Modeling (General Concepts)

Modeling is a tool used by engineers to make decisions regarding design and operation of an environmental system. Models can be used to forecast future conditions in response to those decisions, select a best set of decisions based on some desired criterion, or determine the most likely physical values that explain an observed condition.

Because most real systems are far too complicated to model as they are, a set of simplifying assumptions is posed to make the modeling problem tractable - this is often called the "conceptual model".

On the basis of these simplifying assumptions a "mathematical model" (usually balance equations) is created. The solution of the mathematical model yields the behavior of the system being studied.

After the model is created, it is "calibrated". This is the process of adjusting model parameters (transmissivity, storativity, etc.), forcing inputs, and geometry until the model response is identical (within some tolerance) to the observed historical response of the real system. Multiple calibrations can produce identical responses, so great care must be taken in calibrating and testing a model before using it - once acceptably calibrated the model can be used for forecasting.

Finite-Difference Method (Introduction)

Most problems in environmental modeling require the solution of differential equations, either ordinary or partial. Two common numerical methods of approximating solutions to ODEs and PDEs are finite element and finite difference methods. The finite-difference method (FDM) estimates the values of one or more functions at characteristic locations (nodes) of the solution domain. The estimation is achieved by discritization of the space-time domain through a two, three, or four dimensional grid and the approximation of the differential equation by a difference equation.

The differential problem thus becomes an algebraic problem and the computation of the field variable values at the nodes of the grid is a matter of the solution of the algebraic equations (either linear or non-linear).

One procedure to generate finite difference schemes is based on Taylor-series expansions:

$$f(x+Dx)=f(x) + Dx\frac{df}{dx} + \frac{Dx^2}{2!}\bullet\frac{d^2f}{dx^2} + ... + \frac{Dx^n}{n!}\bullet\frac{d^nf}{dx^n}$$

Rearrange

$$\frac{df}{dx} = \frac{f(x+Dx)-f(x)}{Dx} - Dx\bullet\frac{d^2f}{dx^2} - ...$$

Truncate at second term

$$\frac{df}{dx} \quad \frac{f(x+Dx)-f(x)}{Dx}$$

This expression is called a "first-order" forward finite difference approximation. Error is proportional to Dx.

Now consider a backward discritization:

$$f(x-Dx)=f(x) - Dx\frac{df}{dx} + \frac{Dx^2}{2!}\bullet\frac{d^2f}{dx^2} + ... \pm \frac{Dx^n}{n!}\bullet\frac{d^nf}{dx^n}$$

Rearrange and truncate to obtain:

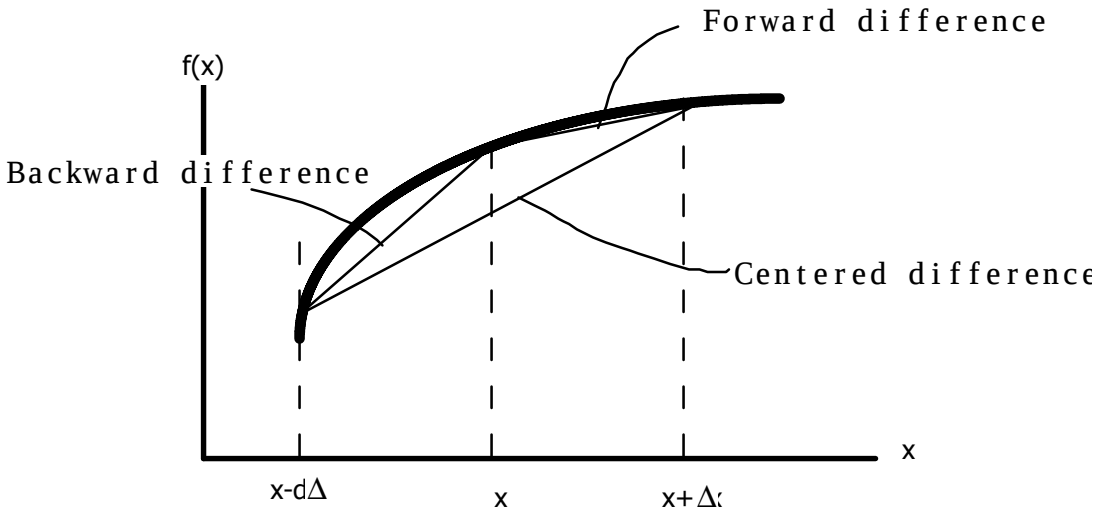
$$\frac{df}{dx} \quad \frac{f(x)-f(x-Dx)}{Dx}$$

This expression is called a "first-order" backward finite difference approximation. Error is proportional to Dx.

If we take the average of these two expressions we obtain

$$\frac{df}{dx} \quad \frac{f(x+Dx)-f(x-Dx)}{2Dx}$$

This expression is called a "second-order" centered finite difference approximation. Error is proportional to Dx^2 .



Because Dx is supposed to represent small purturbations from the function at x, then Dx^2 < Dx, so that the error in the centered difference approximation is smaller.

Why is the error reduced?

Consider the two difference schemes (forward and backward)

$$\text{FD:}\quad f(x+Dx)=f(x) + Dx\frac{df}{dx} + \frac{Dx^2}{2!}\bullet\frac{d^2f}{dx^2} + \ldots. + \frac{Dx^n}{n!}\bullet\frac{d^nf}{dx^n}$$

$$\text{BD:}\quad f(x-Dx)=f(x) - Dx\frac{df}{dx} + \frac{Dx^2}{2!}\bullet\frac{d^2f}{dx^2} + \ldots. \pm \frac{Dx^n}{n!}\bullet\frac{d^nf}{dx^n}$$

The averaging scheme simply adds these two series and divides the result by two. Observe that the Dx term cancels, leaving the next highest term in the truncated part as Dx^2 which determines the truncation error!

Common Difference Schemes

$$\frac{df}{dx} \qquad \frac{f(x+Dx)-f(x)}{Dx} \qquad E(Dx)$$

$$\frac{df}{dx} \qquad \frac{f(x+Dx)-f(x-Dx)}{2Dx} \qquad E(Dx^2)$$

$$\frac{d^2f}{dx^2} \qquad \frac{f(x+Dx)-2f(x)+f(x-Dx)}{Dx^2}$$

$$E(Dx^2)$$

$$\frac{d^3f}{dx^3} \qquad \frac{-f(x-2Dx)+2f(x-Dx)-2f(x+Dx)+f(x+2Dx)}{2Dx^3}$$

$$E(Dx^6)$$

The procedure is generic and can be used to construct approximations of any accuracy. The resulting algebraic equations are then used to relate new values of f to preceding values.

When time is a variable the evaluation requires the analyst to choose which time level to evaluate the functions. If the new values are completely determined by old values the scheme is called "explicit". If the values are determined by other new values and some old values the scheme is called "implicit".

The quality of the schemes depends on:

Consistency - does the scheme exactly replace the differential in the limit as Dx -> 0.
Convergence - do the numerical values exactly duplicate the analytical values when Dx -> 0.
Stability - does any error in the scheme remain bounded (stable) or are errors amplified (unstable).

Practical considerations include:

(1) What is the best discritization (grid, mesh , etc.) selection and orientation.
(2) What is the best scheme for the problem.
(3) Initial and boundary conditions: Geometry and difference representations of different boundary types.
(4) How to obtain solutions: FORTRAN, spreadsheets, graphical methods.

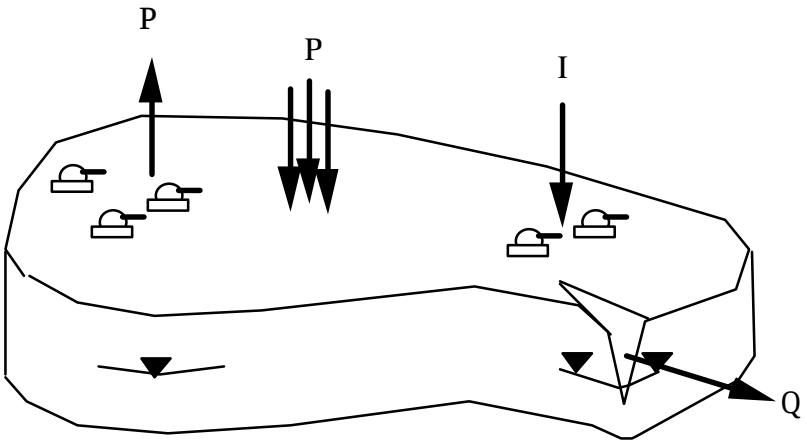
Cell Balance Methods

Cell balance methods are an alternative approach for developing numerical models of physical systems - they have the advantage of being somewhat more intuitive to create although they are roughly equivalent to "integrated finite-

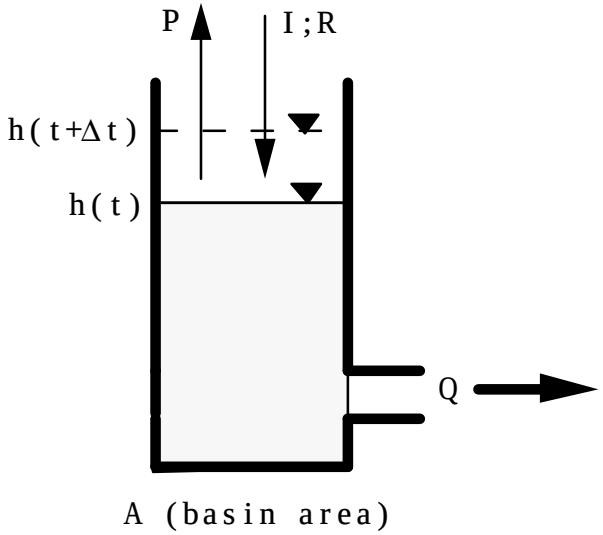
difference" developments.

Single Cell Model

The single cell model visulaizes an entire groundwater system as a single cell.



