TRAINING COURSE

ON

COMPUTER APPLICATIONS IN HYDROLOGY

(UNDER WORLD BANK AIDED HYDROLOGY PROJECT)

Module 14

MODFLOW

for

Ground Water Modelling

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MODFLOW FOR GROUNDWATER MODELLING

1.0   INTRODUCTION

MODFLOW (MODular 3-dimensional finite difference groundwater FLOW model) is originally developed by McDonald and Harbaugh of the USGS, USA in 1984. As the name suggests, the model simulates flow in three dimensions. This lecture intends to present briefly about the development of the model and its capabilities in general.

Brief description is provided on the physical concepts on which the model is based while avoiding complex mathematics involved. 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 hydrological 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.

The division of the program into modules permits the user to examine specific hydrologic features of the model independently. This also facilitates development of additional capabilities because new modules or packages can be added to the program without modifying the existing modules or packages. The input and output systems of the computer program are also designed to permit maximum flexibility.

Ground-water flow within the aquifer is simulated using a block-centred finite-difference approach. Layers can be simulated as confined, unconfined, or a combination of confined and unconfined. Flow from external stresses, such as flow to wells, areal recharge, evapotranspiration, flow to drains, and flow through river beds, can also be simulated. The finite-difference equations can be solved using either the Strongly Implicit Procedure or Slice-Successive Over-relaxation methods.

Because of the modular structure, new options can be added without the necessity of changing existing subroutines. The model may be used for either two-or three-dimensional applications. Generalised input and output procedures have been adopted to suit particular applications.

The major options that are available include procedures to simulate the effects of wells, recharge, rivers, drains, evapotranspiration, and general-head boundaries. The solution algorithms available include two iteration techniques.

2.0   MODEL FORMULATION

The three dimensional unsteady groundwater flow through heterogeneous and anisotropic porous earth material is given by the partial differential equation:

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

where,

K_{xx}, K_{yy}, K_{zz} : hydraulic conductivities along the major axes

h : potentiometric head

W : volumetric flux per unit volume and represents sources and or sinks

S_s : is the specific storage of the aquifer

t : time

In general, S_s, K_{xx}, K_{yy} and K_{zz} are functions of space, for example: $K_{xx} = K(x,y,z)$, whereas h and W are functions of space and time (eg: h = h(x,y,z,t). Thus, the above equation describes groundwater flow under non-equilibrium conditions in a heterogenous and anisotropic medium. Hence this equation together with specification of flow conditions at the boundaries of an aquifer system and specification of initial head conditions, constitutes a mathematical model of ground water flow.

Generally analytical solutions of the equation referred above are rarely possible. So various numerical methods may be used to arrive at approximate solutions. The well known finite difference method is one such approach. With this method, the continuous system is replaced by a system of simultaneous linear algebraic difference equations and their solution yields values of head at specific points and time. Obviously, these constitute an approximation to the time varying head distribution that would be given by an analytical solution of the flow equation.

2.1 Model Description

Development of the groundwater flow equation in finite difference form follows from the application of the continuity equation: the sum of all flows into and out of a cell must be equal to the rate of change in storage within the cell. The finite difference approximation for any cell (i,j,k) in the grid may be obtained as:

$$\begin{aligned}
&CR_{i,j-\frac{1}{2},k}\,(h_{i,j-1,k} - h_{i,j,k}) + CR_{i,j+\frac{1}{2},k}\,(h_{i,j+1,k} - h_{i,j,k}) + CC_{i-\frac{1}{2},j,k}\,(h_{i-1,j,k} - h_{i,j,k}) \\
&+ CC_{i+\frac{1}{2},j,k}\,(h_{i+1,j,k} - h_{i,j,k}) + CV_{i,j,k-\frac{1}{2}}\,(h_{i,j,k-1} - h_{i,j,k}) + CV_{i,j,k+\frac{1}{2}}\,(h_{i,j,k+1} - h_{i,j,k}) \\
&+ P_{i,j,k}\,h_{i,j,k} + Q_{i,j,k} = SS_{i,j,k}(\Delta r_j\Delta c_i\Delta v_k)\Delta h_{i,j,k}\,/\Delta t \quad\dots\dots\dots\dots\dots\dots\dots\text{(2)}
\end{aligned}$$

where,

$CR_{i,j-\frac{1}{2},k}$: the conductance in row i and layer k between nodes

: i,j-1, k and i,j,k

$CC_{i-\frac{1}{2},j,k}$: the conductance in column j and layer k between modes : i-1,j,k and i,j,k.

