Groundwater review

Part II



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Solutions to the Governing Flow Equations

Anderson and Woessner, pp. 20-25

With the Aquifer Viewpoint, we can use Analytical solutions

- Analytical equations are closed form calculus solutions
- Allow us to calculate values for unknowns (head) at any point in the domain.
- Remember that Theis used the Taylor's expansion series.

$$h_0 - h = \frac{Q}{4\pi T} \left[-0.5772 - \ln U + U - \frac{U^2}{2 \times 2!} + \frac{U^3}{2 \times 3!} - \frac{U^4}{2 \times 4!} + \dots \right]$$

- With the System Viewpoint, we use **Numerical** solutions.
- Numerical solutions yield values for only predetermined, finite number of points in the problem domain (N)
- Need to create N algebraic solutions involving the unknowns (hydraulic head) at the locations x, y, and z
- Set up a regular grid with all of the x, y, and z locations specified.



Finite-difference grid

 $h_{i,j}$ = head at point i, j

- Note: there is a different notation for MODFLOW.
- In finite difference approximation, derivatives are replaced by differences between nodal points.
- The smaller the distances x and y, the better the approximate solution is to the actual solution.
- The more grid cells, the greater the number of unknowns.
- Remember Darcy's Law and Laplace's Equation.

FINITE DIFFERENCE METHOD DEVELOPMENT

Obtain a central approximation to at the point (x_0, y_0) of $\frac{\partial^2 h}{\partial x^2}$ by approximating the first derivative at $\left(x_0 + \frac{\Delta x}{2}, y_0\right)$ and

$$\left(x_0-\frac{\Delta x}{2},y_0\right).$$

Then obtain the second derivatives by taking first derivatives at these points.

Start with the definition of a first derivative

$$\frac{dh}{dx} \cong \lim_{\Delta x \to 0} \frac{h(x + \Delta x) - h(x)}{(x + \Delta x) - x} = \lim_{\Delta x \to 0} \frac{h(x + \Delta x) - h(x)}{\Delta x}$$

FD approximation of a first derivative can be viewed as the above equation without the limit process. Furthermore, when employing the FDM, the locations x and $x+\Delta x$ are chosen to coincide with nodes.

Derivatives may be approximated using one of three basic schemes:

1- Forward Difference	→	$\left. \frac{dh}{dx} \right _{x_i} \cong \frac{h_{i+1} - h_i}{x_{i+1} - x_i} = \frac{h_{i+1} - h_i}{\Delta x}$
2- Backward Difference	→	$\left. \frac{dh}{dx} \right _{x_i} \cong \frac{h_i - h_{i-1}}{x_i - x_{i-1}} = \frac{h_i - h_{i-1}}{\Delta x}$
3- Central Difference	→	$\left. \frac{dh}{dx} \right _{x_i} \cong \frac{h_{i+1} - h_{i-1}}{x_{i+1} - x_{i-1}} = \frac{h_{i+1} - h_{i-1}}{2\Delta x}$

Second derivatives are typically approximated using the central difference scheme:

$$\frac{d^{2}h}{dx^{2}} = \frac{d}{dx} \left(\frac{dh}{dx} \Big|_{x_{i}} \right) \cong \frac{\frac{dh}{dx} \Big|_{x_{i+\frac{1}{2}}} - \frac{dh}{dx} \Big|_{x_{i+\frac{1}{2}}}}{x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}} \qquad \dots \#$$

Where, $x_{i\pm 1/2}$ represents the x-location of the midpoint between x_i and $x_{i\pm 1}$

$$\frac{dh}{dx}\Big|_{x_{i+\frac{1}{2}}} \cong \frac{h_{i+1} - h_i}{x_{i+1} - x_i} = \frac{h_{i+1} - h_i}{\Delta x}$$
 (Central difference WRT $x_{i+1/2}$)
$$\frac{dh}{dx}\Big|_{x_{i+\frac{1}{2}}} \cong \frac{h_i - h_{i-1}}{x_i - x_{i-1}} = \frac{h_i - h_{i-1}}{\Delta x}$$

$$\frac{d^2h}{dx^2} = \frac{\frac{h_{i+1} - h_i}{\Delta x} - \frac{h_i - h_{i-1}}{\Delta x}}{\Delta x}$$
$$\frac{d^2h}{dx^2} = \frac{h_{i+1} - 2h_i + h_{i-1}}{\Delta x^2}$$
For solving the second derivative

ve in 2D: or solving the second de

$$\frac{\partial^2 h}{\partial y^2} = \frac{h_{i,j-1} - 2h_{i,j} + h_{i,j+1}}{\Delta y^2} \qquad \dots \dots \# 2$$

