbaugh, 1988)

column have the same width, and there is one value of DELR for each of the NCOL columns in the model grid. Similarly, DELCi is the width of cells (from the top to the bottom in plan view) in rows i, and there is one value of DELC for each of the NROW rows in the model grid.

Layers are numbered starting from the top layer and going down (Fig. 2B). Elevation of the top of layer 1 is defined in addition to the bottom elevation of every layer. The elevation information can be used to calculate the thickness of all cells. Below each layer except the

bottom layer, there can also be a confining bed through which only vertical flow is simulated. Simulating confining beds by this method often is called the Quasi-Three-Dimensional (Quasi-3D) Approach (McDonald and Harbaugh, 1988). There is no requirement to use the Quasi-3D Approach; that is, any confining bed can be simulated using one or more distinct model layers as desired.

Time Discretization

The fundamental component of time discretization is the time step. Time steps are grouped into stress periods (Fig. 3). Time dependent input data can be changed every stress period. For each stress period, the user specifies the total length (PERLEN), the number of time steps (NSTP), and the multiplier for the length of successive time steps (TSMULT). The length of the first time (Δt_1) step can be determined from the following equation:

$$\Delta t_1 = \text{PERLEN}\left(\frac{\text{TSMULT}-1}{\text{TSMULT}^{\text{NSTP}}-1}\right) \tag{4}$$

MODFLOW is designed to simulate steady state or transient conditions. For steady state, the storage term in the groundwater flow equation is set to zero. This is the only part of the flow equation that depends on length of time, so the stress-period length does not affect the calculated heads in a steady-state simulation. However, it is required in MODFLOW that the length of a steady-state stress period be specified, partly so that the same input mechanism for all stress periods can be used. A single time step is all that is required for steady-state stress periods.

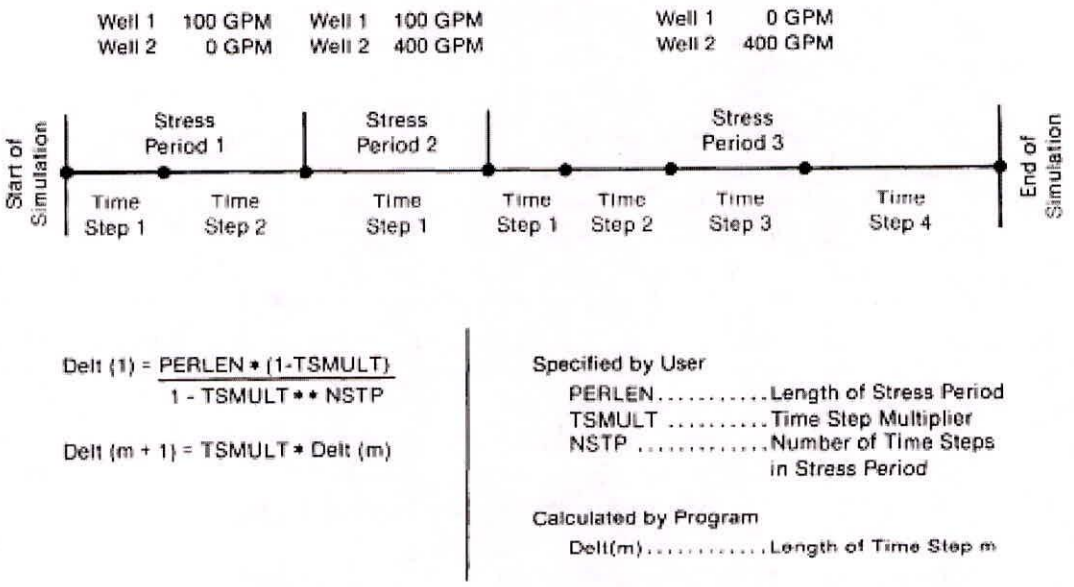

Fig. 3 Division of simulation time into stress periods and time steps (McDonald and Harbaugh, 1988)

Units of Length and Time – The program formulates the groundwater flow equation without using prescribed length and time units. Any consistent units of length and time can be used when specifying the input data for a simulation. It is expected that other processes will generally work with consistent length and time units; however, there could be situations in which there is a requirement to specify the length or time units. In such situations, the input instructions will state the requirements.

Use of Parameters

Many of the numerous data values that must be specified for each model cell can be specified using parameters. A parameter is a single value that can be used to determine data values for multiple cells. Parameters can often make data input more convenient because of the multi-cell capability. For example, parameters can make it easier to adjust model data when manually calibrating a model or making multiple projection simulations in which many data values must be modified by prescribed amounts. Also, parameters are required when using some other processes. For example, the Parameter-Estimation Process requires parameters to be defined because it is generally impossible to estimate the optimum values for all the types of data at all cells. Even in a small model, thousands of data values are used, yet the available observation data are typically only sufficient to estimate a relatively small number of values. Thus, the Parameter-Estimation Process estimates the optimum value for a more limited number of parameters.

The most common and direct approach for determining data values from parameters is to have the value for an individual cell be defined by one parameter. A more complex approach can also be used in which the data value for a single cell is determined by adding contributions from multiple parameters. This additive approach allows interpolation techniques, such as kriging, to be used to produce smooth variations of data values throughout a region based upon the multiple parameter values.