The single aquifer can be further schematized as:



Model assumes averaged conditions throughout the entire system - spatially averaged head, recharge, discharge, etc.

$$AS\frac{h(t+Dt) - h(t)}{Dt} = AR + I - P - Q$$

where

A = aquifer area
S = aquifer storativity
h = averaged aquifer head at time t
I = water injection rate

R = aquifer recharge rate/unit area
P = aquifer pumping rate
Q = aquifer discharge rate (to surface)

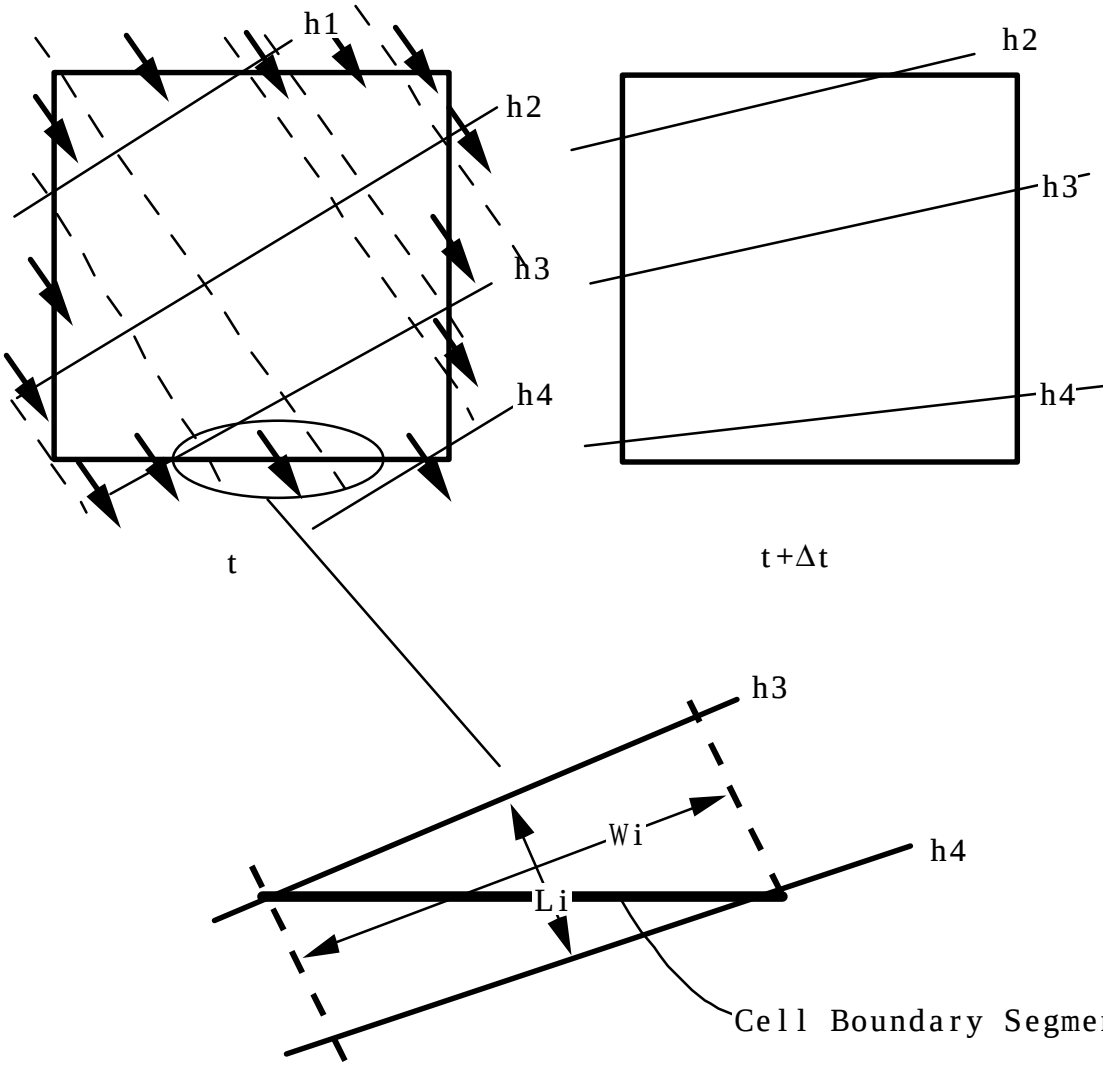
The model also assumes the the rates of recharge, discharge, etc. remain constant over the time interval Dt.

The unknown parameters required for calibration are S and R (implicitly assuming records of pumping, injection, and average head are available). Sometimes Q = Q(h) also requires calibration.

Average values for h are obtained from contour maps at time t and t+ Dt. If A is large, it is subdivided into

subdomains (DA_i), and $h = \sum_i h_i \, DA_i / A$.

When groundwater inflow and outflow are a component of the water balance, the single cell model is modified:



$$\text{Outflow through i-th segment} = T_i \frac{h_3 - h_4}{L_i} W_i$$

where T_i = transmissivity near/at i-th segment.

If contours change significantly over Dt, then one needs to use care to obtain a correct time-averaged flux.

The modified balance is expressed as:

$$AS\frac{h(t+Dt) - h(t)}{Dt} = AR + I - P - Q + \sum_i W_i T_i J_i$$

when justified, other components can be added to the single cell model:

(1) evapo-transpiration
(2) infiltration
(3) drainage
(4) leakage
(5) irrigation return flow

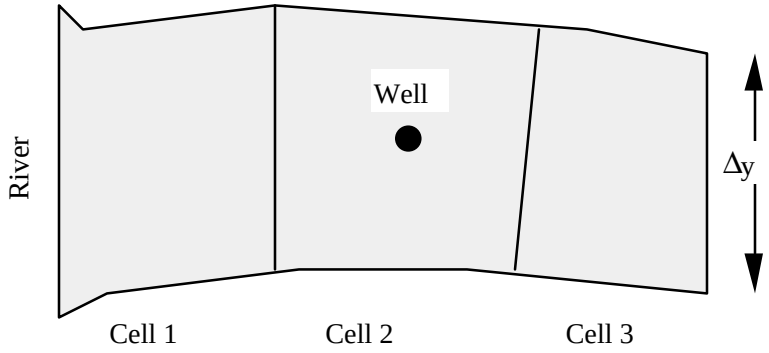
Despite its apparent simplicity this type of model is very useful. In fact, the regional mass balance obtained with this model should be fairly close to that obtained by more complex methods and single cell models serve as nice checks on more complex models.

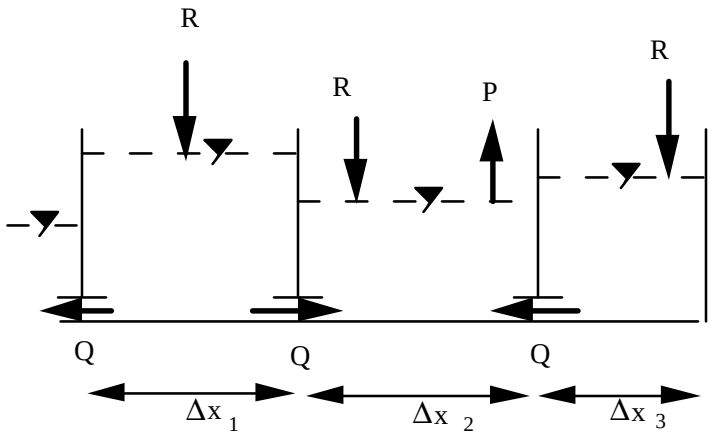
The next step is to join several single cell models through various flux terms - when each cell size is small, and many cells are considered one can obtain a realistic flow model for many types of problems.

Multiple Cell Balance Model

The multiple cell balance model links a number of single cell models by various representations of hydrualics and transport theory.

Consider an aquifer system that can be represented by three cells:





Approach to "model" this system is:

Write single cell models for each cell

$$A_1 S_1 \frac{h(t+Dt)_1 - h(t)_1}{Dt} = A_1 R_1 + I_1 - P_1 - Q_{out1} + Q_{in1}$$

$$A_2 S_2 \frac{h(t+Dt)_2 - h(t)_2}{Dt} = A_2 R_2 + I_2 - P_2 - Q_{out2} + Q_{in2}$$

$$A_3 S_3 \frac{h(t+Dt)_3 - h(t)_3}{Dt} = A_3 R_3 + I_3 - P_3 - Q_{out3} + Q_{in3}$$

Use Darcy's law to link the cells:

$$Q_{in2} = \frac{Dx_2 + Dx_3}{Dx_2/T_2 + Dx_3/T_3} \quad Dy \quad \frac{h_3 - h_2}{(Dx_2 + Dx_3)/2}$$

Then "generalize" these expressions for all three cells:

$$A_i \, S_i \frac{h(t+Dt)_i - h(t)_i}{Dt} = A_i \, R_i + I_i - P_i +$$

$$T_{i-1/2} \quad Dy \quad \frac{h_{i-1} - h_i}{(Dx_{i-1} + Dx_i)/2} + T_{i+1/2} \quad Dy$$

$$\frac{h_{i+1} - h_i}{(Dx_{i+1} + Dx_i)/2}$$

Divide both sides by the cell area $A_i = Dx_i \, Dy_i$

$$S_i \frac{h(t+Dt)_i - h(t)_i}{Dt} = R_i + I_i / A_i - P_i / A_i +$$

$$T_{i-1/2} \quad \frac{1}{Dx} \quad \frac{h_{i-1} - h_i}{(Dx_{i-1} + Dx_i)/2} +$$

$$T_{i+1/2} \, \frac{1}{Dx} \quad \frac{h_{i+1} - h_i}{(Dx_{i+1} + Dx_i)/2}$$

Where

$$T_{i-1/2} = \frac{Dx_{i-1} + Dx_i}{Dx_{i-1}/T_{i-1} + Dx_i/T_i}$$

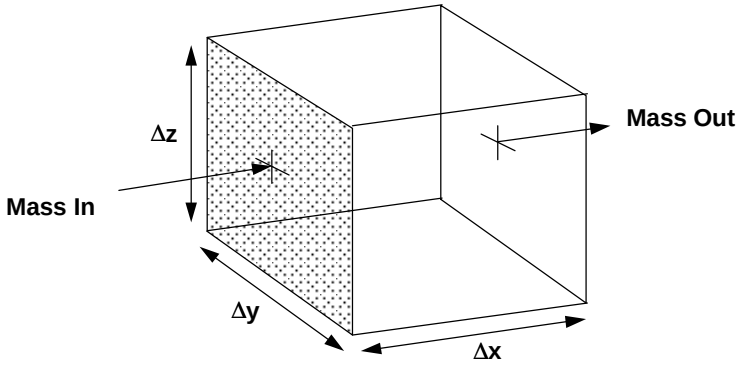
$$T_{i+1/2} = \frac{Dx_i + Dx_{i+1}}{Dx_i/T_i + Dx_{i+1}/T_{i+1}}$$

Remarkably, the MCB method leads to identical expressions as a typical centered finite difference method will if the cells are rectangular.

However, unlike FDM, MCB does not require a particular cell geometry - thus it may be more useful for certain geometrically challenging problems.

