

MODEL

- **A three dimensional replica of an object typically on a smaller scale**
- **A simplified mathematical description of a system or process.**
- **“A major purpose of scientific investigation is to describe reality through models”, Gauch, 1993, *Am. Sci.*, 81, 468.**

WHAT DO MODELS DO?

- “..predict the future state of a system with tolerable certainty” Denning, 1990, *Am. Sci.*, 78, 496.
- “..what some researchers are calling the ‘third branch of science’ - using...computers to simulate physical processes..” Pool, 1993, *Science*, 260, 1077.

PRECAUTIONS

(Denning, 1990, *American Scientist*, 78, 498)

- “We must come to understand the domains over which a given model is reliable..”
- “Systems whose rules can...change in unpredictable ways are unlikely to have a reliable...model.”

GROUNDWATER MODELS

- **Broadly Groundwater Models are grouped into two categories:**
 - **Groundwater quantity (flow) models, and**
 - **Groundwater quality models**

WATER QUANTITY MODELS

(FLOW MODELS)

- **These models are used for:**
 - **aquifer management,**
 - **well field design,**
 - **groundwater recharge enhancement,**
 - **determination of optimum aquifer yield,**
 - **well interference studies,**
 - **studies of groundwater - streamflow interactions, and similar problems.**

WATER QUALITY MODELS

- **These models are used:**
 - **to study the consequences of groundwater contamination, and**
 - **To design the remediation measures.**

Strategies in Model Development

- Definition of Aim (what, why, which knowledge to be acquired, numerically solvable, enough Data?)
- Conceptual Model
 - location, areal extent, thickness aquifers and confining layers
 - Hydrogeological system analysis
- Collected data:
 - (Hydrostratigraphy, Water balance, Aquifer parameter, Morphology, Geology)

Strategies in Model Development

- **Model Design (Geometry, Boundary Conditions, Discretisation)**
- **Calibration**
- **Verification/Validation (Plausibility)**
- **Sensitivity Analysis**
- **Prediction/Decision Making**
- **Visualization**

What is MODFLOW?

Widely used ground-water flow simulation program that runs on any platform (Windows, Sun, Unix, Linux).

Mostly written in standard FORTRAN

Solves the ground-water flow equation with different possible properties, boundary conditions, and initial conditions

First version, 1983, McDonald and Harbaugh. Written to serve USGS needs. Education emphasized.

Public domain (Free)

Open source (Anyone can check and change the source code)

- Changed versions are sometimes commercial - it's up to the developer

Well documented - Modularly constructed (More later)

What is MODFLOW?

Many other programs use results from or are based on MODFLOW:

- Public domain/open source

- MT3DMS (multi-species solute or heat transport, some reactions, dual porosity) (Chunmiao Zheng, U Alabama)
- MODPATH (particle tracking) (Dave Pollock, USGS)
- SEAWAT (density-dependent transport using MODFLOW and MT3DMS) (Chris Langevin, USGS)
- PHT3D (= MT3DMS + PHREEQC) (Henning Prommer)

- Commercial

- MODHMS, MODFLOW-Surfact (Integrated sw/gw/unsat)
- GUI's: PMwin, VisualMF, Groundwater Vistas, GMS, Triwaco*

What is MODFLOW?

Program organized into MODules

- Activate the capabilities you need; no overhead from other capabilities (execution time, RAM)
- The structure is clear and documented for adding additional capabilities such as new equations
- Modularity in 'Processes' and 'Packages'

Summary of MODFLOW capabilities

- Single Phase, Saturated Flow
- Constant Density
- Porous Media (Darcy's Law applies)
- 1, 2, Or 3 Dimensional (2D areal or cross-section OR Quasi-3D)
- Steady State or Transient Flow
- Heterogeneous, Anisotropic (aligned with grid), Layered Units
- Block-Centered Finite-Difference with variable grid spacing
- Layers can be Confined, Unconfined or Convertible
- Boundary conditions include: Dirichlet, Neuman, Cauchy, and Phreatic Surface
- Boundary condition packages include Wells, Recharge, Evapotranspiration, Rivers, Drains, Thin Barriers to Horizontal Flow, Re-wetting, and others.
- Many Solver options
- Monitoring of simulated values comparable to field observations
- Sensitivity analysis and parameter estimation to be accomplished by UCODE

MODFLOW DEVELOPMENT

- Originally organized in modules
 - Modules grouped into packages that perform calculations either specific to the behavior of a geohydrologic feature or a numerical modeling task
 - Packages allow
 - examination of specific hydrologic features independently
 - facilitates development of additional capabilities
- Originally solely a ground-water flow model

MODFLOW DEVELOPMENT

- Scope broadened to allow capabilities such as transport and parameter estimation
- Expansion of modular design required (MODFLOW-2000)
 - addition of “Process”
- MODFLOW-2005 is similar in design to MODFLOW-2000
 - Incorporates different approach for managing internal data
 - Fortran modules are used to declare data that can be shared among subroutines
 - MODFLOW subroutines were originally called modules
 - generic term module has been eliminated and replaced by the term subroutine

ORIGINAL MODULAR STRUCTURE (1988):

- BAS - basic package
 - general tasks - gridding, constant head and no-flow boundaries, initial conditions, time stepping
- OC - output control package
 - controls the information and format of results
- BCF - block centered flow package
 - layer types, grid dimensions, material properties
- WEL - well package
 - locations and flow rates of wells
- RCH - recharge package
 - recharge rates and locations
- RIV - river package
 - locations, river bed material properties, and river stages
- DRN - drain package
 - location, material properties surrounding drains, and elevation of drains
- EVT - evapotranspiration package
 - parameters describing evapotranspiration rate with depth to water table
- GHB - general head boundary package
 - locations, local material properties, and elevation of specified heads
- SOLVERS
 - SIP - strongly implicit procedure package
 - SOR - slice-successive over-relaxation package