Layer Data and List Data

Layer data refers to any type of data for which a value is required for every cell in one or more horizontal layers of the grid. Examples of layer data include areal recharge flux, hydraulic conductivity, and specific storage. One approach for defining layer data is to directly read it as input data. This direct approach is implemented by utility modules, which provide a common mechanism for reading the layer data required for any package. When layer data are required for multiple layers, the utility modules read the data a layer at a time. For each layer, the user can specify either a single value that will apply to all of the cells in the layer or individual values for each cell, which are read row by row starting at row 1. Some layer data can be defined using parameters. For layer data, the user can usually choose between either directly reading the data (through the utility modules) or using parameters, but the same method must be used consistently for any type of input data. That is, if parameters are used to define hydraulic conductivity in a layer, parameters must be used to define hydraulic conductivity for all layers.

List data refers to any type of data for which data values are required for only some of the cells in the grid. Examples include the well recharge rate as simulated by the Well Package and the riverbed conductance as simulated by the River Package. As with layer data, one approach for defining list data is to directly read it as input data. One line of data is read for each

cell for which data are required. For most of the packages that read list data, each line of data includes the layer, row, and column of the cell for which the data applies and one or more types of data. For example, the River Package requires three types of data for each cell at which a river interacts with the ground-water system (river stage, riverbed conductance and riverbed bottom elevation), and each line of data includes all three data types. Some list data to be defined using parameters. When parameters are allowed for defining list data, it is generally possible to define some values in a list by directly reading and other values in the same list through parameters.

OVERALL STRUCTURE OF MODFLOW

The flowchart in Fig. 4 shows the overall functioning of the program for a simulation run. Thus, within a simulation, there are three nested loops: a stress-period loop, within which there is a time-step loop, which in turn contains an iteration loop.

MODFLOW Packages

Various modules are provided in MODFLOW to deal with various field situations, as given below:

- Basic package (BAS)
- Block-centered flow package (BCF)
- River package (RIV)
- Recharge package (RCH)
- Well package (WEL),
- Drain package (DRN)
- Evapotranspiration package (EVT)
- General head boundary package (GHB)

Conceptualization and implementation of these modules are briefly discussed in subsequent sections.

BASIC PACKAGE

The Basic Package handles a number of administrative tasks for the model. It reads data on the number of rows, columns, layers, and stress periods, on the major options to be used, and on the location of input data for those options. It allocates space in computer memory for model arrays; it reads data specifying initial and boundary conditions; it reads and implements data establishing the discretization of time; it sets up the starting head arrays for each time step; it calculates an overall water budget; and it controls model output according to user specification.

Initial Conditions - A head distribution at the beginning of each time step is required to calculate the head distribution at the end of that time step. For each time step after the first, the head distribution at the start of one time step is set equal to the head distribution at the end of the previous time step. For the first time step, "starting heads" are specified by the user. These specified initial heads are used for head calculation only in the first time step; however, they may also be saved, and used to calculate drawdown, the difference between the starting head distribution and some later head distribution.