h,j,k : the head in cell i,j,k

$CV_{i,j,k-½}$: the conductance in row i and column j between modes : i,j,k-1 and i,j,k

$P_{i,j,k}$: certain constant for cell i,j,k

$SS_{i,j,k}$: specific storage of cell i,j,k.

$Q_{i,j,k}$: flow rate into cell i,j,k.

$\Delta r_j \Delta c_i \Delta v_k$: volume of cell i,j,k is recent in time.

Δt : increment in time

The above equation can be rewritten in backward-difference form by specifying flow terms at t_m, end of the time interval, and approximating the time derivative of head over the interval t_{m-1} to t_m as:

$$vCR_{i,j-½,k}(h^m_{i,j-1,k} - h^m_{i,j,k}) + CR_{i,j+½,k}(h^m_{i,j+1,k} - h^m_{i,j,k}) + CC_{i-½,j,k}(h^m_{i-1,j,k} - h^m_{i,j,k})$$
$$+ CC_{i+½,j,k}(h^m_{i+1,j,k} - h^m_{i,j,k}) + CV_{i,j,k-½}(h^m_{i,j,k-1} - h^m_{i,j,k}) + CV_{i,j,k+½}(h^m_{i,j,k+1} - h^m_{i,j,k})$$
$$+ P_{i,j,k}h^m_{i,j,k-1} + Q_{i,j,k} = SS_{i,j,k}(\Delta r_j \Delta c_i \Delta v_k) \{ (h^m_{i,j,k} - h^{m-1}_{i,j,k}) / (t_m - t_{m-1}) \} \quad \dots\dots\dots \quad (3)$$

If an equation of this type is formulated for each of the 'n' cells in the gridded system, then we are left with a system of 'n' equations in 'n' unknowns and the set of equations can be solved for obtaining the unknown head values for each of the cells.

2.2 Discretisation Convention

In the finite difference method, the continuous system described by the governing equation is replaced by a finite set of discrete points in space and time and the partial derivatives are replaced by differences between functional values at these points.

This requires discretisation of the aquifer system into grids forming rows, columns and layers. To conform with computer allay conventions an i, j, k, coordinate system is used (Fig.2.2.1); where i is the now index j is the column index and k is the layer index.

Conceptually, nodes represent cell within which the hydraulic properties are constant. So that any value associated with a mode is distributed over the above extent of the cell.

In fig. 1 the width of the cells along row is designated as Δj for the jth column and that along the column is Δc_i for the ith row. Now the volume of the cell located at (i,j,k) is $\Delta r_j \Delta c_i \Delta v_k$ where Δv_k is the thickness of the layer k.