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = \frac{h_{i-1,j} - 2h_{i,j} + h_{i+1,j}}{\Delta x^2} + \frac{h_{i,j-1} - 2h_{i,j} + h_{i,j+1}}{\Delta y^2}$$

If we take these two equations and set them equal to zero, we have the finite difference form of Laplace's Equation, and we have equal spacing in both x, and y directions:

Then this is the steady-state, finite difference, ground-water flow equation. We must write a form of this equation for each interior point (i,j) of the problem domain. If we then solve this equation for $h_{i,j}$, we get the following equation

$$h_{i,j} = \frac{h_{i-1,j} + h_{i+1,j} + h_{i,j-1} + h_{i,j+1}}{4}$$





BOUNDARY CONDITIONS

To solve this equation also requires specification of boundary conditions. Boundaries constrain the problem domain. Boundaries make the solutions unique for a specific problem.

DIRICHLET conditions:

Hydraulic head is known for surfaces bounding the flow regime. For instance, the surface of the ocean on an island ground-water flow system.

NEUMANN conditions :

Flow across a surface bounding the flow regime is known. For instance, baseflow into a river from a regional aquifer.

MIXED conditions

A combination of Dirichlet and Neumann conditions.

Classification of Boundaries

Physical Boundaries: are formed by the physical presence of an impermeable body of rock or large body of surface water.

Hydraulic Boundaries: are invisible boundaries dependent upon hydrologic conditions. These may include groundwater divides and flow lines and can be altered or moved depending upon the stresses within the system at a given time.

Three types:

Specified Head: (Dirichlet conditions) \rightarrow h = constant or given function.

Specified Flow: (Neumann conditions)
$$\rightarrow \frac{\partial h}{\partial x_i} = const$$
 or given function

Head-dependent Flux: (Cauchy or mixed conditions): Flow is calculated in or out of system depending upon specified boundary head and conductance value between active grid and boundary head.

Implementation:

Specified Head: all steady-state models should have at least one boundary node with a specified head in order for the model to have a reference elevation from which to calculate heads. If flow boundaries are used everywhere, this derivative condition will prevent the model from calculating a unique solution.

In two-dimensional areal models, specified head cells represent fully penetrating surface-water bodies, or the vertically averaged head in the aquifer at hydraulic boundaries.

In three-dimensional models, specified head cells may represent the water table, or surface water bodies.

It is important to note that specified head boundaries represent an inexhaustible supply of water. Hence, the aquifer can potentially pull an infinite amount of water from this source without changing its head value.

Specified-Flux Boundaries: typically are no-flow boundaries, but can also be constant flux boundary conditions where flow can be measured or estimated to be nonzero.

 $\frac{\partial h}{\partial x} = -\frac{q_x}{K}$ (Known flux) from Darcy's equation q = Ki

Finite-Difference Approximation:

$$\frac{\partial h}{\partial x} = \frac{h_{i+1,j} - h_{i-1,j}}{2\Delta x} = -\frac{q_x}{K}$$

$$h_{i-1,j} = 2\Delta x \frac{q_x}{K} + h_{i+1,j}$$

No-flow boundaries can represent:

 $\underline{\mathbf{1}}$. Impermeable bedrock. A conductivity change of as little as two orders of magnitude may result in sufficient enough restriction of flow to be represented as a no-flow condition in certain cases.

2. Impermeable fault zone. Faults tend to be narrow linear features that generally don't coincide with the grid network size or orientation. The best way to simulate these features is with the HFB package in MODFLOW-2000.

<u>3.</u> Groundwater Divide. These hydrologic boundaries may or may not be permanent flow-system features. They tend to be fixed under unstressed conditions. However, if pumping occurs in the vicinity of divides or if the cone of depression reaches the divide, their location can migrate causing the divide to be displaced farther from the pumping well. The presence or absence of precipitation can alter the location of a divide. In some cases, even evapotranspiration can influence the location of a groundwater divide.



<u>4.</u> Streamlines. These hydrologic features are valid for model boundaries when the location of the streamline does not fluctuate significantly. Thus, they are generally good to use as boundaries in steady-state simulations where a natural flow gradient is present.

Because the location of streamlines can fluctuate greatly during transient simulations, particularly when pumping is present, great care must be exercised in their application, and in most cases this boundary condition is violated.

Streamline boundaries are used to separate local, intermediate, and regional flow systems. They are also used as lateral boundaries between two known head conditions.

Typically, larger model domains are used to identify the flowpaths and then more detailed models are developed to isolate flow between a set of flow paths.