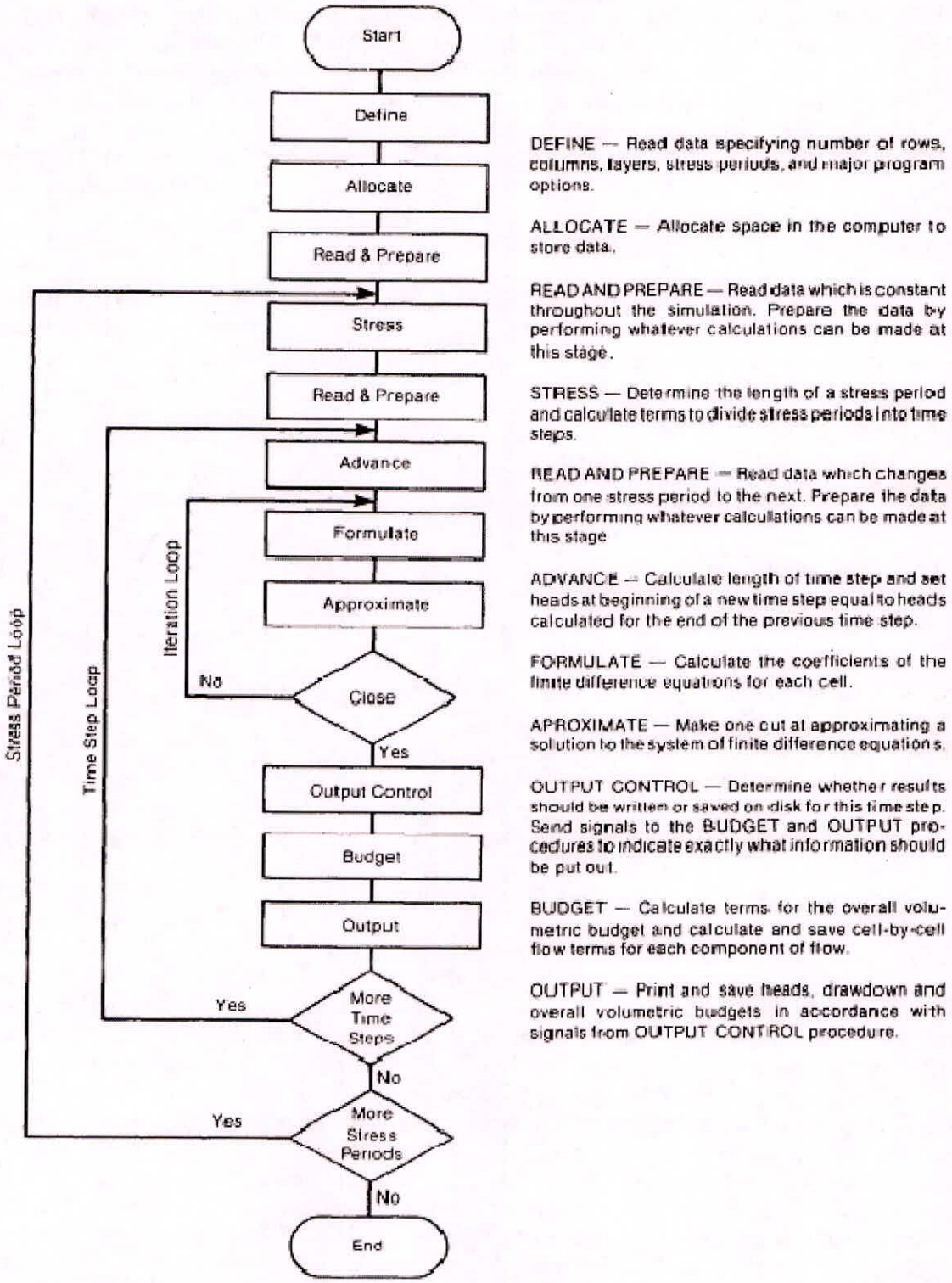

Fig. 4 Overall program structure (McDonald and Harbaugh, 1988)

Output - The primary output of the program is head distribution. The user may control the frequency at which heads are printed or saved on disk through the "Output Control" option. Other output items include drawdowns and volumetric budget terms; the Output Control option also provides for storage or printing of these terms. If Output Control is not utilized, a default output option is invoked—the head distribution and the overall volumetric budget are printed at the end of each stress period, and drawdowns are also printed if starting heads were saved.

BLOCK-CENTERED FLOW PACKAGE

The Block-Centered Flow (BCF) Package computes the conductance components of the finite-difference equation which determine flow between adjacent cells. It also computes the terms that determine the rate of movement of water to and from storage. To make the required calculations, it is assumed that a node is located at the center of each model cell.

Data Requirements

The fundamental variables controlling cell-to-cell flow and storage in the model are entered through the Block-Centered Flow Package input. These variables, depending on the options which are invoked, may include transmissivity, hydraulic conductivity, specific yield, confined storage coefficient, aquifer bottom elevation and aquifer top elevation. Within each layer the required parameters should be specified for every cell, including constant-head and no-flow cells. For no-flow cells, the entered values are never used in calculation, and thus any values may be specified; for constant head cells, the storage terms are not used but the other parameters are, and realistic values for those parameters must be entered.

In the formulation of storage terms, the program distinguishes between layers in which storage coefficient values remain constant throughout the simulation, and those in which the storage coefficient may "convert" from a confined value to a water table value, or vice-versa, as the water level in a cell falls below or rises above the top of the cell. This distinction is made through the use of a layer flag. In all, the model recognizes the following four types of layers, incorporating various combinations of the options provided by the BCF Package:

Layer-type 0 - In this category there is no provision for modification of transmissivity as water level varies, for storage term conversion, or for limitation of vertical flow from above if water level falls below the top of the cell. This layer type is normally used to simulate confined conditions, but could also be used to simulate a layer in which unconfined conditions will always prevail, provided drawdowns are expected to be a small fraction of layer thickness and flow from the overlying layer (if present) is expected to be negligible. If the simulation is transient, storage coefficient or specific yield values are also entered in the input array.

Layer-type 1 - This layer type is utilized only in a single-layer model or in the uppermost layer of a model, and only where unconfined conditions are expected to persist in the layer throughout the entire period of simulation. No provision is made for storage term conversion, by virtue of the assumption that water table conditions will always prevail; and no provision is made for limiting flow from above under dewatered conditions, since layer-type 1 is used only for the uppermost layer of a model. However, transmissivities are computed at each iteration as the products of hydraulic conductivity and saturated thickness values within the layer. Thus the input

data includes hydraulic conductivity and cell bottom elevation, rather than transmissivity. If the simulation is indicated as transient, specific yield values are entered in the input array.

Layer-type 2 - This layer type is used where the situation may alternate between confined and unconfined conditions, so that storage term conversion and limitation of flow from above under dewatered conditions are both desirable; but where the saturated thickness is expected to remain everywhere a high fraction of the layer thickness throughout the period of simulation, so that recalculation of transmissivity as the product of hydraulic conductivity and saturated thickness is not necessary. The storage term conversion option requires that both a confined storage coefficient and a specific yield value be specified for each cell, and that the top elevation be specified for each cell; the top elevation is also used in the option to limit flow from above under dewatered conditions.

Layer-Type 3 - This layer type incorporates all of the BCF options associated with water table conditions. Transmissivities are recalculated at each iteration using hydraulic conductivities and layer bottom elevations, and both storage term conversion and limitation of flow from above under dewatered conditions are implemented. The required data thus includes hydraulic conductivities, layer bottom elevations, confined storage coefficients (if transient), specific yields (if transient), vertical leakances and layer top elevations.

RIVER PACKAGE

Rivers and streams contribute water to the ground-water system or drain water from it depending on the head gradient between the stream and the ground-water regime. The purpose of the River Package is to simulate the effects of flow between surface-water features and ground-water systems. To accomplish this, terms representing seepage to or from the surface features must be added to the groundwater flow equation for each cell affected by the seepage.