The block-centred formulation is used for defining the configuration of cells for the present study. The cells are formed by parallel lines and the points are the modes. For each block, the hydraulic properties are uniform over the extent of a cell.
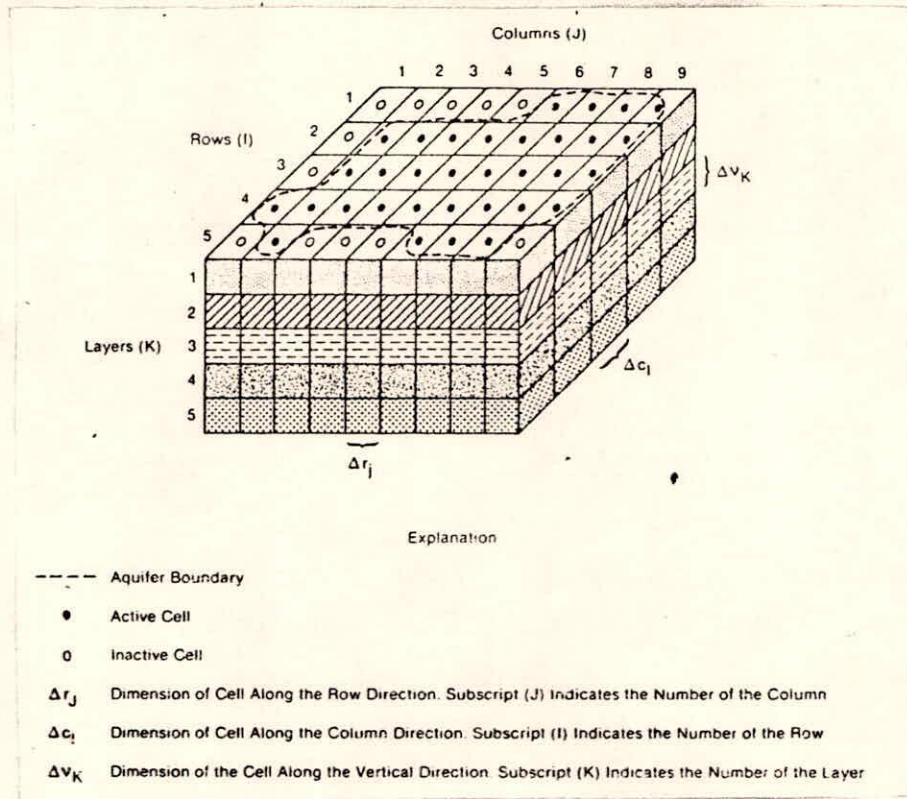
Fig 1 A discretized hypothetical aquifer system

2.3   Boundary Conditions

In the discretized aquifer system, the number of equations is equal to the number of *variable-head cells*. Variable-head cells are those in which head may vary with time. Cells that are not variable-head cells may be either *constant head* or *no-flow cells* (Fig. 2)

Constant head cells are those in which head remains constant with time and noflow cells are those to which there is no flow from adjacent cells. The type of boundaries that may be imposed in the model include, constant head, no-flow, constant-flow and head-dependent flow.

2.4   Solution techniques

In most cases, the actual number of equations will be less than the total number of model cells. The number of equations is equal to the number of "variable-head cells". Finite difference equation of the form given in section (2.1) is required for each variable-head cell. Cells that are not variable-Head cells may be either constant head or no flow and as such, do not require and equation.

An iterative method starting with an initial trial solution is used. An interim solution (approximate) is obtained and it becomes the new trial solution and the procedure is repeated until the

closure criterion is met. in the present if work, an iterative solution package called the strongly Implicit procedure (SIP) is used.
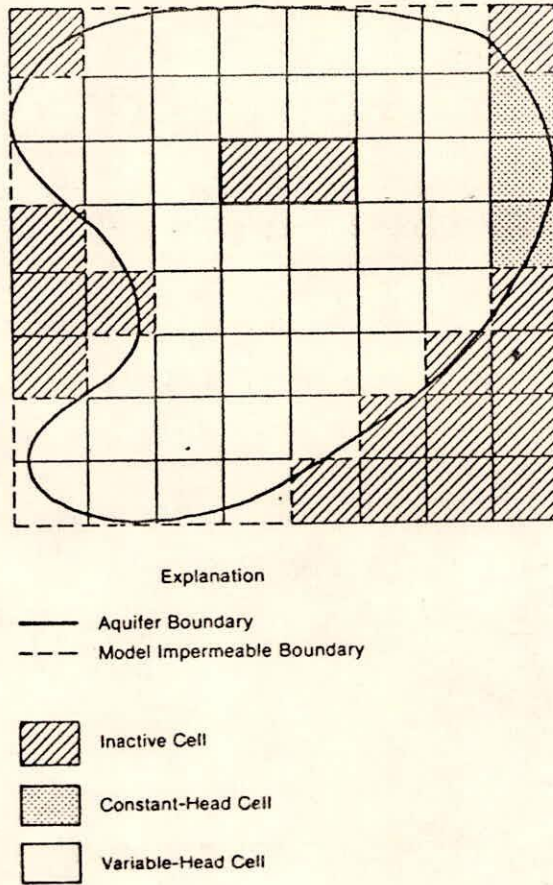