Cell Balance Model for Steady Confined Groundwater Flow

Single Liquid Phase; Fully Saturated Porous Medium



$V_{cell} = \Delta x \Delta y \Delta z$ $V_{pore} = \omega \, \Delta x \Delta y \Delta z$

$V_{solid} = (1-\omega) \Delta x \Delta y \Delta z$ $M_{solid} = \rho_s (1-\omega) \, \Delta x \Delta y \Delta z$

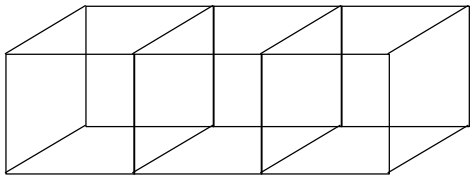
Mass Balance Expression:

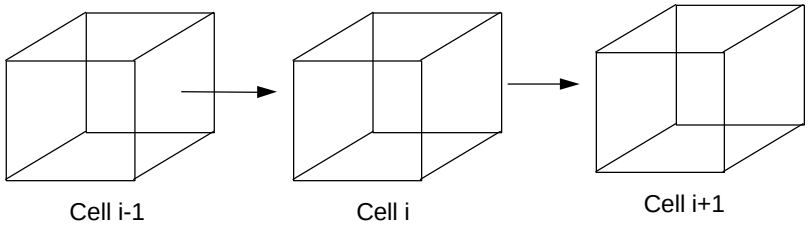
Rate of Change of Mass in Cell =
Mass Flow Into Cell - Mass Flow Out of Cell +
Rate of Mass Transferred

Steady State, No sources or sinks:

0 = Mass Flow Into Cell - Mass Flow Out of Cell

Schematic of Multiple Cells (One-Dimensional Flow)





Balance Expressions for i-th Cell

Mass Flow Into Cell

$K\,\Delta y\Delta z\,[h_{i-1} - h_i]/\Delta x$

Mass Flow Out of Cell

$K\,\Delta y\Delta z\,[h_i - h_{i+1}]/\Delta x$

Complete Balance Equation for i-th Cell

$0 = K\Delta y\Delta z[h_{i-1} - h_i\,]\,/\Delta x - K\Delta y\Delta z[h_i - h_{i+1}]\,/\Delta x$

Group like terms, divide by cell volume:

$0 = K[h_{i-1} - 2h_i + h_{i+1}]/\Delta x^2$ (i)

Using the definition of partial derivative from calculus we can take limits as Δx vanishes and (i) in the limit is

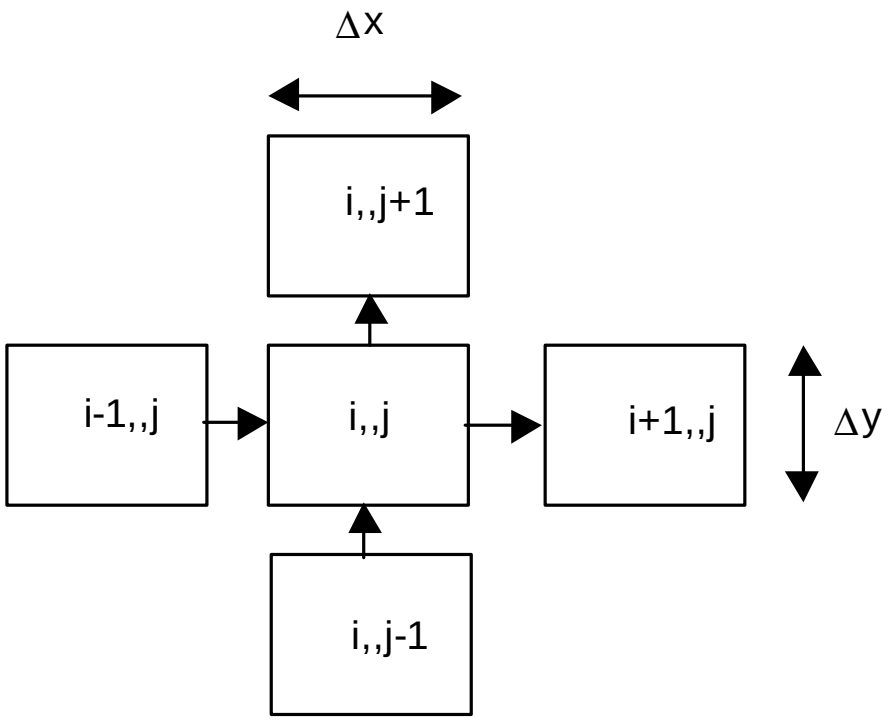
$$0 = \frac{\partial}{\partial x}[K\frac{\partial h}{\partial x}] \qquad \text{(ii)}$$

Observe that this last expression is exactly the governing equation of groundwater flow (Steady State, 1D, Confined Aquifer).

The equation (i) is the algebraic difference approximation to the equation (ii).

$$K[h_{i-1} - 2h_i + h_{i+1}]/\Delta x^2 \approx \frac{\partial}{\partial x}[K\frac{\partial h}{\partial x}]$$

Schematic of Multiple Cells (Two-Dimensional Flow)



Balance Expressions for i,j-th Cell

Mass Flow Into Cell

$$K\,\Delta y\; b[h_{i-1,j} - h_{i,j}]/\Delta x + K\,\Delta x\, b\,[h_{i,j-1} - h_{i,j}]/\Delta y$$

Mass Flow Out of Cell

$$K\,\Delta y\; b[h_{i,j} - h_{i+1,j}]/\Delta x + K\,\Delta x\, b\,[h_{i,j} - h_{i,j+1}]/\Delta y$$

Complete Balance Equation for i,j-th Cell, Substitute T=Kb

$$0 = T\,\Delta y\,[h_{i-1,j} - h_{i,j}]/\Delta x + T\,\Delta x\,[h_{i,j-1} - h_{i,j}]/\Delta y$$
$$-\{T\,\Delta y\,[h_{i,j} - h_{i+1,j}]/\Delta x + T\,\Delta x\,[h_{i,j} - h_{i,j+1}]/\Delta y\}$$

Group like terms, divide by cell area:

$$0 = T[h_{i-1,j} - 2h_{i,j} + h_{i+1,j}]/\Delta x^2 + T[h_{i,j-1} - 2h_{i,j} + h_{i,j+1}]/\Delta y^2$$

Using the definition of partial derivatives from calculus we can take limits as Δx and Δy vanish and in the limit the difference equation is

$$0 = \frac{\partial}{\partial x}[T\frac{\partial h}{\partial x}] + \frac{\partial}{\partial y}[T\frac{\partial h}{\partial y}]$$

Observe that this last expression is exactly the governing equation of 2D, steady-state confined aquifer flow.

Again the difference equation is the algebraic difference approximation to the partial differential equation.

$$T[h_{i-1,j} - 2h_{i,j} + h_{i+1,j}]/\Delta x^2 + T[h_{i,j-1} - 2h_{i,j} + h_{i,j+1}]/\Delta y^2 \approx \frac{\partial}{\partial x}[T\frac{\partial h}{\partial x}] + \frac{\partial}{\partial y}[T\frac{\partial h}{\partial y}]$$

The difference equations can be "solved" using a computer program (e.g. a spreadsheet) for reasonably complicated geometry and boundary conditions.

To account for spatially varying formation properties (K or T) the difference equations are usually written using average values at the cell interfaces.

Mass Flow Into Cell (anisotropic,inhomogeneous)

$$[T_{x\ i-1,j} + T_{x\ i,j}]/2\ \Delta y\ b[h_{i-1,j} - h_{i,j}]/\Delta x +$$
$$[T_{y\ i,j-1} + T_{y\ i,j}]/2\ \Delta x\ b\ [h_{i,j-1} - h_{i,j}]/\Delta y$$

Mass Flow Out of Cell (anisotropic,inhomogeneous)

$$[T_{x\ i,j} + T_{x\ i+1,j}]/2\ \Delta y\ b[h_{i-1,j} - h_{i,j}]/\Delta x +$$
$$[T_{y\ i,j} + T_{y\ i,j+1}]/2\ \Delta x\ b\ [h_{i,j} - h_{i,j+1}]/\Delta y$$

Let

$$A_{ij}=[T_{x\ i-1,j} + T_{x\ i,j}]/2\Delta x^2$$
$$B_{ij}=[T_{x\ i,j} + T_{x\ i+1,j}]/2\Delta x^2$$
$$C_{ij}=[T_{y\ i,j-1} + T_{y\ i,j}]/2\Delta y^2$$
$$D_{ij}=[T_{y\ i,j} + T_{y\ i,j+1}]/2\Delta y^2$$

When we write the complete balance equation for i,j-th cell, collect like terms and divide by the cell volume we obtain:

$$0 = A_{ij}h_{i-1,j} - (A_{ij}+B_{ij}+C_{ij}+D)h_{i,j} + B_{ij}h_{i+1,j} + C_{ij}h_{i,j-1} + D_{ij}h_{i,j+1}$$

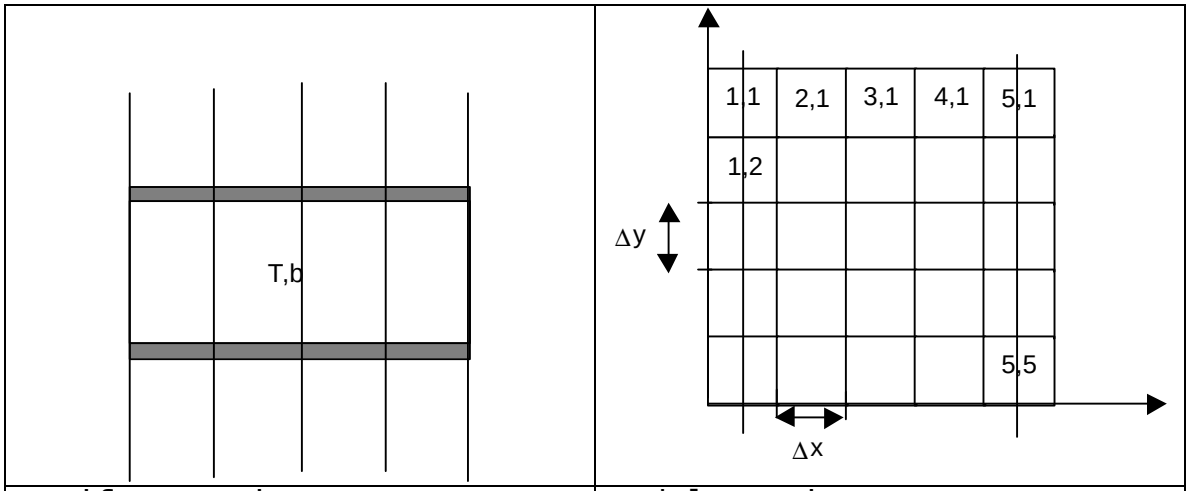
This difference equation can be written as an explicit equation for h as

$$h_{i,j} = [A_{ij}h_{i-1,j} + B_{ij}h_{i+1,j} + C_{ij}h_{i,j-1} + D_{ij}h_{i,j+1}]/(A_{ij}+B_{ij}+C_{ij}+D)$$

This difference equation represents an approximation to the governing flow equation, the accuracy depending on the cell size.

Boundary conditions are applied directly into the analogs (another name for the difference equations) at appropriate locations on the computational grid.