PACKAGES WRITTEN AFTER ORIGINAL MODFLOW:

- PCG2 - preconditioned conjugate-gradient 2 package
 - alternative matrix solver
- STR1 - stream routing package
 - differs from the river package in that the surface water stage varies based on the surface water flow and the Manning equation
- BCF2 - block-centered flow 2 package
 - allows for re-wetting of cells that have gone dry
- BCF3 - block-centered flow 3 package
 - a supplement to the BCF2 package, allowing alternative interblock transmissivity formulations
- HFB1 - horizontal flow barrier package
 - simulation of thin, vertical, low permeability features that impede horizontal flow
- TLK1 - transient leakage package
 - simulates transient leakage and storage changes in confining units of quasi-3D models
- GFD1 - general finite difference flow package
 - substitutes for the BCF package, allows user to enter conductance rather than calculating with MODFLOW
- IBS1 - interbed storage package
 - simulates compaction of compressible, fine-grained units within or adjacent to aquifers in response to pumping
- CHD1 - time-variant specified head boundary package
 - allows time varying specified head

PACKAGES WRITTEN FOR MODFLOW-2000 and since:

- **rapidly growing long list**

GWF1 - ground water flow process (GWF in name file)

finite difference simulation of saturated porous media flow

OBS1 - observation process (OBS in name file)

monitors value of head or flow at specified locations

SEN1 - sensitivity process (SEN in name file)

calculates the change in simulated head and flows at observation locations PES1 -

parameter estimation process (PES in name file)

estimates values of parameters by nonlinear regression to minimize the weighted sum of squared residuals for observations

DIS - discretization package (DIS in name file)

gridding, defining division of space and time for the numerical solution

MULT - multiplier file (MULT in name file)

defines the spatial distribution of multipliers in the grid that act on parameter values specified in those zone

PACKAGES WRITTEN FOR MODFLOW-2000

and since: (continued)

ZON - zone file (ZONE in name file)

defines the spatial distribution of zones in the grid where specified parameters apply

BAS6 - basic package (BAS6 in name file)

constant head and no-flow boundary conditions; and initial conditions

OC - output control package (OC in name file)

controls the information and format of results

BCF6 - block centered flow package (BCF6 in name file)

defines material properties with some parameters being dependent on grid dimensions (e.g. transmissivity), thus this package ignores the discretization information in DIS for some purposes -- the parameter method of inputting data cannot be used -- method of interblock conductance calculations can be selected

LPF1 - layer property flow package (LPFin name file)

an alternative to BCF6 defines material properties with all parameters independent of grid dimensions (e.g. hydraulic conductivity) -- the parameter method of inputting data can be used -- method of interblock conductance calculations can be selected

HFB6 - horizontal flow barrier package (HBF6 in name file)

represents thin barriers that occur between model cells by defining their hydraulic conductivity divided by their thickness and specifying where they occur

PACKAGES WRITTEN FOR MODFLOW-2000

and since: (continued)

WEL6 - well package (WEL in name file)

locations and flow rates of wells

RCH6 - recharge package (RCH in name file)

recharge rates and locations

RIV6 - river package (RIV in name file)

locations, river bed material properties, and river stages

STR6 - stream routing package (STR in name file)

differs from the river package in that the surface water stage varies based on the surface water flow (calculated as specified flow and ground water flux to/from stream) and the Manning equation

DRN6 - drain package (DRN in name file)

location, material properties surrounding drains, and elevation of drains (this update allows a fraction [0-1] of the drain outflow to be returned to a specified cell)

EVT6 - evapotranspiration package (EVT in name file)

parameters describing evapotranspiration rate with depth to water table

GHB6 - general head boundary package (GHB in name file)

locations, local material properties, and elevation of specified heads

CHD6 - time-variant specified head boundary package (CHD in name file)

allows time varying specified head

PACKAGES WRITTEN FOR MODFLOW-2000 and since: (continued)

SOLVERS (SIP SOR PCG DE4 LMG in name file)

SIP5 - strongly implicit procedure package

SOR5 - slice-successive over-relaxation package

PCG2 - preconditioned conjugate gradient package

DE45 - direct solution by alternating diagonal ordering package

LMG1 - multigrid solver speeds execution for large grids and high degree of heterogeneity

ADV2 - advective transport observation package (ADV2 in name file)

allows use of travel time observations for parameter observations

RES1 - reservoir package (RES in name file)

simulates leakage between reservoir and aquifer as reservoir area changes in response to stage changes

FHB1 - flow and head boundary package (FHB in name file)

allows flow and head boundary conditions that vary at times other than starting and ending times of stress periods

IBS6 - interbed storage (subsidence) (IBS in name file)

simulates compaction related to hydraulic head decline

HUF1 - hydrologic-unit flow package (HUF in name file)

calculates effective hydraulic properties for cells based on geometric description of hydrologic units

PACKAGES WRITTEN FOR MODFLOW-2000 and since: (continued)

LAK3 - lake package (LAK in name file)

allows variation of lake stage based on water budgets

ETS1 - evapotranspiration package with segment ET function (ETS in name file)

allows function describing evapotranspiration rate with depth to water table to be piece-wise linear

DRT1 - drain package with return flows (DRT in name file)

allows user to allocate proportions of drain flow to be recharge to specified cells