Explanation

——— Aquifer Boundary

— — — Model Impermeable Boundary

▨ Inactive Cell

▦ Constant-Head Cell

☐ Variable-Head Cell

Fig. 2 Discretized aquifer system showing boundaries and type of cells

2.5 Transient simulation

The objective of transient simulation, available in MODFLOW, is to predict head patterns at successive times when given the initial-head distribution and the boundary conditions. The initial-head distribution consists of a value of $h^1_{i,j,k}$ at each point in mesh at time t_1, the beginning of the first of the discrete time step into which the time axis is divided in the finite-difference process. The first step in the solution process is to calculate values of $h^2{i,j,k}$ that is, heads at time t_2 which mark the end of the first time step. In the finite difference equation of section (2.1), therefore, the subscript m is taken as 2, while the subscript m-1, which appears in only one head term, is taken as 1.

When the heads for time t_2 have been obtained, the process is repeated to obtain heads at time t_3, the end of the second time step. To do this, the finite difference equation is reapplied, now using 2 as time subscript m-1 and 3 as time subscript m. Again, a system of n equations in n unknowns is

formulated where the unknowns are now the heads at t_3; and this set of equations is solved simultaneously to obtain the head distribution at t_3. This process is continued for as many time steps as necessary to cover the time range of interest.

It is important to note that the set of finite-difference equations is reformulated at each time step; that is, at each step there is new system of simultaneous equations to be solved. The heads at the end of the time step make up the unknowns for which this system must be solved; the heads at the beginning of the step are among the known terms in the equations. The solution process is repeated at each time step yielding a new array of heads for the end of the time step.

The solution at each time step might be obtained by direct algebraic methods yielding exact solution to the set of equations. However, numerical problems associated with their use tend to make them less desirable than iterative methods. An iterative method starts with an initial trial solution to calculate an interim solution. The interim solution becomes the new trial solution. The process repeated until a closure criterion is met wherein successive solutions may be considered nearly equal.

3.0   DESCRIPTION OF VARIOUS PACKAGES

The are about eleven modules provided in MODFLOW to deal with various field situations. Those are the basic package, block centred package, river package, recharge package, well package, drain package, evapotranspiration package, general-head boundary package, SIP package, SSOR package and utility modules. Conceptualization and implementation of these modules are briefly described through the following sections.

3.1   Basic Package

The Basic Package handles the administrative tasks of the model. The major tasks for which it is responsible are the discretisation of space and time into cells and time steps, specification of initial and boundary conditions, specification of heads for the beginning of each time step, specification of program options to be used, calculation of the volumetric budget, and control of the output of results.

In the finite-difference method, a rectilinear grid is used to divide the region to be studied into rows, columns, and layers, forming cells with rectangular faces. The properties of the cells, which are assumed to be homogenous, are used to formulate the coefficients of the finite-difference equations. Generally, the grid is superimposed on a flow system contained in a sequence of stratigraphic units which are not quite horizontal (Fig. 3).