Rectangular Aquifer Example



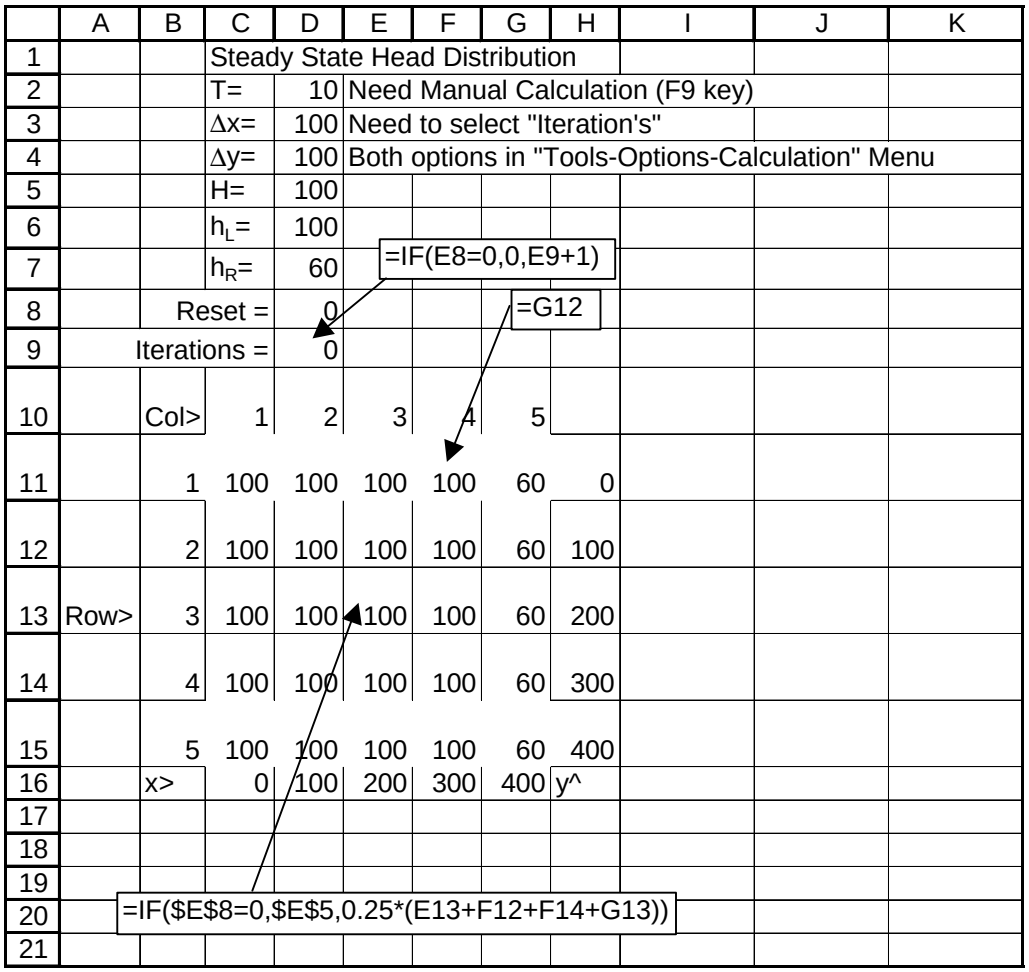
Aquifer Domain | Model Domain

Simulate the Aquifer with the 5 x 5 model shown. The left and right boundaries will be treated as specified head boundaries. The upper and lower boundary will be treated as no flow boundaries.

The difference equations are entered into spreadsheet cells corresponding to the appropriate location in the model domain.

Boundary conditions are incorporated by explicit entering of the conditions.

An example spreadsheet is shown on the next figure.

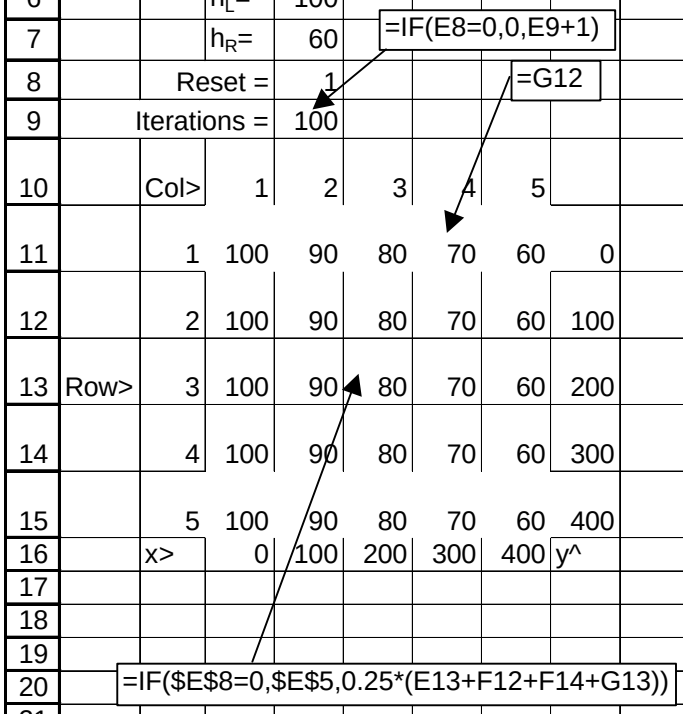


Observe that the cell formula depends on the value of cell D8. This feature allows you to reset the calculations in case something goes wrong. Once D8 is changed to non-zero and you instruct the program to make calculations, it will automatically update the cell values until the solution converges. The value in cell D5 is just some starting value to begin the iterations.

Please observe that the automatic recalculation feature must be disabled and the iterations feature selected. Both these options can be selected from the "Tools-Options-Calculation" dialog box in the spreadsheet (EXCEL).

The result for this example is shown on the next figure.

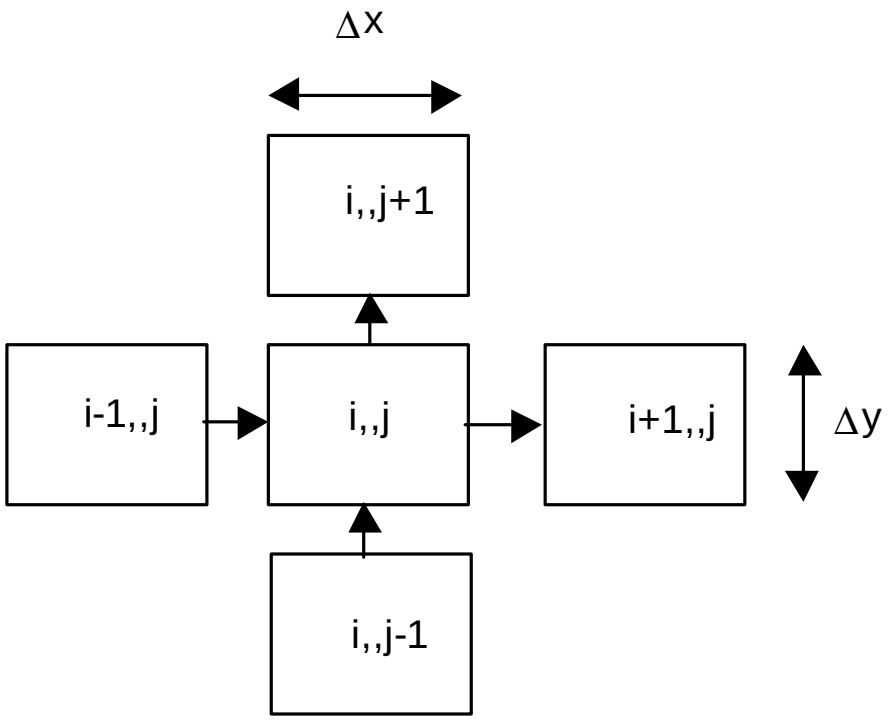
	A	B	C	D	E	F	G	H	I	J	K
1			Steady State Head Distribution								
2			T=	10	Need Manual Calculation (F9 key)						
3			Δx=	100	Need to select "Iteration's"						
4			Δy=	100	Both options in "Tools-Options-Calculation" Menu						
5			H=	100							
6			h_L=	100							
7			h_R=	60							
8		Reset =		1							
9		Iterations =		100							
10		Col>	1	2	3	4	5				
11		1	100	90	80	70	60	0			
12		2	100	90	80	70	60	100			
13	Row>	3	100	90	80	70	60	200			
14		4	100	90	80	70	60	300			
15		5	100	90	80	70	60	400			
16		x>	0	100	200	300	400	y^			
17											
18											
19											
20											
21											



Thus we now have a tool to allow us to approximate the solution to

$$0 = \frac{\partial}{\partial x}[T\frac{\partial h}{\partial x}] + \frac{\partial}{\partial y}[T\frac{\partial h}{\partial y}]$$

Cell Balance Model for Transient Confined Groundwater Flow



Balance Expressions for i,j-th Cell

Mass Flow Into Cell

$K\ \Delta y\ b[h_{i-1,j} - h_{i,j}]/\Delta x + K\ \Delta x\ b\ [h_{i,j-1} - h_{i,j}]/\Delta y$

Mass Flow Out of Cell

$K\ \Delta y\ b[h_{i,j} - h_{i+1,j}]/\Delta x + K\ \Delta x\ b\ [h_{i,j} - h_{i,j+1}]/\Delta y$

Rate of Mass Stored in Cell

$S\ \Delta x \Delta y\ [h^{t+\Delta t}_{i,j} - h^{t}_{i,j}]/\Delta t$

Rate of Internal Mass Transferred (Recharge - Pumpage)

$R-Q = (r-q)\Delta x \Delta y$

(R,Q is volumetric rate over entire cell, r,q is rate per unit area of cell)

Complete Balance Equation for i,j-th Cell, Substitute T=Kb

$$S\,\Delta x\Delta y\,[h^{t+\Delta t}_{i,j} - h^{t}_{i,j}]/\Delta t = (r-q)\Delta x\Delta y + T\,\Delta y\,[h_{i-1,j} - h_{i,j}]/\Delta x + T\,\Delta x\,[h_{i,j-1} - h_{i,j}]/\Delta y - T\,\Delta y\,[h_{i,j} - h_{i+1,j}]/\Delta x - T\,\Delta x\,[h_{i,j} - h_{i,j+1}]/\Delta y$$

Group like terms, divide by cell area:

$$S\,[h^{t+\Delta t}_{i,j} - h^{t}_{i,j}]/\Delta t = T[h_{i-1,j} - 2h_{i,j} + h_{i+1,j}]/\Delta x^2 + T[h_{i,j-1} - 2h_{i,j} + h_{i,j+1}]/\Delta y^2 + (r-q)$$

Using the definition of partial derivatives from calculus we can take limits as Δx and Δy vanish and in the limit the difference equation is

$$S\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left[T\frac{\partial h}{\partial x}\right] + \frac{\partial}{\partial y}\left[T\frac{\partial h}{\partial y}\right] + r - q$$

Observe that this last expression is exactly the governing equation of 2D, confined aquifer flow.

Again the difference equation is the algebraic difference approximation to the partial differential equation.

$$T[h_{i-1,j} - 2h_{i,j} + h_{i+1,j}]/\Delta x^2 + T[h_{i,j-1} - 2h_{i,j} + h_{i,j+1}]/\Delta y^2 \approx \frac{\partial}{\partial x}\left[T\frac{\partial h}{\partial x}\right] + \frac{\partial}{\partial y}\left[T\frac{\partial h}{\partial y}\right]$$

The difference equations can be "solved" using a computer program (e.g. a spreadsheet) for reasonably complicated geometry and boundary conditions.

To account for spatially varying formation properties (K or T) the difference equations are usually written using average values at the cell interfaces.