No-Flow Boundary condition:

$$q_x = -K \frac{\partial h}{\partial x} = 0 \qquad \qquad \Rightarrow \frac{\partial h}{\partial x} = 0$$
$$q_y = -K \frac{\partial h}{\partial y} = 0 \qquad \qquad \Rightarrow \frac{\partial h}{\partial y} = 0$$

Finite-Difference Approximation

Using central difference approximation for the LHS of the model grid:

$$\frac{\partial h}{\partial x} = \frac{h_{i+1,j} - h_{i-1,j}}{2\Delta x} = 0 \qquad \text{or,} \qquad h_{i+1,j} = h_{i-1,j}$$

The no-flow boundary is defined for column #2, and 12 (i = 2, and i = 12) of the nodes, and j is variable from 1 to 6.

<u>General-Head Boundaries</u>: are used whenever the head of a surface-water body or other known head is separated from the aquifer by material or deposits having different hydrogeologic properties than the aquifer (model cell representing the aquifer).

If the conductance is set to a very high value, this boundary condition behaves like a constant-head boundary. However, the head can be changed for each stress period, unlike a constant-head boundary.

The conductance value results in a time lag for equilibrium conditions to be reached between the boundary head and the head in the aquifer.

Special Conditions:

<u>Water table</u>: Free surface where flux can pass across boundary. Nonlinear boundary condition. How do we handle this so that we can accurately incorporate unconfined flow (parabolic water table)?

There are a number of ways in which we can simulate a water table numerically. One way is to use the expression:

$\frac{\partial^2 h}{\partial h}$	$\frac{\partial^2 h}{\partial h}$	$-\underline{R}$	(Boisson's equation)
∂x^2	∂y^2	T	(Boisson's equation)

R recharge T Transmissivity

The transient equation is a bit more complex:

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = -\frac{R}{T} + \frac{S}{T}\frac{\partial h}{\partial t}$$

Assuming constant spacing in both the x and y directions and constant areal recharge over the entire domain, what is the finite difference approximation to the Poisson equation?

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y x^2} = -\frac{R}{T}$$

$$\frac{h_{i-1,j} - 2h_{i,j} + h_{i+1,j}}{\Delta x^2} + \frac{h_{i,j-1} - 2h_{i,j} + h_{i,j+1}}{\Delta y^2} = -\frac{R}{T}$$

for $\Delta x = \Delta y$, $h_{i-1,j} + h_{i+1,j} + h_{i,j-1} + h_{i,j+1} - 4h_{i,j} = \Delta^2 \left(-\frac{R}{T}\right)$

<u>Region near a well</u>: Drawdowns can be incorrectly calculated. Precision of results is dependent upon grid size, number of wells, areal distribution of wells, and degree of drawdown. This will be discussed later in the course when we look at individual packages for MODFLOW.

Unconfined Aquifer with Dupuit Conditions

Continuity for a steady-state condition with areal recharge is:

$$Q_2 - Q_1 = R\Delta x \Delta y$$

Recall that our governing equation is

$$-K\frac{\partial}{\partial x}\left(h\frac{\partial h}{\partial x}\right) - K\frac{\partial}{\partial y}\left(h\frac{\partial h}{\partial y}\right) = R$$

And we made the transformation

$$h\frac{\partial h}{\partial x} = \frac{\partial \left(\frac{h^2}{2}\right)}{\partial x} = \frac{1}{2}\frac{\partial h^2}{\partial x}$$
$$\frac{\partial h^2}{\partial x} = 2h\frac{\partial h}{\partial x}$$

We obtain an expression now

$$\frac{K}{2} \left(\frac{\partial^2 h^2}{\partial x^2} + \frac{\partial^2 h^2}{\partial y^2} \right) = -R$$

$$\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} = -\frac{2R}{K}$$
(Where

Where $v = h^2$)

How do we solve this?

Solve for (v) which is now the dependant variable, then the final FORTRAN expression is:

$$h(i, j) = SQRT(v(i, j))$$

What does the transient case look like? Use a Crank-Nicolson formulation.

$$K\frac{\partial}{\partial x}\left(h\frac{\partial h}{\partial x}\right) + K\frac{\partial}{\partial y}\left(h\frac{\partial h}{\partial y}\right) = S_{y}\frac{\partial h}{\partial t} - R(x, y, t)$$

Evaluating Error

How does one determine the error associated with a given derivative approximation and hence, the nodal values of h? Given <u>Taylor's theorem</u>, FD approximation can be analyzed, starting with:

$$f(x) = f(x_0) + (x - x_0)f'(x_0) + \frac{(x - x_0)^2}{2!}f''(x_0) + \dots + \frac{(x - x_0)^n}{n!}f^{(n)}(x_0) + R_n$$

Then:

$$h(x_{i+1}) = h(x_i) + \frac{dh}{dx}\Big|_{x_i} (x_{i+1} - x_i) + \frac{d^2h}{dx^2}\Big|_{x_i} \frac{(x_{i+1} - x_i)^2}{2!} + \dots$$