Thus some cells may represent two very different rock types, making specification of physical properties difficult. It is convenient, therefore, to deform the grid so that grid layers follow the contours of the stratigraphic units. Simulation time is divided into stress periods--time intervals during
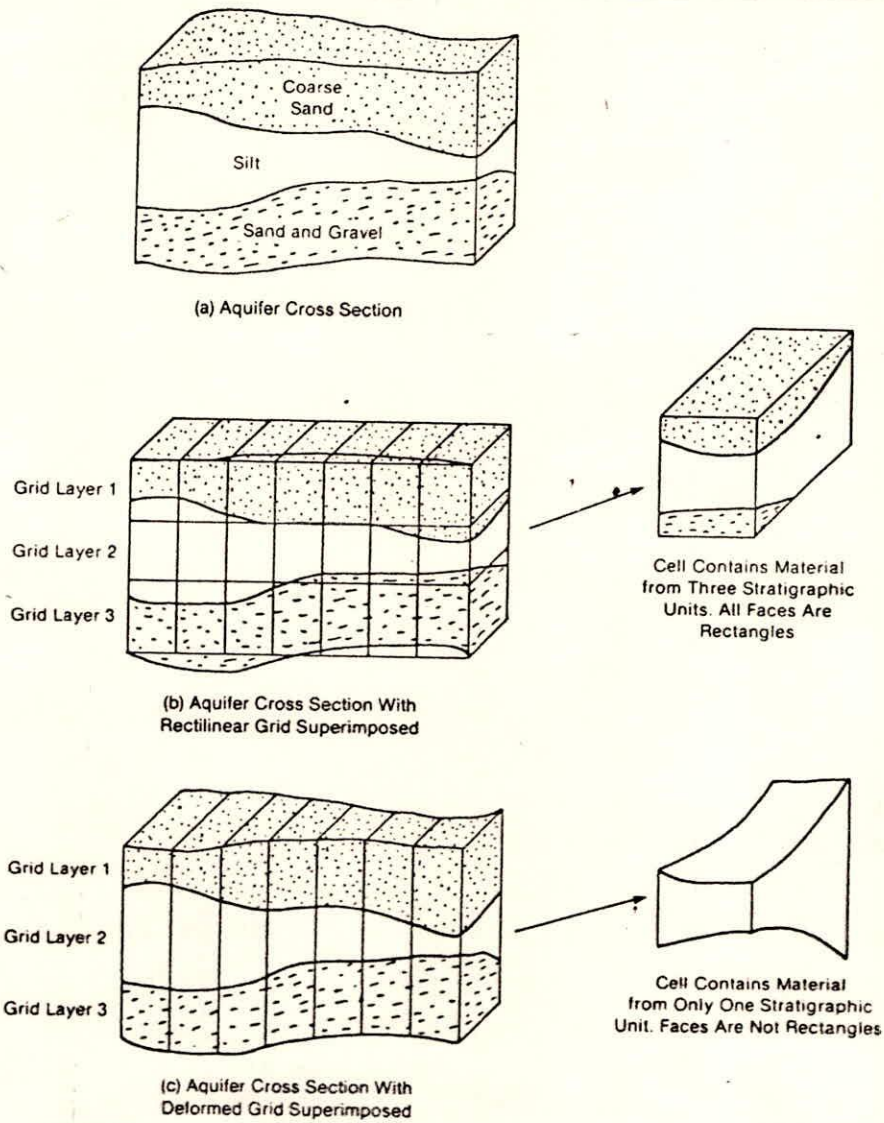
(a) Aquifer Cross Section

Grid Layer 1

Grid Layer 2

Grid Layer 3

Cell Contains Material
from Three Stratigraphic
Units. All Faces Are
Rectangles

(b) Aquifer Cross Section With
Rectilinear Grid Superimposed

Grid Layer 1

Grid Layer 2

Grid Layer 3

Cell Contains Material
from Only One Stratigraphic
Unit. Faces Are Not Rectangles

(c) Aquifer Cross Section With
Deformed Grid Superimposed

Fig. 3 Rectilinear and deformed grids

which all external stresses are constant--which are, in turn, divided into time steps. The length of each stress period is specified explicitly by the user. Within the stress period, the time steps form a geometric series in which the parameters of the series, the number of elements, and the multiplier are specified by the user. The program uses those parameters along with the length of the stress period to calculate the length of each time step.

3.2   Block-Centred Flow Package

The Block Centred Flow (BCF) Package computes the conductance components of the finite-difference equation which determines flow between adjacent cells. It also computes the terms that