LMT6 - link to MT3D (LMT in name file)

allows printing of file to be read by MT3D for contaminant transport

SFR - Streamflow-Routing package (SFR in name file)

is used to simulate streams in a model (provides greater flexibility in how streams are specified than STR)

UZF - Unsaturated Zone Flow Package (UZF in name file)

simulates vertical flow of water through the unsaturated zone to the saturated zone

Basic MODFLOW input and output

BASIC INPUT ITEMS INCLUDE:

- Grid
- Time stepping
- Hydraulic parameters
- Boundary Conditions
- Stresses
- Solution parameters

BASIC OUTPUT ITEMS:

- Hydraulic Heads
- Drawdown
- Flow rates
- Mass Balance

Binary files containing output in compressed form

MODEL FORMULATION

The 3D unsteady GW flow through heterogeneous and anisotropic porous material is given by the partial differential equation:

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

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

S_s : specific storage of the aquifer

h : potentiometric head

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

t : time

S_s , K_{xx} , K_{yy} and K_{zz} are functions of space,

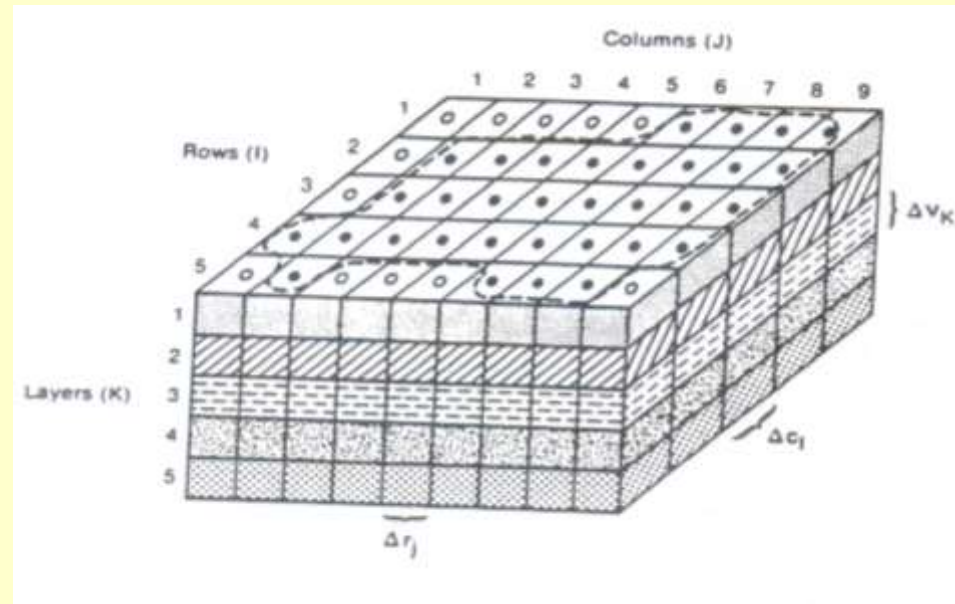
h and W are functions of space and time

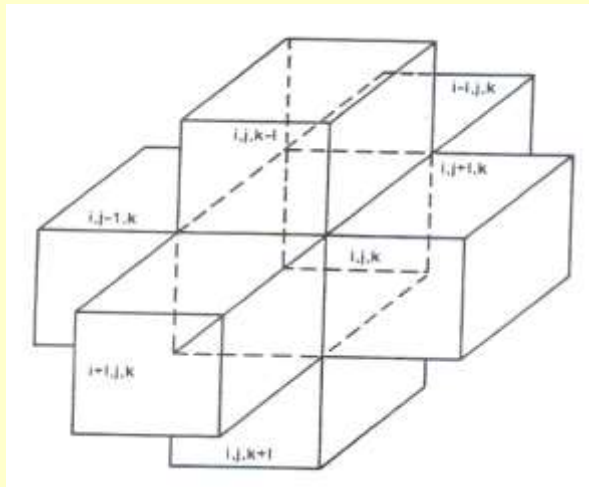
MODEL FORMULATION(...2)

- The equation describes groundwater flow under non-equilibrium conditions in a heterogeneous and anisotropic medium. So, 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.
- Analytical solutions of the equation is rarely possible
- Numerical methods (Finite Difference) are employed to solve the equation

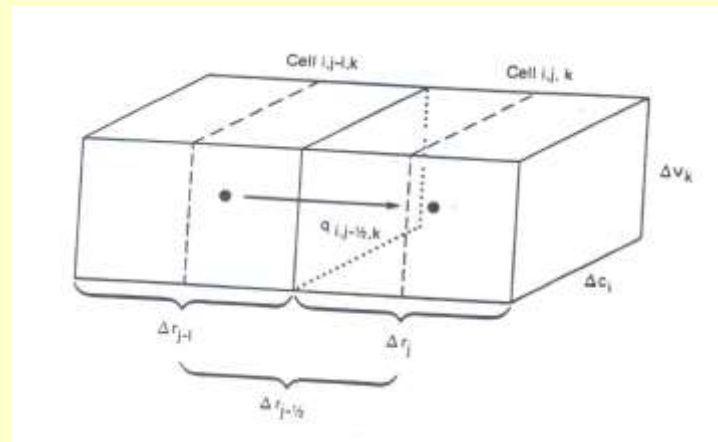
DISCRETISATION CONVENTION

- Continuous system is replaced by a finite set of discrete points in space and time.
- Partial derivatives are replaced by differences between functional values at these points.
- The aquifer system is discretized into grids forming rows, columns and layers.
- Node represent a cell within which the hydraulic properties are constant.
- Block-centred formulation is used for defining the configuration of cells.