Mass Flow Into Cell (anisotropic,inhomogeneous)

$$[T_{x\ i-1,j} + T_{x\ i,j}]/2\ \Delta y\ b[h_{i-1,j} - h_{i,j}]/\Delta x +$$
$$[T_{y\ i,j-1} + T_{y\ i,j}]/2\ \Delta x\ b\ [h_{i,j-1} - h_{i,j}]/\Delta y$$

Mass Flow Out of Cell (anisotropic,inhomogeneous)

$$[T_{x\ i,j} + T_{x\ i+1,j}]/2\ \Delta y\ b[h_{i-1,j} - h_{i,j}]/\Delta x +$$
$$[T_{y\ i,j} + T_{y\ i,j+1}]/2\ \Delta x\ b\ [h_{i,j} - h_{i,j+1}]/\Delta y$$

Let

$$A_{ij}=[T_{x\ i-1,j} + T_{x\ i,j}]/2\Delta x^2$$
$$B_{ij}=[T_{x\ i,j} + T_{x\ i+1,j}]/2\Delta x^2$$
$$C_{ij}=[T_{y\ i,j-1} + T_{y\ i,j}]/2\Delta y^2$$
$$D_{ij}=[T_{y\ i,j} + T_{y\ i,j+1}]/2\Delta y^2$$

When we write the complete balance equation for i,j-th cell, collect like terms and divide by the cell volume we obtain:

$$S\ [h^{t+\Delta t}_{\ i,j} - h^{t}_{\ i,j}]/\Delta t$$
$$= A_{ij}h_{i-1,j} -(A_{ij}+B_{ij}+C_{ij}+D)h_{i,j} + B_{ij}h_{i+1,j} + C_{ij}h_{i,j-1} + D_{ij}h_{i,j+1} + r - q$$

This difference equation can be rearranged as an explicit update expression if all the values of h on the right hand side are evaluates at time level t.

$$h^{t+\Delta t}_{\ i,j} =$$

$$h^{t}_{\ i,j} + \Delta t/S\ *\{\ r - q +$$
$$[A_{ij}\ h^{t}_{\ i-1,j} + B_{ij}\ h^{t}_{\ i+1,j} + C_{ij}\ h^{t}_{\ i,j-1} + D_{ij}\ h^{t}_{\ i,j+1}]/(A_{ij}+B_{ij}+C_{ij}+D)\}$$

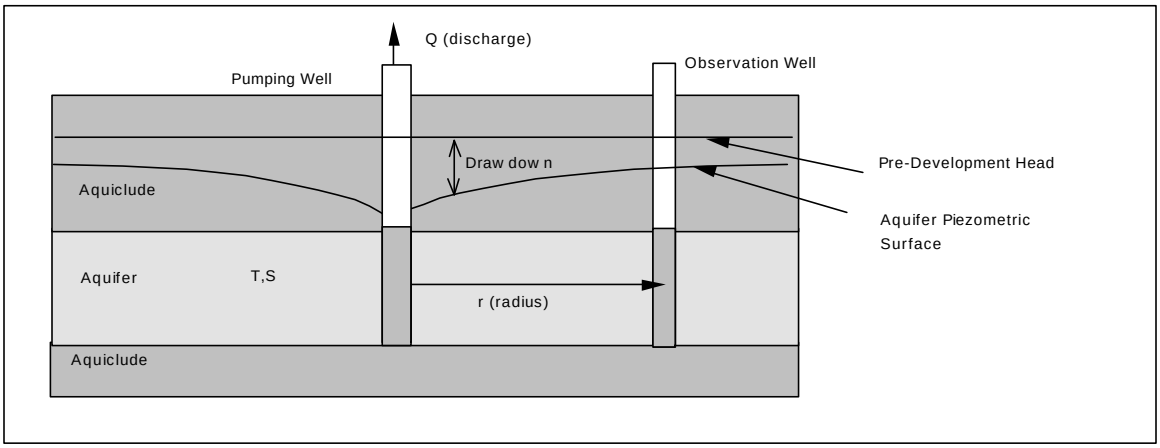
This difference equation represents an approximation to the governing flow equation, the accuracy depending on the cell size.

The time step Δt depends on the values of T, Δx, Δy and S for a stable solution. More robust difference equations are generally used (implicit, Crank_Nicholsen; etc.) but the representation presented here is very simple to program – even in a spreadsheet.

Example

Flow to a Well in a Leaky-Confined Aquifer

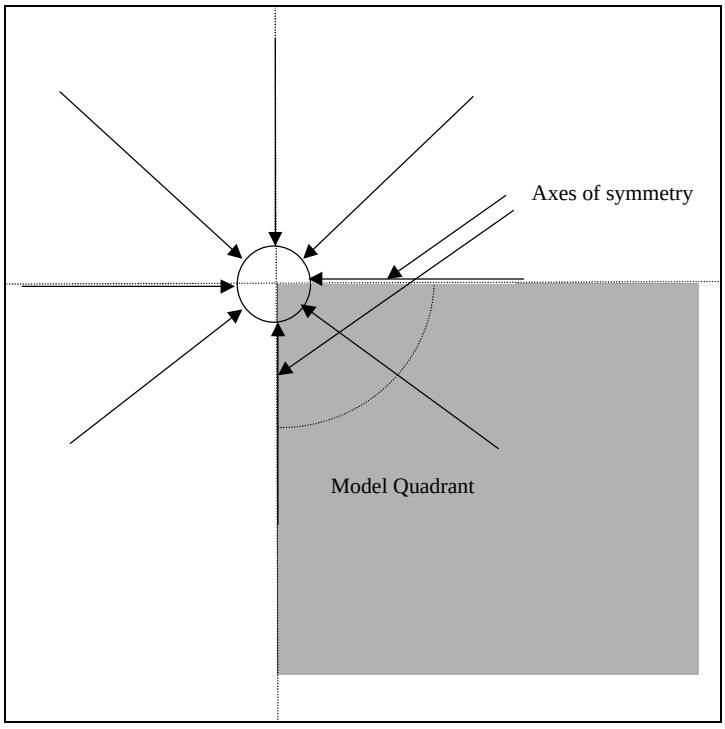
Conceptual Model



Homogeneous-isotropic aquifer, well pumps at constant rate.

Determine distance-drawdown by numerical model and compare to analytical (Theis) solution.

Grid Design



Observe that there are two axes of symmetry. The flow domain is mapped onto the quadrant shown and only 1/4 of the flow is considered.

A spreadsheet model of this situation is depicted below. Observe the arrays for material properties (T,S) and recharge/discharge.

Flow to Well in Aquifer										
Δx	2									
Δy	2									
Δx^2	4									
Δy^2	4									
	Transmissivity Array			sq. meters/day						
	Column									
Row	0	1	2	3	4	5	6	7	8	0
0	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023
1	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023
2	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023
3	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023
4	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023
5	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023
6	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023
7	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023
8	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023
0	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023
	Storage Coefficient Array									
	Column									
Row	0	1	2	3	4	5	6	7	8	0
0	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075
1	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075
2	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075
3	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075
4	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075
5	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075
6	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075
7	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075
8	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075
0	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075	0.0075
	Recharge Array			cu .meters/day						
	Column									
Row	0	1	2	3	4	5	6	7	8	0
0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
	Pumpage Array			cu. meters/day						
	Column									
Row	0	1	2	3	4	5	6	7	8	0
0	0	0	0	0	0	0	0	0	0	0
1	0	0.004	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
	Initial Head Array			meters						
	Column									
Row	0	1	2	3	4	5	6	7	8	0
0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
1	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
2	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
3	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
4	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
5	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
6	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
7	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
8	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0

continued .....

..... from previous sheet

Restart	1									
Iteration	2917									
Dt	0.1									
Time	291.7	sec								
Pumpage	1.1668									
	Head (Iteration -1)			meters						
	Column									
Row	0	1	2	3	4	5	6	7	8	0
0	97.5	97.5	98.3	98.9	99.2	99.4	99.6	99.8	99.9	100.0
1	97.5	97.5	98.3	98.9	99.2	99.4	99.6	99.8	99.9	100.0
2	98.3	98.3	98.7	99.0	99.3	99.5	99.6	99.8	99.9	100.0
3	98.9	98.9	99.0	99.2	99.4	99.5	99.7	99.8	99.9	100.0
4	99.2	99.2	99.3	99.4	99.5	99.6	99.7	99.8	99.9	100.0
5	99.4	99.4	99.5	99.5	99.6	99.7	99.8	99.9	99.9	100.0
6	99.6	99.6	99.6	99.7	99.7	99.8	99.8	99.9	100.0	100.0
7	99.8	99.8	99.8	99.8	99.8	99.9	99.9	99.9	100.0	100.0
8	99.9	99.9	99.9	99.9	99.9	99.9	100.0	100.0	100.0	100.0
0	99.9	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
	Head (Iteration)			meters						
	Column									
Row	0	1	2	3	4	5	6	7	8	0
0	97.5	97.5	98.3	98.9	99.2	99.4	99.6	99.8	99.9	100.0
1	97.5	97.4893	98.3482	98.8536	99.1891	99.43	99.6132	99.7601	99.8852	100
2	98.3	98.3482	98.6813	99.0046	99.2668	99.4736	99.6385	99.7742	99.8916	100
3	98.9	98.8536	99.0046	99.1984	99.3838	99.5454	99.6824	99.7995	99.9032	100
4	99.2	99.1891	99.2668	99.3838	99.5098	99.629	99.7362	99.8316	99.9181	100
5	99.4	99.43	99.4736	99.5454	99.629	99.7134	99.7931	99.8665	99.9347	100
6	99.6	99.6132	99.6385	99.6824	99.7362	99.7931	99.8488	99.9016	99.9516	100
7	99.8	99.7601	99.7742	99.7995	99.8316	99.8665	99.9016	99.9356	99.9682	100
8	99.9	99.8852	99.8916	99.9032	99.9181	99.9347	99.9516	99.9682	99.9843	100
0	99.8852	100	100	100	100	100	100	100	100	100
◄	Drawdown (Iteration)			meters						
	Column									
Row	0	1	2	3	4	5	6	7	8	0
0	2.5	2.5	1.7	1.1	0.8	0.6	0.4	0.2	0.1	0.0
1	2.5	2.5	1.7	1.1	0.8	0.6	0.4	0.2	0.1	0.0
2	1.7	1.7	1.3	1.0	0.7	0.5	0.4	0.2	0.1	0.0
3	1.1	1.1	1.0	0.8	0.6	0.5	0.3	0.2	0.1	0.0
4	0.8	0.8	0.7	0.6	0.5	0.4	0.3	0.2	0.1	0.0
5	0.6	0.6	0.5	0.5	0.4	0.3	0.2	0.1	0.1	0.0
6	0.4	0.4	0.4	0.3	0.3	0.2	0.2	0.1	0.0	0.0
7	0.2	0.2	0.2	0.2	0.2	0.1	0.1	0.1	0.0	0.0
8	0.1	0.1	0.1	0.1	0.1	0.1	0.0	0.0	0.0	0.0
0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

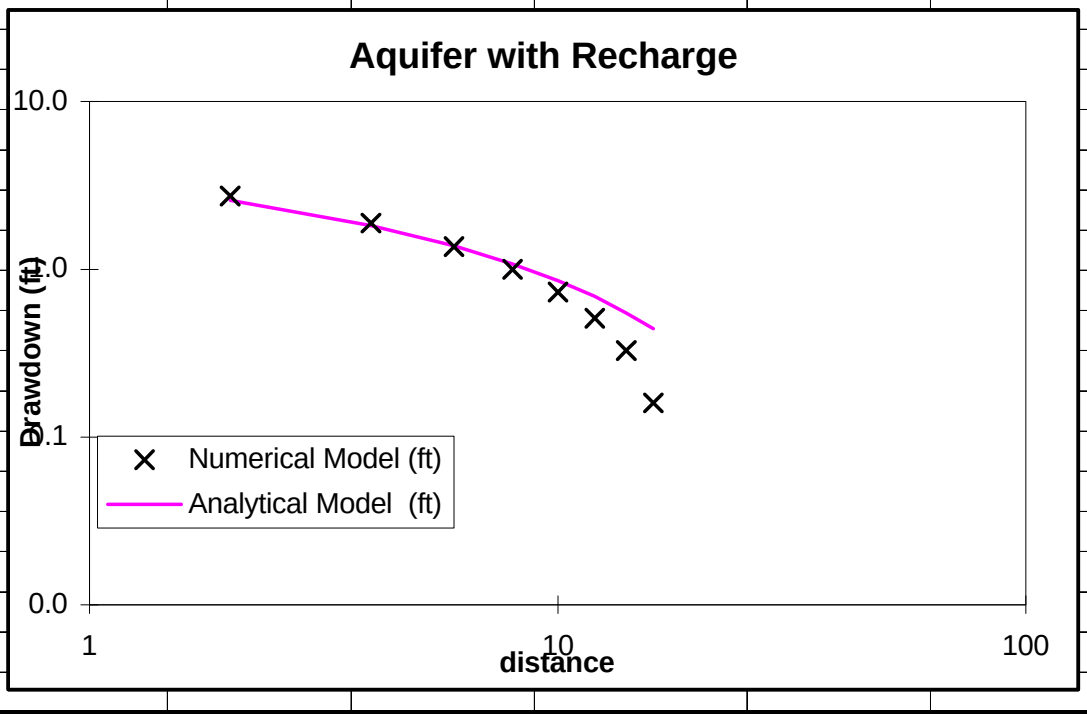
The next sheet shows a close-up of the computation portion of the spreadsheet.