Figure 5 shows a stream divided into reaches so that each reach is completely contained in a single cell. Stream aquifer seepage is simulated between each reach and the model cell that contains that reach.

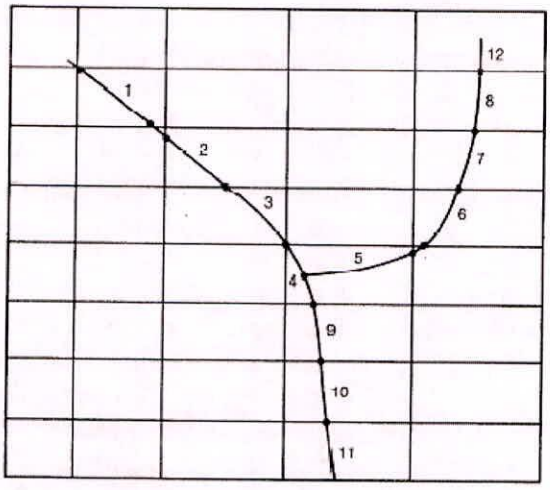

Fig. 5 Discretization of a stream into reaches (McDonald and Harbaugh, 1988)

The cross-section of Fig. 6a shows a situation in which the open water of a stream is separated from the ground-water system by a layer of low permeability streambed material. Figure 6b shows an idealization of this system in which the stream-aquifer interconnection is represented as a simple conductance through which one-dimensional flow occurs. The system of Fig. 6 is helpful in conceptualizing and describing the simulation of stream-aquifer interaction; however, it must be recognized that, in many instances, no discrete low-permeability streambed layer is present. The techniques of simulation developed through the conceptualization of Fig. 6 can still be applied to represent these situations, provided proper interpretation is placed on the various terms and parameters that are used.

The length of an idealized streambed conductance block is taken as the length of the stream, L, as it crosses the node; the width is taken as the stream width, W; the distance of flow is taken as the thickness, M, of the streambed layer; and the hydraulic conductivity of the streambed material is designated K. The assumption is made that measurable head losses between the stream and the aquifer are limited to those across the streambed layer itself--that is, that there is no significant head loss between the bottom of the streambed layer and the point represented by the underlying model node. It is further assumed that the underlying model cell remains fully saturated--that is, that its water level does not drop below the bottom of the streambed layer. Under these assumptions, flow between the stream and the ground-water system is given by

$$QRIV = CRIV (HRIV - hi,j,k) \tag{5}$$

where QRIV is the flow between the stream and the aquifer, taken as positive if it is directed into the aquifer; HRIV is the head in the stream; CRIV is the hydraulic conductance of the stream-aquifer interconnection (KLW/M), and hi,j,k is the head at the node in the cell underlying the stream reach.

Equation (5) provide an acceptable approximation of stream-aquifer interaction over a certain range of aquifer head values. In most cases, however, if water levels in the aquifer fall below a certain point, seepage from the stream ceases to depend on head in the aquifer. Thus, water level in the aquifer may fall below the bottom of the streambed layer, leaving an unsaturated interval beneath that layer; in this case if it is assumed that the streambed layer itself remains saturated, the head at its base will simply be the elevation at that point. If this elevation is designated RBOT, the flow through the streambed layer is given

$$QRIV = CRIV (HRIV - RBOT) \tag{6}$$

The program utilizes these concepts in simulating stream-aquifer interaction--that is, flow between a stream and a node i,j,k is simulated according to the equation set

$$QRIV = CRIV (HRIV - hi,j,k), \quad hi,j,k > RBOT \tag{7}$$

$$QRIV = CRIV (HRIV - RBOT), \quad hi,j,k < RBOT \tag{8}$$

The simplified model of stream-aquifer interaction utilized here assumes that this interaction is independent of the location of the stream reach within the cell, and that the level of water in the stream is uniform over the reach, and constant over each stress period. The latter

assumption implies that conditions of flow in the stream do not vary significantly during the stress period-- for example, that the stream does not go dry or overflow its banks, or that such events are of such short duration as to have no effect on stream-aquifer interaction.

Data describing each river are specified by the user for each stress period. Input consists of six entries for each river reach, specifying the layer, row, and column of the cell containing the reach, and the three parameters needed to calculate seepage--stream level or stage, the conductance of the stream-aquifer interconnection, and the bottom elevation or level at which the limiting value of stream seepage is attained.