represent 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 centre of each model cell and thus the name Block-Centred Flow is given to the package.
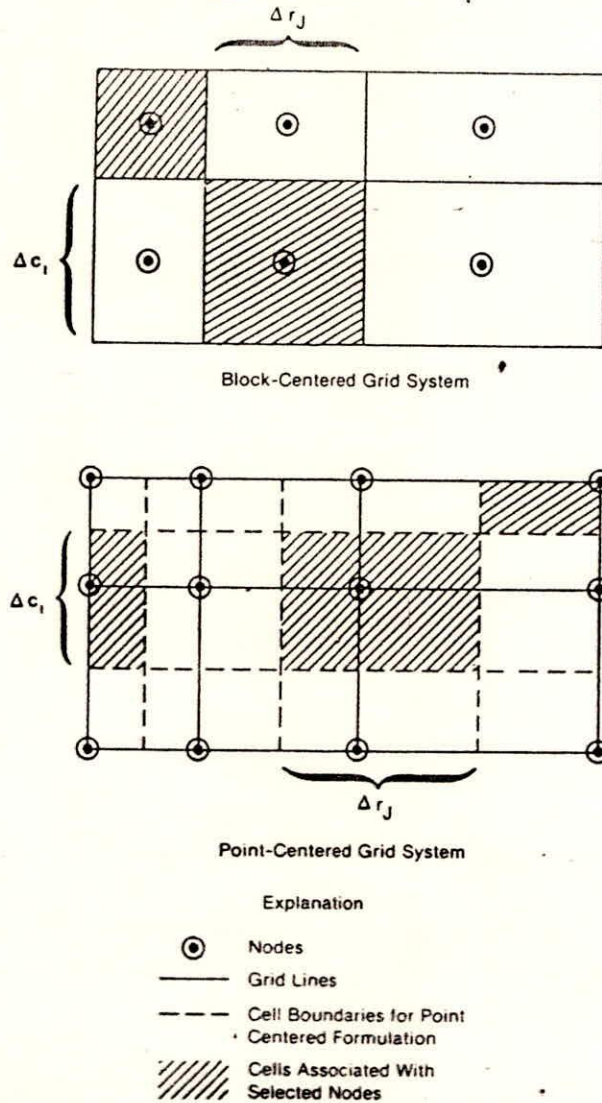

Fig. 4 A block centred grid system with node points located at the centre of the blocks.

3.3   River Package

Rivers may contribute water to the aquifer or drain water from the aquifer depending on the head gradient between the river and the aquifer. The effect of leakage through the river bed on the shape of the water table is shown in Fig. 5 The purpose of the River Package is to simulate the effect of that leakage. To simulate the effect of river leakage in the model, terms representing the leakage are added to the ground-water flow equation for each cell. The river is divided into reaches, each of which is completely contained in a single cell. River/aquifer leakage is defined between each river

reach and the model cell that contains the reach. Fig. 6 shows a cross section of a grid cell containing a river reach. The river bed has been exaggerated to illustrate that water must pass through the bed to get from the river into the aquifer cell. A block diagram of the same situation has also been shown in Fig. 6 (bottom); the river bed has been represented by a rectilinear prism of homogeneous porous material.
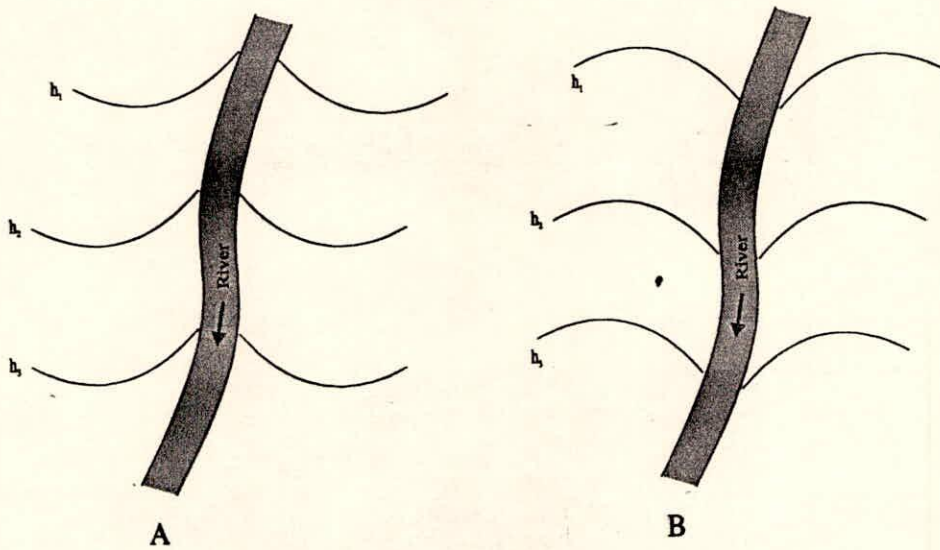