Restart	1									
Iteration	2917									
Dt	0.1									
Time	291.7	sec								
Pumpage	1.1668									
	Head (Iteration -1)			meters						
	Column									
Row	0	1	2	3	4	5	6	7	8	0
0	97.5	97.5	98.3	98.9	99.2	99.4	99.6	99.8	99.9	100.0
1	97.5	97.5	98.3	98.9	99.2	99.4	99.6	99.8	99.9	100.0
2	98.3	98.3	98.7	99.0	99.3	99.5	99.6	99.8	99.9	100.0
3	98.9	98.9	99.0	99.2	99.4	99.5	99.7	99.8	99.9	100.0
4	99.2	99.2	99.3	99.4	99.5	99.6	99.7	99.8	99.9	100.0
5	99.4	99.4	99.5	99.5	99.6	99.7	99.8	99.9	99.9	100.0
6	99.6	99.6	99.6	99.7	99.7	99.8	99.8	99.9	100.0	100.0
7	99.8	99.8	99.8	99.8	99.8	99.9	99.9	99.9	100.0	100.0
8	99.9	99.9	99.9	99.9	99.9	99.9	100.0	100.0	100.0	100.0
0	99.9	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
	Head (Iteration)			meters						
	Column									
Row	0	1	2	3	4	5	6	7	8	0
0	97.5	97.5	98.3	98.9	99.2	99.4	99.6	99.8	99.9	100.0
1	97.5	97.4893	98.3482	98.8536	99.1891	99.43	99.6132	99.7601	99.8852	100
2	98.3	98.3482	98.6813	99.0046	99.2668	99.4736	99.6385	99.7742	99.8916	100
3	98.9	98.8536	99.0046	99.1984	99.3838	99.5454	99.6824	99.7995	99.9032	100
4	99.2	99.1891	99.2668	99.3838	99.5098	99.629	99.7362	99.8316	99.9181	100
5	99.4	99.43	99.4736	99.5454	99.629	99.7134	99.7931	99.8665	99.9347	100
6	99.6	99.6132	99.6385	99.6824	99.7362	99.7931	99.8488	99.9016	99.9516	100
7	99.8	99.7601	99.7742	99.7995	99.8316	99.8665	99.9016	99.9356	99.9682	100
8	99.9	99.8852	99.8916	99.9032	99.9181	99.9347	99.9516	99.9682	99.9843	100
0	99.8852	100	100	100	100	100	100	100	100	100
	Drawdown (Iteration)			meters						
	Column									
Row	0	1	2	3	4	5	6	7	8	0
0	2.5	2.5	1.7	1.1	0.8	0.6	0.4	0.2	0.1	0.0
1	2.5	2.5	1.7	1.1	0.8	0.6	0.4	0.2	0.1	0.0
2	1.7	1.7	1.3	1.0	0.7	0.5	0.4	0.2	0.1	0.0
3	1.1	1.1	1.0	0.8	0.6	0.5	0.3	0.2	0.1	0.0
4	0.8	0.8	0.7	0.6	0.5	0.4	0.3	0.2	0.1	0.0
5	0.6	0.6	0.5	0.5	0.4	0.3	0.2	0.1	0.1	0.0
6	0.4	0.4	0.4	0.3	0.3	0.2	0.2	0.1	0.0	0.0
7	0.2	0.2	0.2	0.2	0.2	0.1	0.1	0.1	0.0	0.0
8	0.1	0.1	0.1	0.1	0.1	0.1	0.0	0.0	0.0	0.0
0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

```
=C82+$B$73*((0.5/$B$4)*((D11+C11)*(D82-C82)-(C11+B11)*
   (C82-B82))+(0.5/$B$5)*((C10+C11)*(C81-C82)-(C11+C12)*(C82-C83))+
    (C37-C50)/($B$2*$B$3))/C24
```

Finally the results of the numerical model and the analytical model are compared in the spreadsheet below:

Q	0.016	m^3/day	Pumping well discharge (L^3/t)		
T	0.0023	m^2/day	Aquifer transmissivity (L^2/t)		
S	0.0075		Aquifer storage coefficient		
K'	0.0000001	m/day	Aquitard vertical hydraulic conductivity (L/t)		
b'	1000000	m	Thickness of aquitard (L)		
B	151657.5089				
		Time	Drawdown		
r (m)	r/B	t (sec)	Numerical Mode	Analytical Model (ft)	
2	1.31876E-05	600	2.8	2.570356098	
4	2.63752E-05	600	1.9	1.811892648	
6	3.95628E-05	600	1.4	1.37775644	
8	5.27504E-05	600	1.0	1.079606125	
10	6.5938E-05	600	0.7	0.858173798	
12	7.91257E-05	600	0.5	0.686812466	
14	9.23133E-05	600	0.3	0.551067971	
16	0.000105501	600	0.2	0.442088141	
18	0.000118688	600	0.0	0.353959906	



In the interest of simplicity, some of the more subtle aspects of the use of the difference notation have not been brought out. It is important to note, however, that if one is interested in evaluating or examining $\Delta f/\Delta x$, the notation is assumed to imply that one is keeping the y coordinate and the time coordinate fixed. Obviously, $\Delta f/\Delta x$, which is computed for one small volume, need not have the same value as $\Delta f/\Delta x$ for a volume located somewhere else in space.

3.7. CONSERVATION OF FLUID MASS IN A VOLUME

The most basic of the conservation equations is the conservation-of-mass or continuity equation, which, for the fluid in the volume of aquifer in Figure 3.3, states:

$$\begin{pmatrix}\text{rate of change of}\\ \text{mass of fluid in}\\ \text{a volume with time}\end{pmatrix} = \begin{pmatrix}\text{rate of flow of}\\ \text{fluid mass into}\\ \text{the volume}\end{pmatrix} - \begin{pmatrix}\text{rate of flow of}\\ \text{fluid mass out}\\ \text{of the volume}\end{pmatrix} \quad (3.5)$$

This equation, unlike the general equation (3.1), has no additional terms, because mass cannot be created within a volume. The next task is to account mathematically for all the terms in (3.5).

To develop (3.5) mathematically, we will have to make use of the following quantities:

ρ = density, the mass of fluid per unit volume of fluid. It has units of mass divided by length cubed or M/L^3.

u, v = the velocity of the fluid within the pore space in the x and y directions, respec-

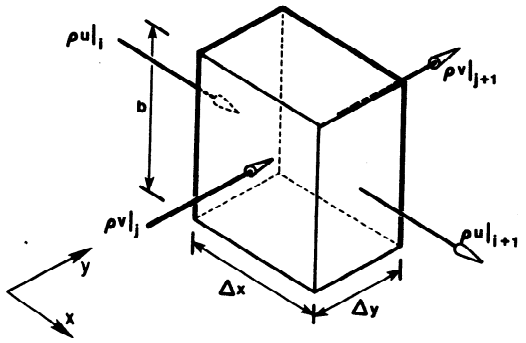


Figure 3.3.
Elemental volume with horizontal mass fluxes indicated.

tively. Velocity has units of length divided by time or L/T.

ϵ = the porosity of the material, the fraction of the volume considered that is not occupied by the solid grains. ϵ is also equal to the fractional areal surface of a boundary face of the volume that is not occupied by the solid material. Thus, ϵ is a measure of the fraction of the surface area across which fluid can flow, as well as a measure of the fraction of the volume available for fluid occupation.

The first term in (3.5) is a measure of the rate of change of fluid in the volume. Experimentally, one might measure this term by weighing the volume at two different times and determining the change in amount of fluid in the volume during the interval. Thus one must measure the mass per volume and multiply by the volume to obtain the mass, or

$$\begin{pmatrix}\text{fluid mass}\\ \text{in the volume}\\ \text{at time } t\end{pmatrix} = (\rho\epsilon b\ \Delta x\ \Delta y)\Big|_{t} \tag{3.6}$$

where $\epsilon\ \Delta x\ \Delta y b$ is the volume occupied by the fluid. Then the fluid mass in the volume at time Δt later is

$$\begin{pmatrix}\text{fluid mass}\\ \text{in the volume}\\ \text{at time } t+\Delta t\end{pmatrix} = (\rho\epsilon b\ \Delta x\ \Delta y)\Big|_{t+\Delta t} \tag{3.7}$$

The rate of change of mass is then equal to the difference in mass at the two times divided by Δt or

$$\begin{pmatrix}\text{rate of change of}\\ \text{fluid mass in the}\\ \text{volume with time}\end{pmatrix} = \frac{(\rho\epsilon b\ \Delta x\ \Delta y)|_{t+\Delta t} - (\rho\epsilon b\ \Delta x\ \Delta y)|_{t}}{\Delta t} = \frac{\Delta(\rho\epsilon b\ \Delta x\ \Delta y)}{\Delta t} \tag{3.8}$$

The next term that needs to be evaluated in (3.5) is the mass of fluid flowing into the volume. This is equal to the mass flow per unit area multiplied by the area. This term has three components: one that accounts for the x-direction inflow, one that accounts for the y-direction inflow, and

one that accounts for net vertical recharge due to leakage from above and below.

$$\begin{pmatrix}\text{rate of flow of}\\ \text{fluid mass into}\\ \text{the volume}\end{pmatrix} = (\rho u \epsilon b\ \Delta y)\Big|_i + (\rho v \epsilon b\ \Delta x)\Big|_j + \rho R\ \Delta x\ \Delta y \qquad (3.9)$$

where $\epsilon b\ \Delta y$ and $\epsilon b\ \Delta x$ are the areas the x and y components of flow cross, R is the recharge rate, and $\Delta x\ \Delta y$ is the area through which the recharge occurs. The outflow expression is similar to (3.9) except that terms are evaluated at $i + 1$ and $j + 1$ instead of i and j, respectively, and instead of net recharge, a term that accounts for pumping wells is included:

$$\begin{pmatrix}\text{rate of flow of}\\ \text{fluid mass out}\\ \text{of the volume}\end{pmatrix} = (\rho u \epsilon b\ \Delta y)\Big|_{i+1} + (\rho v \epsilon b\ \Delta x)\Big|_{j+1} + \rho Q\ \Delta x\ \Delta y \qquad (3.10)$$

where $Q\ \Delta x\ \Delta y$ is the volume of water pumped per unit time from the volume.