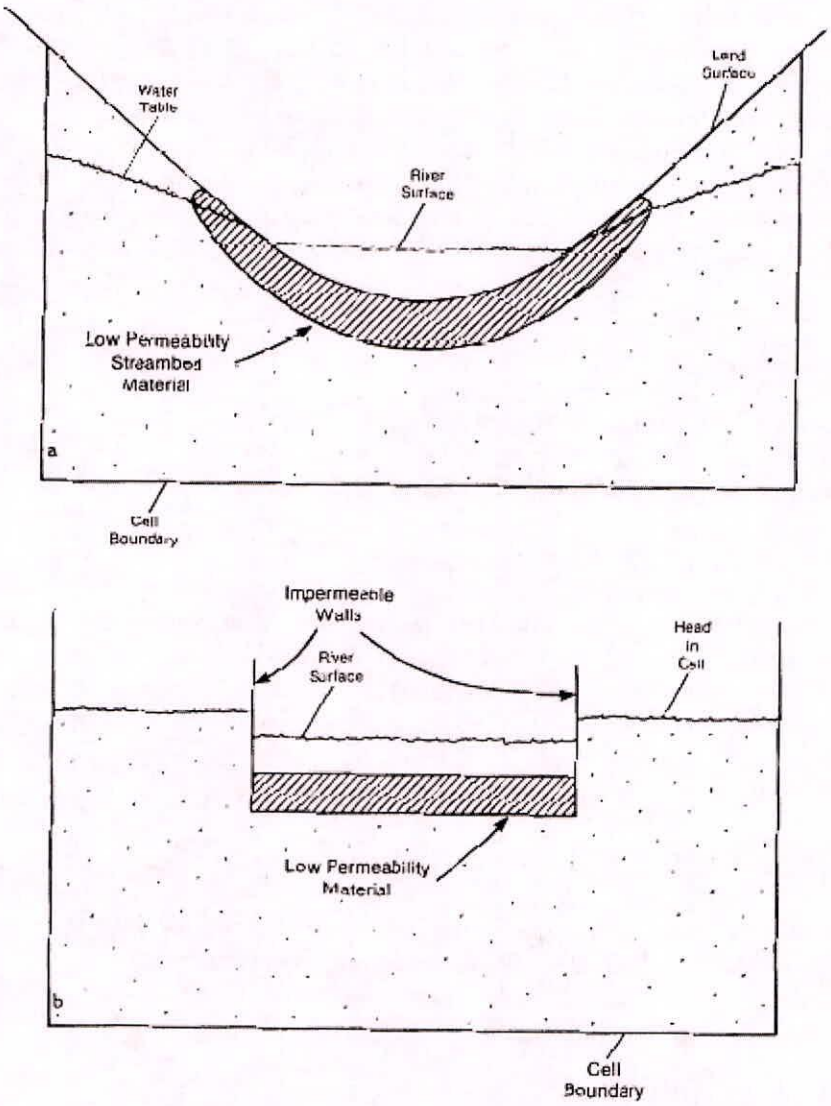

Fig. 6 (a) Cross section of an aquifer containing a stream, and (b) Conceptual representation of stream-aquifer interconnection in simulation (McDonald and Harbaugh, 1988)

RECHARGE PACKAGE

The Recharge (RCH) Package is designed to simulate areally distributed recharge to the ground-water system. Most commonly, areal recharge occurs as a result of precipitation that percolates to the ground-water system. Recharge applied to the model is defined as

$$QR_{i,j} = I_{i,j} * DELR_j * DELC_i \quad (9)$$

where $QR_{i,j}$ is the recharge flow rate applied to the model at horizontal cell location (i,j) expressed as a fluid volume per unit time; and $I_{i,j}$ is the recharge flux (in units of length per unit time) applicable to the map area, $DELR_j * DELC_i$, of the cell. The recharge, $QR_{i,j}$, is applied to a single cell within the vertical column of cells located at (i j). There is no need to allow for recharge to occur simultaneously at multiple depths in the same vertical column because natural recharge enters the ground-water system at its top. In the simplest situation, the top of the ground-water system will occur in model layer 1; however, the vertical position of the top of the system may vary with horizontal location and with time as the water-table rises and falls. The program incorporates three options for specifying the cell in each vertical column of cells that receives the recharge. The RCH Package can potentially be used to simulate recharge from sources other than precipitation -- for example, artificial recharge. If the ability to apply recharge to more than one cell in a vertical column of cells is required, then the Well Package, which allows recharge or discharge to be specified at any model cell, can be used.

The three options include: (1) application of the recharge to model layer 1; (2) application of the recharge to any cell in the vertical column as specified by layer numbers contained in two dimensional array IRCHi,j; and (3) application of the recharge to the uppermost active cell in the vertical column, provided there is no constant head cell above it in the column (Fig. 7). Under options 1 and 2, if a cell designated to receive recharge is no-flow, then no recharge is added. Under the third option, if there is a constant head cell in a vertical column of cells and there is no active cell above, then no recharge is applied to this column because it is assumed that any recharge would be intercepted by the constant head source.

For the typical situation of recharge from precipitation option 3 is the easiest to use. The model user does not have to be concerned about determining which is the highest active cell in a vertical column because the program automatically determines this throughout the simulation. Option 1, however, can be useful in situations where recharge should not pass through the no-flow cells in layer 1. For example, some cell may be designated no-flow because they are impermeable. Any recharge specified for those cells should not pass into layer 2. Of course option 3 could still be used in this situation by specifying that the recharge rate is zero at the impermeable cells. Similarly, option 2 may be useful when layers other than layer 1 have outcrop areas and when recharge to the specified layers should not penetrate through no-flow cells to a lower layer.

WELL PACKAGE

The Well Package is designed to simulate features such as wells which withdraw water from the aquifer (or add water to it) at a specified rate during a given stress period, where the rate is independent of both the cell area and the head in the cell. Well discharge is handled in the Well Package by specifying the rate, Q, at which each individual well adds water to the aquifer or

removes water from it, during each stress period of the simulation. Negative values of Q are used to indicate well discharge, while positive values of Q indicate a recharging well.