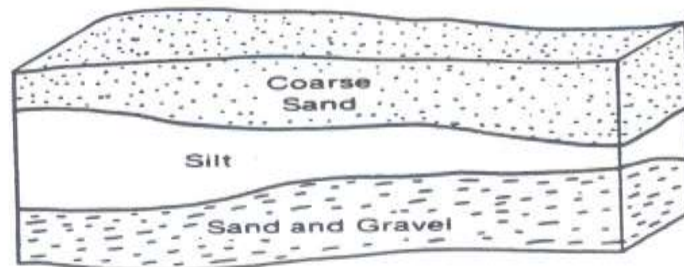




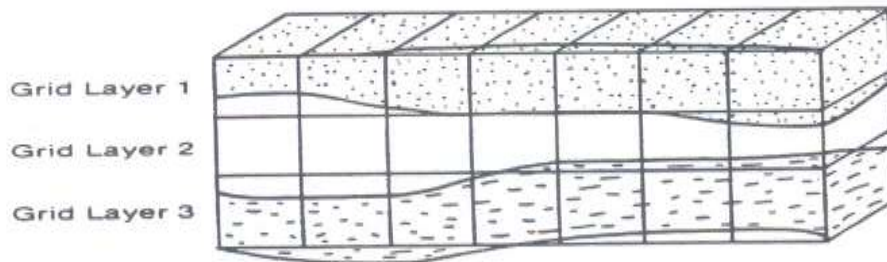
Cell i,j,k and indices for the six adjacent cells



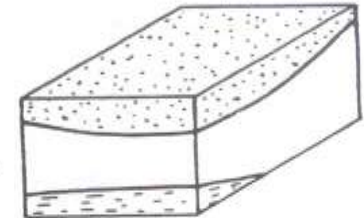
Flow into cell i,j,k from cell $i,j-1,k$



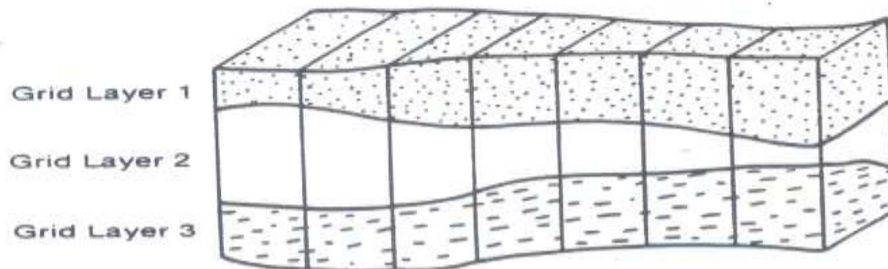
(a) Aquifer Cross Section



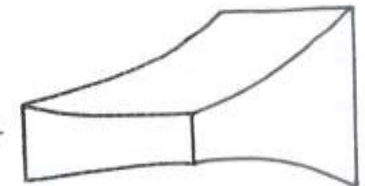
(b) Aquifer Cross Section With Rectilinear Grid Superimposed



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



(c) Aquifer Cross Section With Deformed Grid Superimposed



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

Rectilinear and deformed grids

FINITE DIFFERENCE EQUATION

- Development of the groundwater flow equation in the finite difference form follows the application of continuity equation:

$$\sum Q_i = S_s \frac{\Delta h}{\Delta t} \Delta V$$

i.e., the sum of all flows into and out of the cell must be equal to the rate of change in storage within the cell.

$$q_{i,j-\frac{1}{2},k} = KR_{i,j-\frac{1}{2},k} \Delta c_i \Delta v_k \frac{(h_{i,j-1,k} - h_{i,j,k})}{\Delta r_{j-\frac{1}{2}}}$$

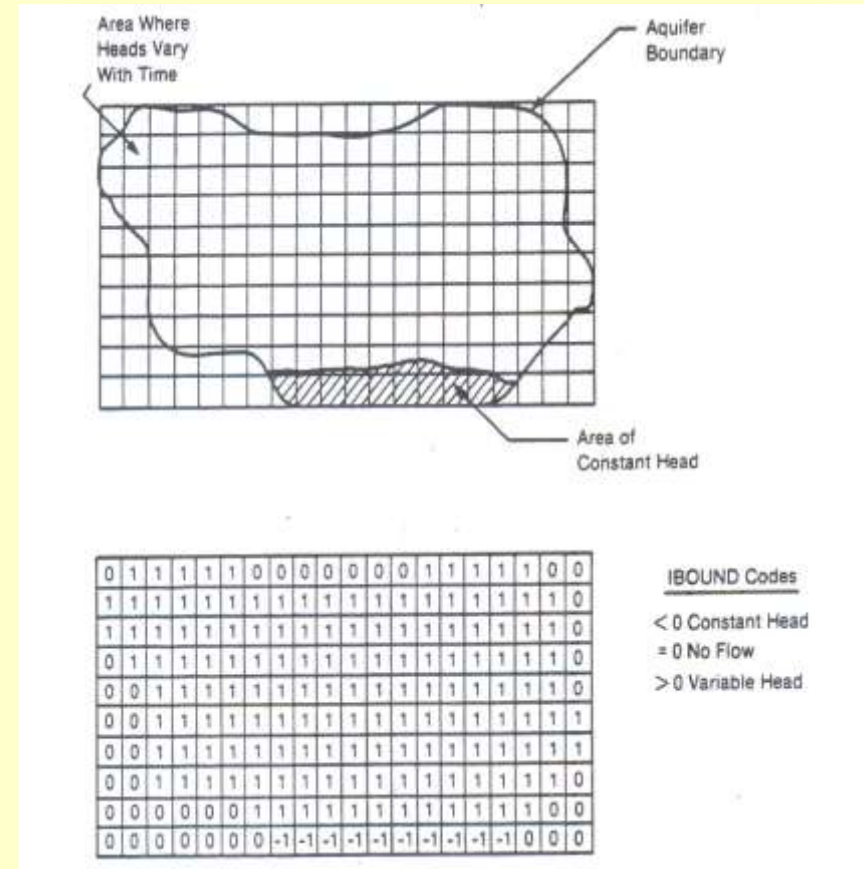
The finite difference approximation for any cell (i,j,k) in the grid may be obtained as:

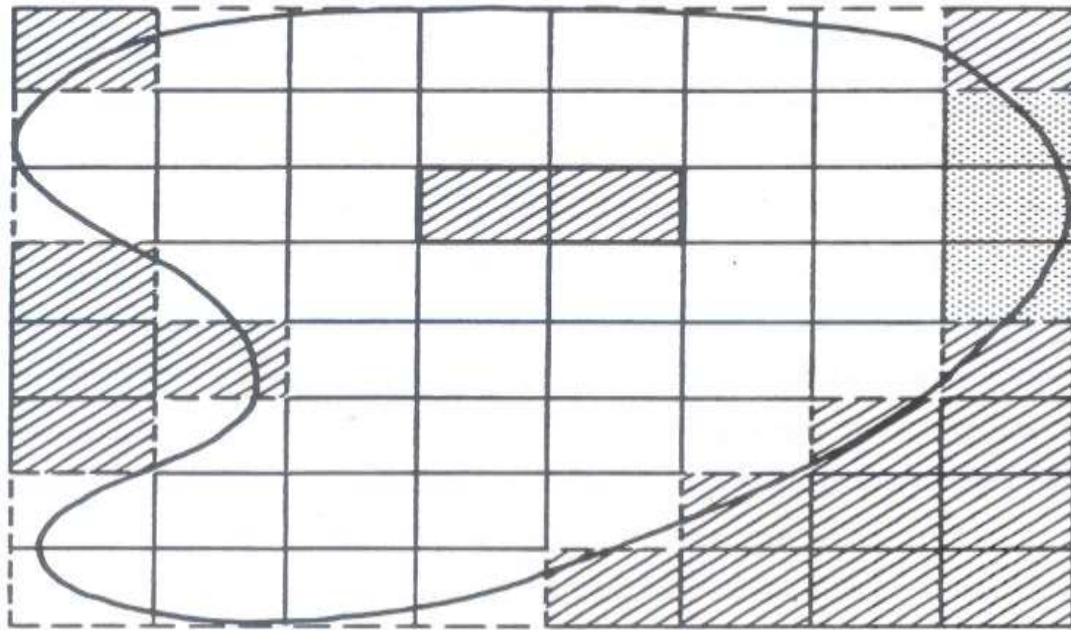
$$\begin{aligned} & CR_{i,j-1/2,k} (h_{i,j-1,k} - h_{i,j,k}) + CR_{i,j+1/2,k} (h_{i,j+1,k} - h_{i,j,k}) \\ & + CC_{i-1/2,j,k} (h_{i-1,j,k} - h_{i,j,k}) + CC_{i+1/2,j,k} (h_{i+1,j,k} - h_{i,j,k}) \\ & + CV_{i,j,k-1/2} (h_{i,j,k-1} - h_{i,j,k}) + CV_{i,j,k+1/2} (h_{i,j,k+1} - h_{i,j,k}) \\ & + P_{i,j,k}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

- $CR_{i,j-1/2,k}$: conductance in row i and layer k between nodes $i,j-1, k$ and i,j,k
- $CC_{i-1/2,j,k}$: the conductance in column j and layer k between modes $i-1,j,k$ and i,j,k .
- $CV_{i,j,k-1/2}$: conductance in row i and column j between modes $i,j,k-1$ and i,j,k
- $h_{i,j,k}$: the head in cell i,j,k
- $P_{i,j,k}$: certain constant for cell i,j,k
- $S_{Si,j,k}$: specific storage of cell i,j,k .
- $Q_{i,j,k}$: flow rate into cell i,j,k .
- $r_j C_i V_k$: volume of cell i,j,k is recent in time.
- Δt : increment in time




BOUNDARY CONDITIONS

- In the discretized aquifer system, the number of equations is equal to the number of *variable-head cells*.
- Cells that are not variable-head cells may be either *constant head* or *no-flow cells*
- The type of boundaries that may be imposed in the model include, constant head, no-flow, constant-flow and head-dependent flow.





Explanation

- Aquifer Boundary
- - - Model Impermeable Boundary
-  Inactive Cell
-  Constant-Head Cell
-  Variable-Head Cell

Discretized aquifer system showing boundaries and type of cells

DESCRIPTION OF VARIOUS PACKAGES

In the original version of MODFLOW, there are about eleven modules (MODFLOW 96/ MODFLOW-2000 have additions).

Those are:

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

List of packages

<u>Package Name</u>	<u>Abbreviation</u>	<u>Package Description</u>	
Basic	BAS	Handles those tasks that are part of the model as a whole. Among those tasks are specification of boundaries, determination of time-step length, establishment of initial conditions, and printing of results.	
Block-Centered Flow	BCF	Calculates terms of finite-difference equations which represent flow within porous medium; specifically, flow from cell to cell and flow into storage.	Flow Component Packages
Well	WEL	Adds terms representing flow to wells to the finite-difference equations.	
Recharge	RCH	Adds terms representing areally distributed recharge to the finite-difference equations.	
River	RIV	Adds terms representing flow to rivers to the finite-difference equations.	
Drain	DRN	Adds terms representing flow to drains to the finite-difference equations.	
Evapotranspiration	EVT	Adds terms representing ET to the finite-difference equations.	
General-Head Boundaries	GHB	Adds terms representing general-head boundaries to the finite-difference equations.	
Strongly Implicit Procedure	SIP	Iteratively solves the system of finite-difference equations using the Strongly Implicit Procedure.	Solver Packages
Slice-Successive Overrelaxation	SOR	Iteratively solves the system of finite-difference equations using Slice-Successive Overrelaxation.	