A   B

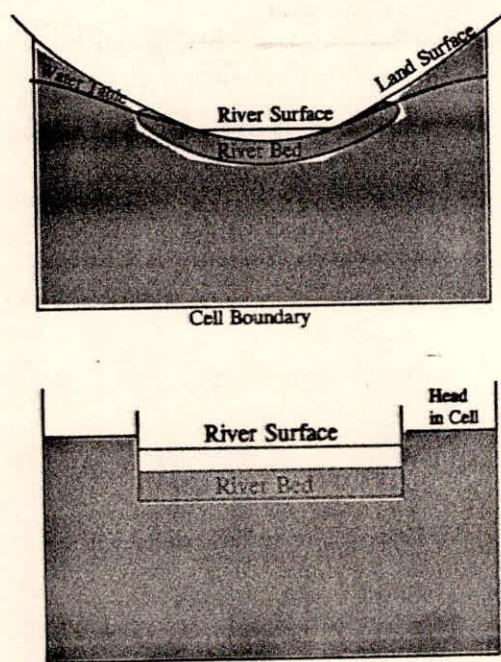Fig. 5 Watertable contours near a gaining (A) and losing stream (B)

Fig. 6 Cross section of an aquifer containing a river and the corresponding block formulation for the model

Leakage through a reach of river bed is approximated by Darcy's law as:

$$QRIV = KLW(HRIV - HAQ)/M \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (4)$$

where

QRIV is the leakage through the reach of the riverbed (L^3t^{-1});

K is the hydraulic conductivity of the riverbed (LT^{-1});

L is the length of the reach (L);

W is the width of the river (L);

M is the thickness of the riverbed (L);

HAQ is the head on the aquifer side of the riverbed (L); and

HRIV is the head on the river side of the riverbed (L).

3.4 Recharge Package

Infiltration from precipitation generally occurs evenly over a large area. Hence, it is called *areally distributed recharge*. It is expressed in terms of flow rate per unit area which reduces to units of length per unit time such as cm/sec or in/hr. The volumetric rate of flow into a cell is the infiltration rate times the horizontal area of the cell. In equation form

$$QRCH_{i,j,k} = I_{ijk} * DELR_j * DELC_i \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (5)$$

Where $I_{i,j,k}$ is the infiltration rate (LT^{-1}). Notice that the recharge rate is independent of the head in the cell.

3.5 Well Package

A recharging well can be viewed as a source of water which is not affected by the head in the aquifer. A discharging well is a recharging well with a negative recharge rate. For the sake of this discussion, the well will be assumed to be screened in only a single cell. Thus for each cell containing a well, the recharge rate must be added to the right side of the finite-difference equation.

3.6 Drain Package

The rate at which water seeps into a drain in the saturated zone of an aquifer is approximated in the model using the equation

$$QD_{i,j,k} = CD_{i,j,k}(h_{i,j,k} - d_{i,j,k}) = CD_{i,j,k}h_{i,j,k} - CD_{i,j,k}d_{i,j,k} \quad \ldots\ldots\ldots\ldots \quad (6)$$

where

$QD_{i,j,k}$ \qquad is the rate water flows into the drain $L^3t^{-1)}$

$d_{i,j,k}$ is the head in the drain (L);

$h_{i,j,k}$ is the head in the aquifer near the drain (L); and

$CD_{i,j,k}$ is the conductance of the interface between the aquifer and the drain (L^2t^{-1}).

The coefficient $CD_{i,j,k}$ (Fig. 7) is the conductance of the interface between the drain and the porous material. It may be affected by size and frequency of openings in a drain tile, chemical precipitation around a tile, difference in permeability between the aquifer material and the backfill around a tile, and a low permeability bed in an open drain or the converging area of flow as the drain is approached. The head in the drain is assumed to be the elevation of the drain. Thus the flow into the drain is assumed to be proportional to the head above the drain. The equation only holds when the head in the aquifer is greater than the head in the drain. When the elevation of the drain is greater than the head in the aquifer, the flow into the drain, $QD_{i,j,k}$ is equal to zero.
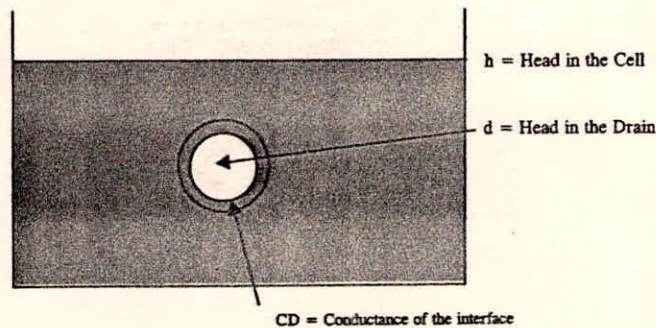
h = Head in the Cell