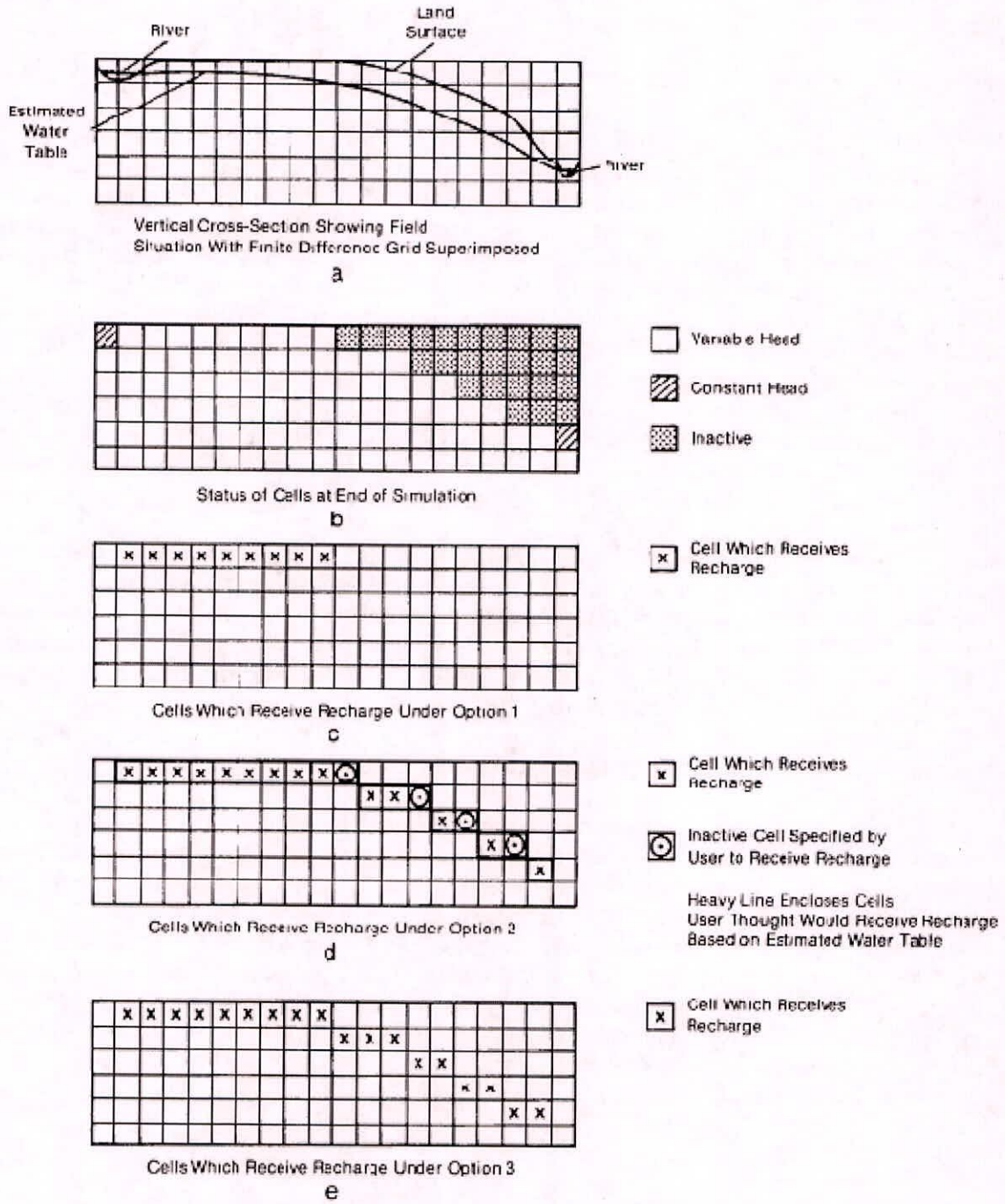

Fig. 7 Hypothetical problem showing which cells receive recharge under the three options available in Recharge Package (McDonald and Harbaugh, 1988)

DRAIN PACKAGE

The Drain Package is designed to simulate the effects of features such as agricultural drains, which remove water from the aquifer at a rate proportional to the difference between the head in the aquifer and some fixed head or elevation, so long as the head in the aquifer is above that elevation, but which have no effect if head falls below that level.

Figure 8 shows a cross section through a cell, illustrating concepts underlying the simulation of drains in the model. The drain is assumed to run only partially full, so that head within the drain is approximately equal to the median drain elevation, $d_{i,j,k}$. The head computed by the model for cell i,j,k ($h_{i,j,k}$) is actually an average value for the cell, and is normally assumed to prevail at some distance from the drain itself. The drain head, $d_{i,j,k}$ prevails only locally, within the drain--it does not characterize the cell as a whole. The head losses between $h_{i,j,k}$ and $d_{i,j,k}$ are assumed to be caused by three flow processes - convergent flow toward the drain, flow through material of different conductivity immediately around the drain, and flow through the wall of the drain. If the total head loss $h_{i,j,k}$-$d_{i,j,k}$ may be taken as proportional to the discharge QD (the discharge from cell i,j,k into the drain), the drain function can be described by the equation pair:

$$QD_{i,j,k} = CD_{i,j,k}(h_{i,j,k} - d_{i,j,k}) \qquad \text{for } h_{i,j,k} > d_{i,j,k} \qquad (10)$$

$$QD_{i,j,k} = 0 \qquad \text{for } h_{i,j,k} \leq d_{i,j,k} \qquad (11)$$

The coefficient $CD_{i,j,k}$ of Eq. (10) is a lumped (or equivalent) conductance describing all of the head loss between the drain and the region of cell i,j,k in which the head $h_{i,j,k}$ can be the assumed to prevail. It depends on the characteristics of the convergent flow pattern toward the drain as well on the characteristics of the drain itself and its immediate environment.