BASIC PACKAGE

It handles the administrative tasks of the model.

The major tasks are:

- the discretization 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.

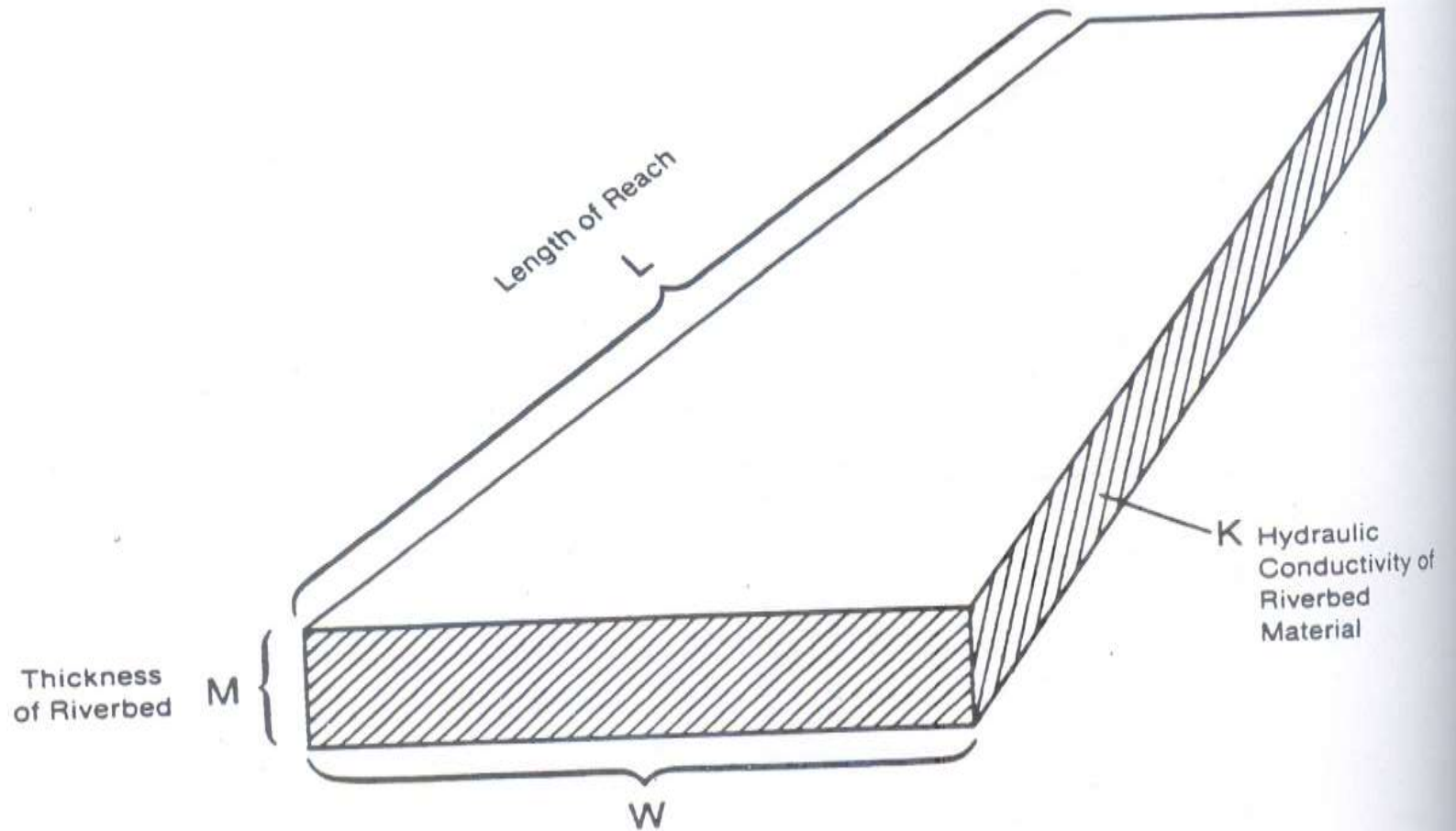
BLOCK-CENTRED FLOW PACKAGE

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.

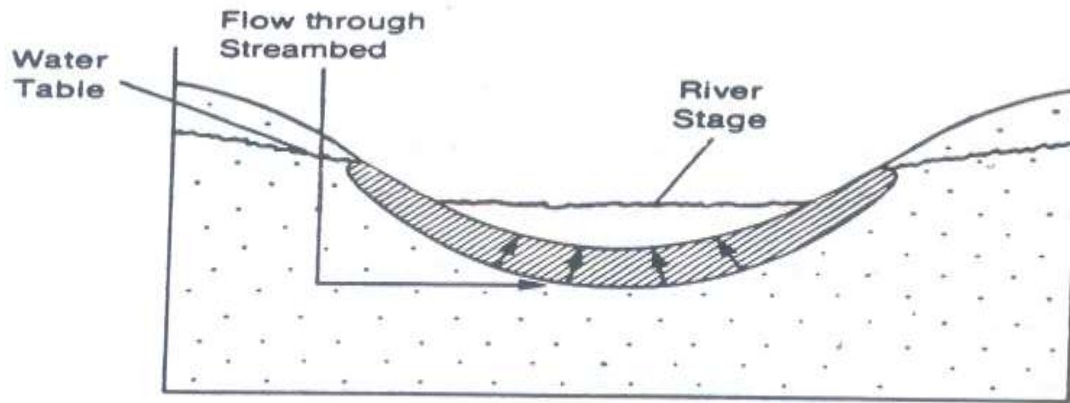
RIVER PACKAGE

- **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 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.**