d = Head in the Drain

CD = Conductance of the interface

Fig. 7 Leakage into a drain as a function of head in the aquifer and elevation of the drain

3.7   Evapotranspiration Package

Evapotranspiration(ET) is the mechanism whereby water is converted from liquid phase to vapour phase. This package simulates this effect. It deals primarily with water removed by the roots of plants.

The ET rate determined by the package depends on the position of the aquifer head relative to two given ET reference elevations: ET surface and ET extinction levels. For a given node the ET rate decreases to zero as the aquifer head declines to the extinction elevation and is set to zero when the aquifer head drops below this elevation. The ET rate increases to a user controlled maximum limit as the aquifer head rises above extinction level to the given ET surface elevation. The ET rate is assumed to be proportional to the saturated thickness above the given ET extinction elevation.

3.8   General-Head Boundary Package

General head boundary consists of a source of water outside the modeled area which supplies water to a cell depending upon the head difference. The rate of water supplied to a cell (i,j,k) is given by:

$$Q_{i,j,k,m} = C_m(HB_m - h_{i,j,k,m}) \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (7)$$

where

$Q_{i,j,k,m}$ rate at which water is supplied to a cell from boundary

C_m proportionality constant for boundary m

HB_m head at source boundary m

$h_{i,j,k,m}$ head in the cell

The source can be a gaining river in which case C_m is the river bed conductance. If the source is buried drain then C_m is a function of drain characteristics and the material around the drain. It could also be the head in the aquifer outside the simulated area wherein the proportionality constant is the hydraulic conductance of the material between head and the boundary of the simulated area.

3.9   Iteration Packages

There are two iteration packages available on MODFLOW; one the Strongly Implicit Procedure (SIP) and the other Slice Successive Over-relaxation Package (SSOR).

The strongly implicit Procedure (SIP) and Slice Successive Over-relaxation Package (SSOR) are methods for iteratively solving a large system of simultaneous linear equations. They solve the finite-difference equations associated with the cells in the finite difference grid. The initial trial solution may either be supplied externally for speedier computations or the module may assume its own value. However, the closure criterion should be specified.

3.10   Utility Modules

Utility modules are those sub-modules which perform general tasks common to several different packages. There are eight utility modules for writing an unformulated record consisting of an array with one real number for each cell in the grid, for writing an unformatted record consisting of an array with one real number for each cell in a layer, for printing two-dimensional arrays which contains one real number for each cell in a layer, for printing in strip form the first N columns of each row and then the next N columns, etc. , for printing column numbers at the top of each page of data printed, for reading a two dimensional array of real numbers, for reading a two dimensional array of integers and for reading a one-dimensional array of real numbers.

4.0   APPLICATION

MODFLOW can be used as an efficient tool in groundwater development and management. Two dimensional or three dimensional modelling is possible. It can model the hydraulic potentials, drawdown or flow in a simple/ complex aquifer system. Steady state as well as transient simulations are possible. Head values, drawdown or flow term for each cell may be obtained at required time steps in any stress period. Also, the volumetric budget may be obtained as and when required. Different scenarios can be modelled to simulate any future changes likely to occur in an aquifer system.

For instance, the effect of changes in pumpage from wells in an aquifer system on the water table can be studied. Similarly the leakage from a reservoir/ canal and its influence on the aquifer can be modelled and studied. As mentioned earlier the effect of recharge, evapo-transpiration, flow across boundaries, drainage, pumpage etc. can be simulated in an 'aquifer system to evolve realistic groundwater management strategies. With the introduction of a particle tracking module, the MODFLOW may be used to investigate contamination transport also.