In practice, it is more common to calculate CD from measured values of QD and h-d using Eq. (10). If h-d is not accurately known, CD is usually adjusted during model calibration in order to match measured values of QD to model calculated values.

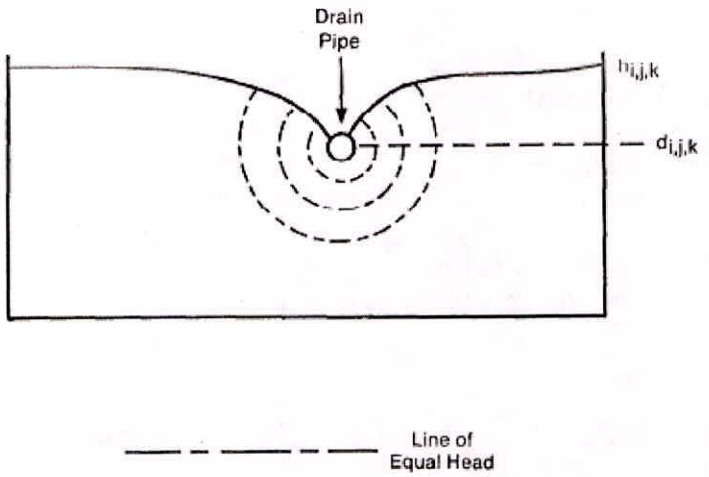

Fig. 8 Cross section through cell i,j,k illustrating head loss in covergent flow drain (McDonald and Harbaugh, 1988)

EVAPOTRANSPIRATION PACKAGE

The Evapotranspiration (ET) Package simulates the effects of plant transpiration and direct evaporation in removing water from the saturated ground water regime. The approach is based on the following assumptions: (1) when the water table is at or above a specified elevation, termed the "ET surface", evapotranspiration loss from the water table occurs at a maximum rate specified by the user; (2) when the depth of the water table below the ET surface elevation exceeds a specified interval, termed the "extinction depth" or "cutoff depth", evapotranspiration from the water table ceases; and (3) between these limits, evapotranspiration from the water table varies linearly with water table elevation. This can be expressed in equation form as

$$R_{ETi,j} = R_{ETMi,j} \qquad h_{i,j,k} > hs_{i,j} \qquad (12)$$

$$R_{ETi,j} = 0 \qquad h_{i,j,k} < (hs_{i,j} - di,j) \qquad (13)$$

$$R_{ETi,j} = R_{ETMi,j}\,[h_{i,j,k} - (hs_{i,j} - d_{i,j})]/d_{i,j} \qquad (hs_{i,j} - d_{i,j}) \le h_{i,j,k} \le hs_{i,j} \qquad (14)$$

where $R_{ETi,j}$ is the rate of loss per unit surface area of water table due to evapotranspiration, in volume of water per unit area per unit time, within the map area DELRj*DELCi; $h_{i,j,k}$ is the head, or water table elevation in the cell from which the evapotranspiration occurs; $R_{ETMi,j}$ is the maximum possible value of $R_{ETi,j}$; $hs_{i,j}$ is the ET surface elevation, or the water table elevation at which this maximum value of evapotranspiration loss occurs; and $d_{i,j}$ is the cutoff or extinction depth, such that when the distance between $hs_{i,j}$ and $h_{i,j,k}$ exceeds $d_{i,j}$ evapotranspiration ceases. In implementing the finite difference approach the volumetric rate of evapotranspiration loss from a given cell is given as the product of the loss rate per unit area, and the horizontal surface area, DELRj*DELCi, of the cell from which the loss occurs, i.e.

$$Q_{ETi,j} = R_{ETi,j} * DELRj * DELCi \qquad (15)$$

where $Q_{ETi,j}$ is the evapotranspiration, in volume of water per unit time, through the area DELRj*DELCi. Evapotranspiration is drawn from only one cell in the vertical column beneath the map area DELRj*DELCi; the user designates the cell (i.e. the layer, k) using one of two options. Under the first option, evapotranspiration is always drawn from the uppermost layer of the model; under the second, the user specifies the cell, within the vertical column at i,j, from which the evapotranspiration is to be taken.

GENERAL-HEAD BOUNDARY PACKAGE

The function of the General-Head Boundary (GHB) Package is mathematically similar to that of the River, Drain and Evapotranspiration packages, in that flow into or out of a cell i,j,k, from an external source is provided in proportion to the difference between the head in the cell, $h_{i,j,k}$, and the head assigned to the external source, $hb_{i,j,k}$. Thus, a linear relationship between flow into t he cell and head in the cell is established, i.e.

$$Qb_{i,j,k} = Cb_{i,j,k}\,(hb_{i,j,k} - h_{i,j,k}) \qquad (16)$$

where $Qb_{i,j,k}$ is the flow into cell i,j,k from the source; $cb_{i,j,k}$ is the conductance between the external source and cell i,j,k; $hb_{i,j,k}$ is the head assigned to the external source; and $h_{i,j,k}$ is the head in cell i,j,k. The relationship between cell i,j,k and the external source is shown schematically in Fig. 9. The constant-head source is represented by the apparatus on the right in

Fig. 9, which holds the source head at the level hb regardless of other factors; the link between the source and cell i,j,k is represented by the block of porous material $Cb_{i,j,k}$. In contrast to the River, Drain and Evapotranspiration packages, the GHB Package provides no limiting value of flow to bound the linear function in either direction; and as the head difference between cell i,j,k and the source increases, flow into or out of the cell continues to increase without limit. Care must accordingly be used in utilizing the GHB Package to insure that unrealistic flows into or out of the system do not develop during the course of simulation.