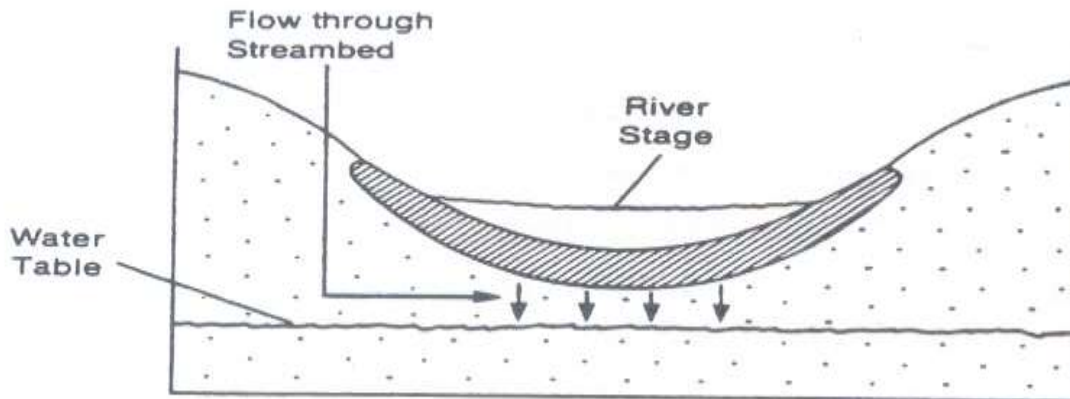
Streambed Conductance = KLW/M

Conductance of river bed defined



Head at the bottom of the streambed is equal to head in the cell.

A



Head at the bottom of the streambed is equal to elevation of bottom of streambed layer.

B

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

RIVER PACKAGE (.2)

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

$$Q_{RIV} = KLW * (H_{RIV} - H_{AQ}) / M$$

Where,

Q_{RIV} : the leakage through the reach of the riverbed

K : the hydraulic conductivity of the riverbed

L : the length of the reach

W : the width of the river

M : the thickness of the riverbed

H_{AQ} : the head on the aquifer side of the riverbed

H_{RIV} : the head on the river side of the riverbed

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:

$$QRCH_{i,j,k} = I_{i,j,k} * \Delta R_j * \Delta C_i$$

Where $I_{i,j,k}$ is the infiltration rate. Notice that the recharge rate is independent of the head in the cell.

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.

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

$$QD_{i,j,k} = CD_{i,j,k} (h_{i,j,k} - d_{i,j,k}) = CD_{i,j,k} h_{i,j,k} - CD_{i,j,k} d_{i,j,k}$$

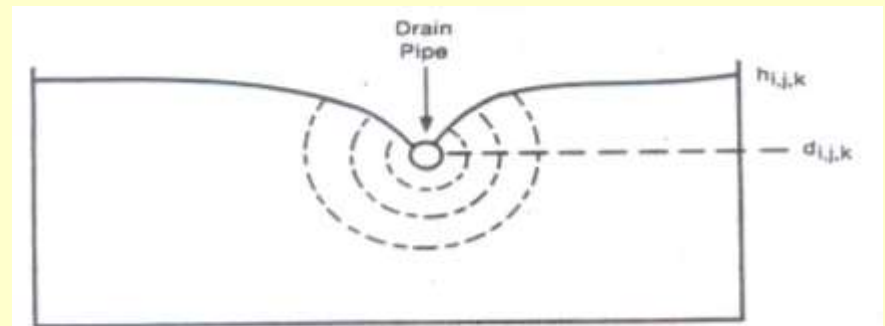
Where,

$QD_{i,j,k}$: the rate water flows into the drain

$d_{i,j,k}$: the head in the drain

$h_{i,j,k}$: the head in the aquifer near the drain

$CD_{i,j,k}$: the conductance of the interface between the aquifer and the drain.