Combination of the terms in (3.8), (3.9), and (3.10) according to equation (3.5) yields the mass-balance equation

$$\frac{\Delta(\rho \epsilon\ \Delta x\ \Delta y b)}{\Delta t} = (\rho u \epsilon b\ \Delta y)\Big|_i - (\rho u \epsilon b\ \Delta y)\Big|_{i+1} + (\rho v \epsilon b\ \Delta x)\Big|_j - (\rho v \epsilon b\ \Delta x)\Big|_{j+1} + \rho R\ \Delta x\ \Delta y - \rho Q\ \Delta x\ \Delta y \qquad (3.11)$$

Although ρ, ϵ, u, v, and b are assumed to vary spatially and temporally, such that, for example, these variables may have different values at i and $i + 1$, Δx and Δy are constants. Thus, equation (3.11) may be divided by Δx and Δy to obtain

$$\frac{\Delta(\rho \epsilon b)}{\Delta t} = \frac{(\rho u \epsilon b)|_i - (\rho u \epsilon b)|_{i+1}}{\Delta x} + \frac{(\rho v \epsilon b)|_j - (\rho v \epsilon b)|_{j+1}}{\Delta y} + \rho R - \rho Q \qquad (3.12)$$

Then, making use of the Δ notation defined in equations (3.2) and (3.3), we obtain

$$\frac{\Delta(\rho \epsilon b)}{\Delta t} = -\frac{\Delta(\rho u \epsilon b)}{\Delta x} - \frac{\Delta(\rho v \epsilon b)}{\Delta y} + \rho R - \rho Q \qquad (3.13)$$

This is the basic form of the continuity equation used in modeling. Subsequently this equation will be modified, and the reader may have difficulty

relating the final version back to the physically meaningful concept of conservation of mass. Nevertheless, if the basic physical premise and the progression of mathematical steps are correct, the final equation derived must also be correct.

One of the most commonly used modifications to (3.13) involves the *storage coefficient,* denoted by S. The storage coefficient is the volume of water that an aquifer will absorb (or release) from storage per unit planar area per unit change in head. The storage coefficient is therefore dimensionless. If we denote the head by ϕ and the change in head by $\Delta\phi$, the quantity $\rho S\,\Delta\phi$ is the mass of water that an aquifer absorbs (or stores) as a result of a head change of $\Delta\phi$ per unit area. As discussed previously, the only way that mass can be added to or subtracted from a volume is via convection or flow of the mass into or out of the volume. Thus the quantity $\rho S(\Delta\phi/\Delta t)$ must equal the left side of equation (3.13), and therefore

$$\rho S \frac{\Delta\phi}{\Delta t} = -\frac{\Delta(\rho u \epsilon b)}{\Delta x} - \frac{\Delta(\rho v \epsilon b)}{\Delta y} + \rho R - \rho Q. \tag{3.14}$$

In equation (3.14), S and ϵ are properties of the aquifer being considered while ρ is the water density. These must be specified. The parameter b is the thickness of a confined aquifer or the depth of flow in an unconfined aquifer (and thus directly related to the water-table elevation). The unknowns that must be solved for in (3.14) are the velocities, u and v, and the head ϕ.

3.8. DARCY'S LAW AND THE GROUNDWATER FLOW EQUATION

In the mid nineteenth century Henri Darcy, a French engineer, performed a series of classical experiments to investigate the behavior of flow in porous media. He found that in flow through a pipe packed with porous material, the flow per unit area is proportional to the head difference between the two ends of the pipe and inversely proportional to the pipe length. The constant of proportionality between the flow and the head gradient is the permeability, and the relation obtained by Darcy is

$$q = -K \frac{\Delta\phi}{\Delta l} \tag{3.15}$$

where

q = the volumetric flow per cross-sectional area,
K = the permeability,
$\Delta\phi$ = the head difference across the length of the pipe, and
Δl = the pipe length.

Equation (3.15), commonly referred to as *Darcy's law,* is not strictly a law but only a useful relation that applies to most (though certainly not all) naturally occurring flows in porous media. Among the effects that may cause non-Darcian behavior are high velocity or the presence of more than one liquid phase (such as oil flowing with water).

Although Darcy's law was developed from experimental evidence for one-dimensional flows in porous media, it has been extended to two- and three-dimensional flows. In systems that have the same permeability in all directions, called *isotropic media,* equation (3.15) is generalized so that the flow in any direction is proportional to the head gradient in that direction. For a two-dimensional system, such as the one that is our primary interest,

$$q_x = \epsilon u = -K \frac{\Delta \phi}{\Delta x} \tag{3.16a}$$

$$q_y = \epsilon v = -K \frac{\Delta \phi}{\Delta y} \tag{3.16b}$$

where q_x and q_y are the volume of flow per unit time per unit cross-sectional area in the x and y direction, respectively. The flow components q_x and q_y are called *Darcy velocities,* or *superficial velocities,* and are smaller than the actual average velocities in the pores by the factor ϵ.

For media that behave according to equation (3.16), the direction of flow is always the same as the head gradient direction. However, in some media, referred to as *anisotropic media,* this is not the case. For example, in a limestone formation, caverns may exist that follow one predominant direction. A head gradient not collinear with this direction may still give rise to flow through the caverns. In an anisotropic material, flow from one point to another moves along the path of least resistance and not necessarily along the straight line connecting the two points. Modeling of anisotropic flows requires that different permeabilities be specified in each direction and that terms be included that account for flow in one direction due to a gradient in an orthogonal direction. Thus, the anisotropic analogue to (3.16) would be

$$q_x = \epsilon u = -K_{xx} \frac{\Delta \phi}{\Delta x} - K_{xy} \frac{\Delta \phi}{\Delta y} \tag{3.17a}$$

$$q_y = \epsilon v = -K_{yx} \frac{\Delta \phi}{\Delta x} - K_{yy} \frac{\Delta \phi}{\Delta y} \tag{3.17b}$$

where

K_{xx} = the permeability in the x direction due to a head gradient in the x direction,

K_{xy} = the permeability in the x direction due to a head gradient in the y direction,

K_{yx} = the permeability in the y direction due to a head gradient in the x direction, and

K_{yy} = the permeability in the y direction due to a head gradient in the y direction.

Available data often are not extensive enough to permit modeling of anisotropy with any significance. For purposes of further discussions here, only the isotropic version of Darcy's law, as in equation (3.16), will be used. The reader should keep in mind, however, that directional differences in permeability, particularly between vertical and horizontal directions, can significantly influence a flow pattern and the rate of transport of contaminants.

The linear relation between velocities and head gradient as given in (3.16) makes it possible to eliminate the velocities from equation (3.14). Substitution of (3.16a) and (3.16b) into (3.14) for ϵu and ϵv results in

$$\rho S \frac{\Delta \phi}{\Delta t} = \frac{\Delta}{\Delta x}\left(\rho K b \frac{\Delta \phi}{\Delta x}\right) + \frac{\Delta}{\Delta y}\left(\rho K b \frac{\Delta \phi}{\Delta y}\right) + \rho R - \rho Q \qquad (3.18)$$

Recall that Kb is equal to the transmissivity T, so that (3.18) becomes

$$S \frac{\Delta \phi}{\Delta t} = \frac{\Delta}{\Delta x}\left(\rho T \frac{\Delta \phi}{\Delta x}\right) + \frac{\Delta}{\Delta y}\left(\rho T \frac{\Delta \phi}{\Delta y}\right) + \rho R - \rho Q \qquad (3.19)$$

If the problem under consideration is one for which the density does not vary spatially, then density may be divided out of equation (3.19) to yield

$$S \frac{\Delta \phi}{\Delta t} = \frac{\Delta}{\Delta x}\left(T \frac{\Delta \phi}{\Delta x}\right) + \frac{\Delta}{\Delta y}\left(T \frac{\Delta \phi}{\Delta y}\right) + R - Q \qquad (3.20)$$

This balance equation is the form most commonly solved to obtain a head profile or the flow field in an aquifer. This equation states that per unit area, the rate of change of fluid volume is equal to the net inflow in the x direction plus the net inflow in the y direction plus the net recharge due to vertical leakage minus the net discharge due to pumping wells.

To model an aquifer, one divides it into a number of adjacent subvolumes and then applies equation (3.20) to each subvolume. This set of equations is supplemented by boundary conditions at the periphery of the aquifer that provide head values or flux conditions. Once this system is solved for the distribution of head, the velocity field may be computed using the difference form of Darcy's law in equation (3.16). The velocities are important, as they give an indication of the rate at which contaminants move, and they are used in the species balance equation to be developed in the next section.

3.10. EXAMPLE OF APPLICATION OF GROUNDWATER FLOW EQUATION

A computer model applies equations (3.20) and (3.30) to a groundwater aquifer that has been subdivided into hundreds or even thousands of small volumes. The computer is important to this model, because it can quickly perform the large number of arithmetic operations required to obtain the head or concentration distribution. The computer possesses no inherent wisdom; it can perform the necessary manipulations only if they are prescribed by the programmer. Thus the quality of computer results depends directly on the quality of the information and commands provided to the computer.

To give the reader a very simplistic view of how equations (3.20) and (3.30) are solved by the computer, we will apply equation (3.20) to the hypothetical confined aquifer depicted areally in Figure 3.4. The aquifer extends 5,000 meters in the x direction and 2,000 meters in the y direction. The aquifer is bounded below by an impermeable formation (aquiclude) but above by an aquitard, which recharges the aquifer uniformly at the rate of 50 cm/yr with water that contains no contaminants. The transmissivity, T, equals 3,000 m²/day. No flow crosses the northern, southern, or eastern edges of the aquifer. At the left edge, the hydraulic head ϕ is equal to 3 m above mean sea level. The aquifer is subdivided such that equations may be applied to the two square volumes in Figure 3.4.