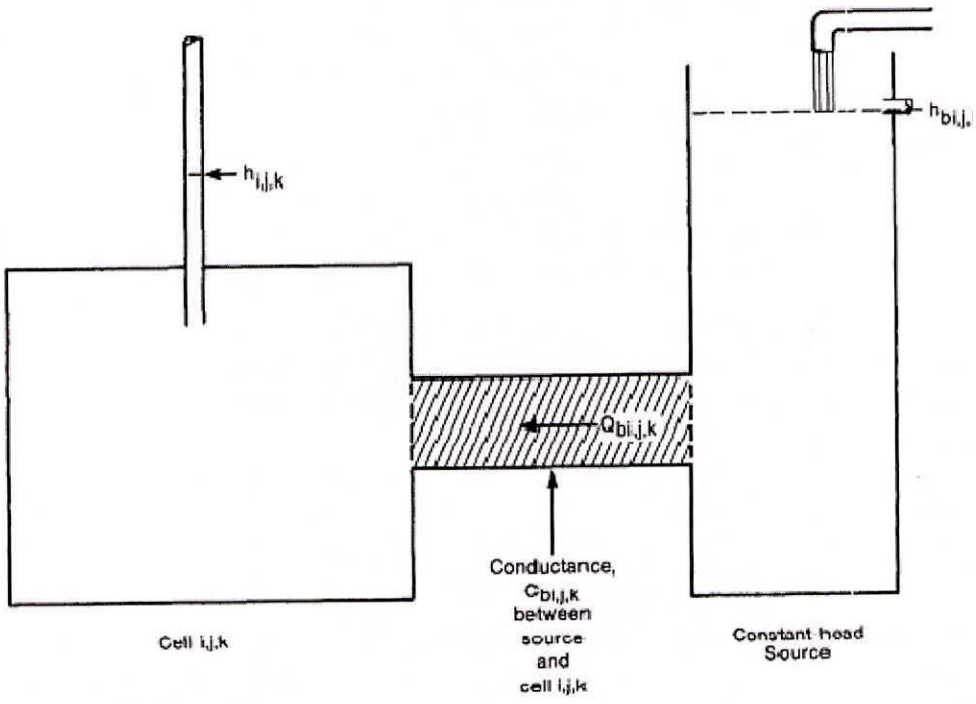

Fig. 9 Schematic diagram illustrating principle of general-head boundary package (McDonald and Harbaugh, 1988)

MODFLOW UPDATES

In recent versions of the program, packages like Horizontal flow package and Layer boundary flow package have been added. Furthermore, in MODFLOW (version 2000) the Source Term Packages have been introduced, wherein the packages are divided according to whether they are head dependent or head independent.

- Head-Dependent Packages: RIV, DRN, GHB, EVT
- Head-Independent Packages: WEL, RCH

Other packages included are the *Time-Variant Specified-Head Package* (CHD), and *Solver Packages* like SIP (strongly implicit procedure), SOR (slice successive overrelaxation), PCG (preconditioned Conjugate Gradient), and DE4 (direct solution based on alternating diagonal ordering).

STEPS FOR GROUNDWATER FLOW MODELLING

Develop a conceptual model of the system. A conceptual model is a simplified representation of the groundwater flow system, frequently in pictorial form that defines the hydrostratigraphic units of interest and all system boundaries. During this step, field data are assembled including information on water balance and data needed to assign values to aquifer parameters and hydrologic stresses. This includes definition of hydrostratigraphic units and system boundaries.

Select the computer code to be used. The code is the computer program that contains an algorithm to numerically solve the mathematical model. Both the governing equation and code should be verified to demonstrate: a) the governing equation accurately describes the physical processes occurring, and b) the computer program accurately solve the equations that make-up the mathematical model.

Design the model. The conceptual model is put into a form suitable for modeling. This step includes grid design, selection of time steps, setting boundary and initial conditions, and preliminary selection of values for aquifer parameters and hydrologic stresses.

Calibrate the model. The purpose of calibration is to establish that the model can reproduce field-measured heads and flows within a reasonable margin of error. Calibration is accomplished by trial-and-error adjustment of parameters or by using an automated parameter estimation code.

Conduct sensitivity analysis. Sensitivity analysis is performed to ascertain the effects of uncertainty on the calibrated model. The model is influenced by uncertainty owing to the inability to define the exact spatial and temporal distribution of parameter values in the problem domain. There is also uncertainty over definition of boundary conditions and stresses.

Use the model for predictive simulations. Prediction quantifies the response of the system to future events. The model is run with calibrated values for parameters and stresses, except for those stresses expected to change in the future. Uncertainty in a predictive simulation arises from uncertainty in the calibrated model and the inability to estimate accurate values for the magnitude and timing of future stresses. Predictive sensitivity analysis quantifies the uncertainty in parameter values on the prediction. Ranges in estimated future stresses are simulated to examine the impact on the model's prediction.

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