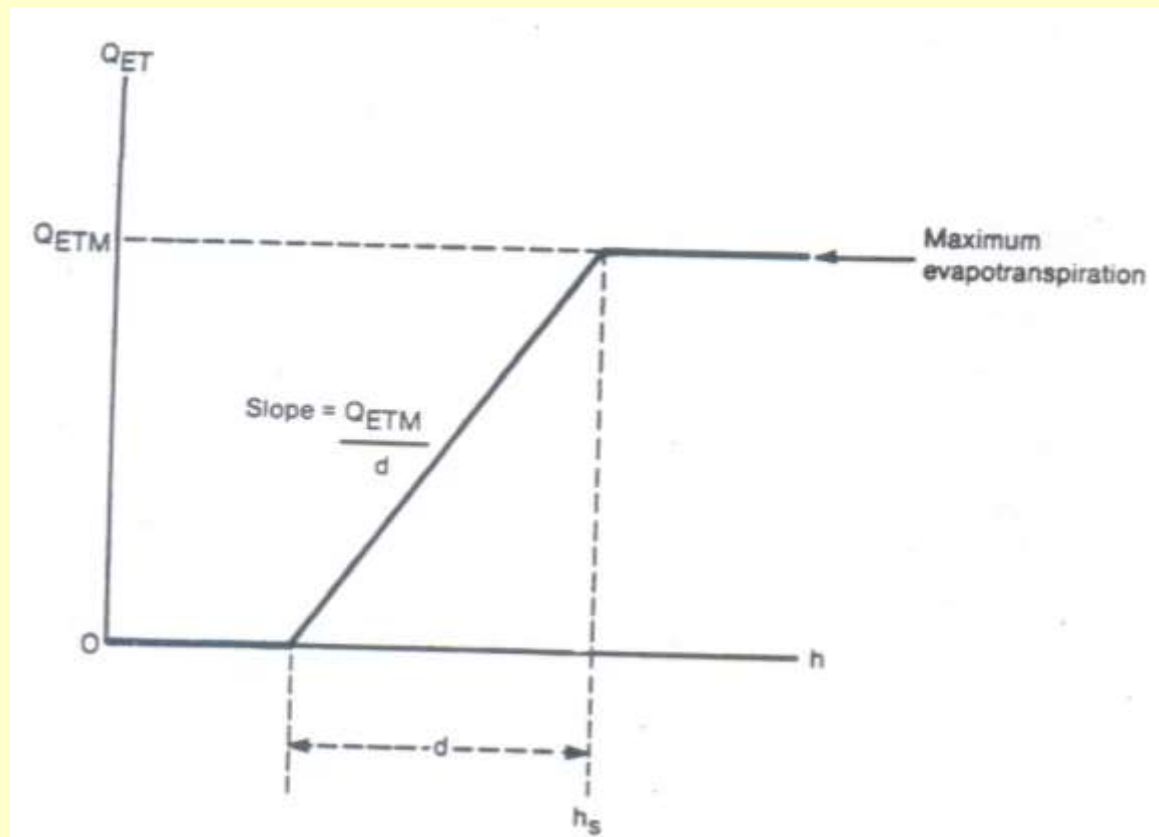
EVAPOTRANSPIRATION PACKAGE

Evapotranspiration (ET) is the mechanism whereby water is converted from liquid phase to vapour phase.

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



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:

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

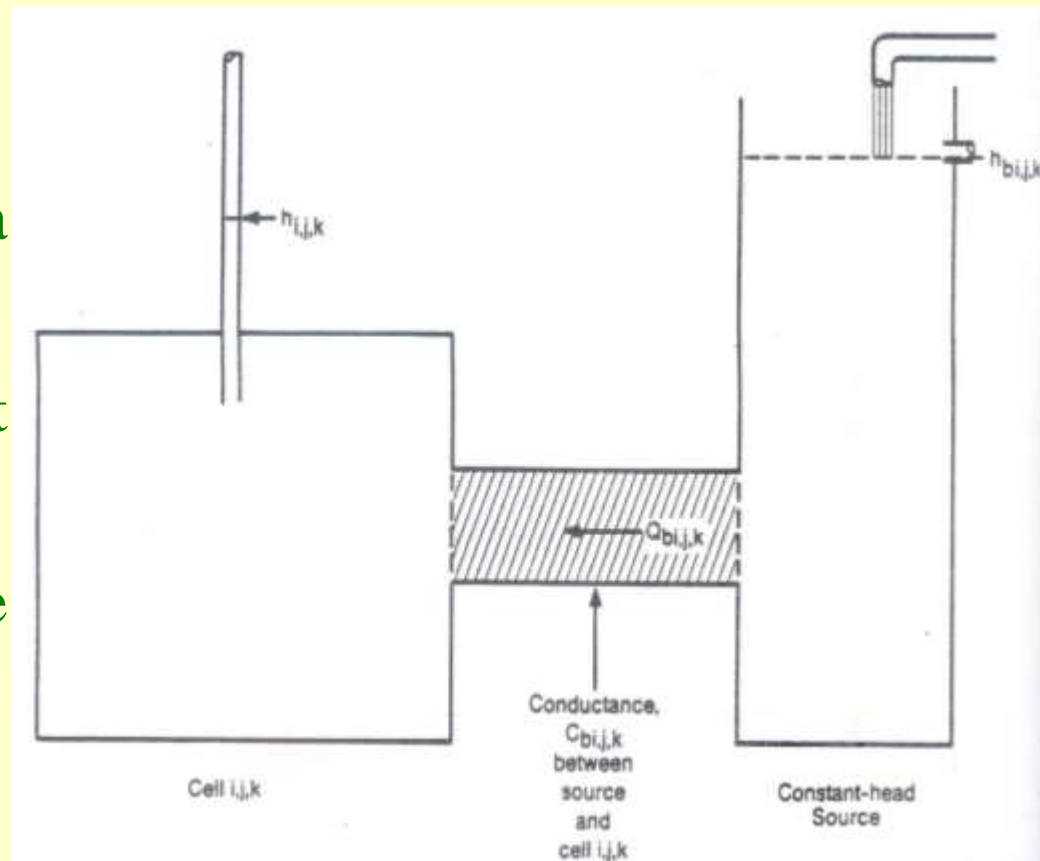
Where,

$Q_{i,j,k,m}$: water supply rate to a cell from boundary

C_m : proportionality constant for boundary

HB_m : head at source boundary m

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



Wall (HFB) Boundary Condition

- The Horizontal-Flow-Barrier (HFB) Package is included to simulate thin, vertical, low-permeability features that impede the horizontal flow of groundwater.
- This package allows such features to be simulated without the need to reduce grid spacing in an excessive number of model cells, thus enhancing model efficiency.
- These features are approximated as a series of horizontal flow barriers conceptually situated on the boundaries between adjacent cells in the finite difference grid.

Thankyou