Because the system is operating at steady state (i.e., conditions at any point in the aquifer do not vary with time), the time-difference term in equation (3.20) will be equal to zero. Further, there are no pumping wells in the system, so (3.20) becomes

$$0 = \frac{\Delta}{\Delta x}\left(T\frac{\Delta\phi}{\Delta x}\right) + \frac{\Delta}{\Delta y}\left(T\frac{\Delta\phi}{\Delta y}\right) + R \tag{3.31}$$

This equation is applied to volumes 1 and 2 with reference to Figure 3.5. In Figure 3.5 values of $\Delta\phi/\Delta x$ at the east and west boundaries of the volume are indicated, and because $q_y = 0$ on the north and south boundaries, $\Delta\phi/\Delta y$ must be zero on these ends. Note that $\Delta x = 2{,}000$ m. For volume 1,

$$\frac{\Delta}{\Delta x}\left(T\frac{\Delta\phi}{\Delta x}\right) = \frac{\left(T\dfrac{\phi_2 - \phi_1}{2{,}000\text{ m}}\right) - \left(T\dfrac{\phi_1 - 3\text{ m}}{2{,}000\text{ m}}\right)}{2{,}000\text{ m}}$$

$$= \frac{3{,}000\text{ m}^2}{\text{day}}\left[\frac{\phi_2 - 2\phi_1 + 3\text{ m}}{(2{,}000\text{ m})^2}\right] \tag{3.32a}$$

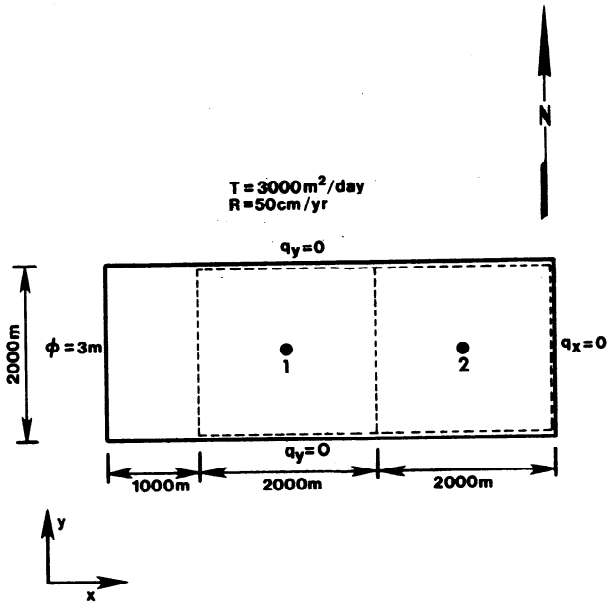


Figure 3.4.
Areal view of a hypothetical rectangular confined aquifer discretized into two elements.

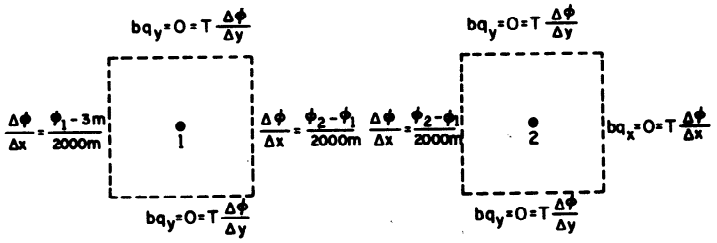


Figure 3.5.
Application of groundwater flow equation (3.31) to the two elements of the horizontal aquifer.

$$\frac{\Delta}{\Delta y}\left(T\frac{\Delta\phi}{\Delta y}\right)=\frac{0-0}{2{,}000\text{ m}}=0 \tag{3.32b}$$

$$R = 50\text{ cm/yr} = .00137\text{ m/day} \tag{3.32c}$$

Insertion of (3.32) into (3.31) yields

$$0=\frac{3{,}000}{(2{,}000)^2}(\phi_2-2\phi_1+3\text{ m})+.00137\text{ m} \tag{3.33}$$

This single equation contains two unknowns and cannot be solved without a supplementary condition. The needed extra condition is provided by the balance over volume 2:

$$\frac{\Delta}{\Delta x}\left(T\frac{\Delta\phi}{\Delta x}\right)=\frac{0-T\dfrac{\phi_2-\phi_1}{2{,}000\text{ m}}}{2{,}000\text{ m}}=-\frac{3{,}000\text{ m}^2}{\text{day}}\left[\frac{\phi_2-\phi_1}{(2{,}000\text{ m})^2}\right] \tag{3.34a}$$

$$\frac{\Delta}{\Delta y}\left(T\frac{\Delta\phi}{\Delta y}\right)=\frac{0-0}{2{,}000\text{ m}}=0 \tag{3.34b}$$

$$R = 50\text{ cm/yr} = .00137\text{ m/day} \tag{3.34c}$$

Combination of (3.34) into the balance equation (3.31) yields

$$0=-\frac{3{,}000}{(2{,}000)^2}(\phi_2-\phi_1)+.00137\text{ m} \tag{3.35}$$

Now equations (3.35) and (3.33) are two simple algebraic equations in the two unknowns ϕ_2 and ϕ_1, which we may solve simultaneously to obtain

$$\phi_1 = 6.65\text{ m}, \qquad \phi_2 = 8.48\text{ m}$$

Because ϕ_2 is greater than ϕ_1, which in turn is greater than the western boundary value of 3.0 m, we can see that flow will move toward the west.

Once the solution for ϕ has been obtained, Darcy's law may be applied to compute the velocity field. This velocity field is used in equation (3.30) for computation of the concentration distribution. The differencing of this equation follows along the same lines as with the flow equation.

11. SUMMARY

This chapter has introduced the concepts behind numerical modeling. Numerical modeling is in no way magical but depends upon basic principles

Modeling with MODFLOW and related tools (A description of one of the more common tools in use)
(Adapted from "Modeling groundwater flow with MODFLOW …, S.A. Leake, USGS Report FS-121-97)

The modular finite-difference groundwater flow model (MODFLOW) developed by the U.S. Geological Survey (USGS) is a computer program for simulating common features in groundwater systems (McDonald and Har- baugh, 1988; Harbaugh and McDonald, 1996). The program was constructed in the ear- ly 1980s and has continually evolved since then with development of many new packages and related programs for groundwater studies. Currently MODFLOW is the most widely used program in the world for simulating ground- water flow. The popularity of the program is attributed to the following factors:

• The finite-difference method used by MODFLOW is relatively easy to under- stand and apply to a wide variety of real-world conditions.
• MODDFLOW works on many different computer systems ranging from personal computers to super computers.
• MODFLOW can be applied as a one- dimensional, two-dimensional, or
quasi- or full three-dimensional model.
• Each simulation feature of MODFLOW has been evensively tested.
• Data input instructions and theory are well documented.
• The modular program design of MODFLOW allows for new simulation features to be added with relative ease.
• A wide variety of computer programs written by the USGS, other federal agencies, and private companies are available to analyze field data and con- struct input data sets for MODFLOW.
• A wide variety of programs are available to read output from MODFLOW and graphically present model results in ways that are easily understood.
• MODFLOW has been accepted in many court cases in the United States as a legitimate approach to analysis of groundwater systems.

SIMULATION CAPABILITIES OF MODFLOW

MODFLOW is designed to simulate aquifer systems in which saturated-flow conditions exist, Darcy's Law applies, the density of ground water is constant, and the principal directions of horizontal hydraulic conductivity or transmissivity do not vary within the system. These conditions are met for many aquifer systems for which there is an interest in analysis of groundwater flow and contaminant movement. For these systems, MODFLOW can simu-

late a wide variety of hydrologic features and processes (Fig. 1).
Steady-state and transient flow can be simulated in unconfined aquifers, confined aquifers, and confining units. A variety of features and processes such as rivers, streams, drains, springs, reservoirs, wells, evapotranspiration, and recharge from precipitation and irrigation also can be simulated. At least four different solution methods have been implemented for solving the finite-difference equations that MODFLOW constructs. The avail- ability of different solution approaches allows model users to select the most efficient method for their problem.

APPLICATION OF MODFLOW

MODFLOW simulates groundwater flow in aquifer systems using the finite-difference method. in this method, an aquifer system is divided into rectangular blocks by a grid (Fig 2.) The grid of blocks is organized into rows, columns, and layers. Each block is commonly called a cell.

MODEL INPUT

For each cell within the volume of the aquifer system, the user must specify aquifer properties. Also, the user specifies information relating to wells, rivers, and other inflow and outflow features for cells corresponding to the location of the features. For example, if the interaction between a river and an aquifer sys- tem is simulated, then for each cell traversed by the river, input information includes layer, row, and column indices; river stage; and hydraulic properties of the river bed.

MODEL OUTPUT

MODFLOW uses the input to construct and solve equations of groundwater flow in the aquifer system. The solution consists of head (groundwater level) at every cell in the aquifer system (except for cells where head was specified as known in the input data sets) at intervals called 'time steps.' The head can be printed and/or saved on a computer storage device for any time step.

Hydrologists commonly use water levels from a model layer to construct contour maps for comparison with similar maps drawn from field data. They also compare computed water levels at individual cells with measured water levels from wells at corresponding locations to determine model error (Fig. 3). The process of adjusting the model input values to reduce the model error is referred to as model calibration.

In addition to water levels, MODFLOW prints a water budget for the entire aquifer sys- tem. The budget lists inflow to and outflow from the aquifer system for all hydrologic features that add or remove water.

Other program output consists of flow rates for each model cell. MODFLOW can write the flow rates onto a computer storage device for any hydrologic feature in a simulation. These cell-by-cell flow rates commonly are read by post-processing programs for detailed analysis of the simulated groundwater system.

INVERSE MODELING WITH MODFLOWP

In conventional or "forward modeling," model parameters (such as aquifer properties) are specified and water levels and flow quantities are computed (Fig. 4). For most aquifer systems, however, more information is available from field data on water levels, flows, and advective transport or groundwater age than on input parameters.

Typically, input parameters are adjusted during model calibration using a trial- and-error process. This calibration process can yield acceptable agreement between computed model results and field data but is time consuming, may not produce parameter values that result in the best fit of field data, and does not result in quantitative estimates of uncertainty in model results and estimated parameter values.

Inverse modeling is a more formal approach to model calibration that includes automatic parameter adjustment in order to match field data. The program MODFLOWP is the USGS version of MODFLOW that includes automatic parameter estimation. MODFLOWP uses a weighted least-squares objective function as a measure of how well model results agree with field measurements. Weights are used to reflect reliability of individual measurements.

Parameters that can be estimated by MODFLOWP include transmissivity; hydraulic conductivity, storage coefficient; vertical leakance; vertical and horizontal anisotropy, hydraulic conductance between aquifer systems and rivers, drains and other features; a real recharge; maximum evapotranspiration; pumping; and water levels at constant-head boundaries. Measured or extemally estimated information on parameters also can be included. Parameter values that minimize the objective function (Fig' 5) are calculated by MODFLOWP using the modified Gauss-Newton method or the

conjugate-direction method. The resulting parameter values are "best-fit" in that they pro- vide the closest match between measured and simulated heads and flows, as measured by the objective function. The task of the modeler is to evaluate how well these calculated values represent the physical system being simulated.

Model output includes estimates of parameters and statistics relating to the parameter estimates. The statistics can be used to quantify the reliability of the resulting model, suggest changes in model construction, and compare results of models constructed in different ways, Post-processors can be used to calculate confidence intervals on predicted heads and flows to
depict prediction uncertainty. To effectively use MODFLOWP, an understanding of principles of groundwater flow and basic statistics is needed.

PARTICLE TRACKING WITH MODPATH

Many studies require information such as the average rate of moveriient of groundwater and contaminants. Also, information often is needed on the recharge or capture areas for water discharging to wells, springs, stream reaches, and other features. Although MOD- FLOW does not compute this information directly, simulation with MODFLOW provides basic information needed for such analyses. The partide-trackng program, MODPATH, is a post-processing program for MODFLOW to estimate flow paths (Fig. 6) and times of travel in groundwater systems. An accompanying program, MODPATH-PLOT, displays particle paths, contours, and model features. MODPATH can be used for studies of steady-state and transient flows. Common applications include studies of paths and time of travel of contaminant movement; and source (recharge) areas of wells, springs, rivers, and other features.

MODPATH can place particles at specified locations or generate starting locations of arrays of particles in selected reoons. Particles can be tracked forward from starting locations to calculate where water is goin or backwards to map where it came from. Multiple particle-release times can be used to simulate "plumes" of contamination.