With additional terms up to and including the remainder term R_N , where N is assumed to be larger then the highest-order derivative written in the expression

For equal grid spacing:
$$h_{i+1} = h_i + \frac{dh}{dx}\Big|_{x_i} \Delta x + \frac{d^2h}{dx^2}\Big|_{x_i} \frac{\Delta x^2}{2!} + \dots$$

Truncation Error

Subtracting h_i from both sides of the first equation yields:

$$h_{i+1} - h_i = \frac{dh}{dx} \bigg|_{x_i} \Delta x + \frac{d^2 h}{dx^2} \bigg|_{x_i} \frac{\Delta x^2}{2!} + \dots$$
 # divide by Δx

Comparison of the above equation with the forward-difference expression indicates that the FD approximation neglects the terms:

$\left.\frac{dh}{dx}\right _{x_i} - \frac{h_{i+1} - h_i}{\Delta x} = \left \frac{d^2h}{dx^2}\right _{x_i} \frac{\Delta x}{2!} + \frac{d^3h}{dx^3}\right _{x_i} \frac{\Delta x^2}{3!} + .$	
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True derivative – Approximation = Error

The truncation error (T.E.) is the difference between the true derivative and the FD approximation to that derivative

Consistency

Def: Consistency is defined by the requirements that:

$\lim_{\Delta x \to 0} T \cdot E = 0$

A fundamental requirement of any FD approximation is when we re-impose the limit process; the actual derivative must be recovered.

Convergence

Def: A solution is said to be convergent if:

$$\lim_{\Delta x \to 0} \left\| \boldsymbol{h}_{i}^{n} - h(x,t) \right\| = 0$$

Where: h_i^n is the solution to the FD expression and h(x,t) is the exact solution to the PDE.

Finite Difference Method – Order of Approximation

Def: The Order of Approximation is determined by the order of the lowest-order term in the residual.

$$\frac{dh}{dx}\Big|_{x_i} - \frac{h_{i+1} - h_i}{\Delta x} = \frac{d^2h}{dx^2}\Big|_{x_i} \frac{\Delta x}{2!} + \frac{d^3h}{dx^3}\Big|_{x_i} \frac{\Delta x^2}{3!} + \dots$$

$$\frac{dh}{dx}\Big|_{x_i} \cong \frac{h_{i+1} - h_i}{\Delta x} \qquad T.E. = \frac{d^2h}{dx^2}\Big|_{x_i} \frac{\Delta x}{2!} + \dots$$

Because power $((\Delta x^p)) = 1$, (i.e., p = 1), the approximation is <u>first order</u>.

The higher the order of approximation, the "faster" the truncation error decreases as Δx goes to zero.

Discretization Error

Def: Difference between the exact solution to the PDE and the exact solution to FD approximation to the PDE.

Round- off Error

Def: Errors due to the fact that variables are represented computationally by a limited number of digits.

Difference between the computed solution and the exact solution.

Stability refers to the growth in error with time. Any numerical scheme that allows growth in error over time, which eventually swamps the solution is called unstable.

Def: Stability is defined by the requirement that:

$$\left|h_{ij}^{n}-h(x,y,t)\right| \rightarrow 0$$
 as $t \rightarrow \infty$

Where h_{ij}^{n} is the solution to the FD expression and h(x, y, t) is the exact solution to the PDE.

Other Sources of Error

Applicable to any numerical method (e.g., FDM, FEM, etc.)

- Errors in formulating the problem
- Errors in translating the PDE into an algorithm suitable for solution
- Errors in program design
- Errors in coding and data (I/O) Preparation

Solver Routines

Remember the general finite-difference approximation for Laplace's Equation at point i,j when solved for head (h).

$$h_{i,j} = \frac{h_{i-1,j} + h_{i+1,j} + h_{i,j-1} + h_{i,j+1}}{4}$$

One of these equations needs to be written for each interior point of the problem domain. The head at point i, j is an average of the four neighbors (five-point operator).



For instance, if i=2 and j=2, then



Instead of simultaneously solving N sets of algebraic equations,

- 1) guess initial heads,
- 2) iterate and adjust head values.

Common Iterative techniques

- 1) Jacobi
- 2) Gauss-Seidel
- 3) Successive over relaxation
- 4) Strongly implicit procedure
- 5) Preconditioned conjugate gradient

Increased efficiency and complexity with the solvers in this list.

Jacobi

$$h_{i,j}^{m+1} = \frac{h_{i-1,j}^m + h_{i+1,j}^m + h_{i,j-1}^m + h_{i,j+1}^m}{4}$$

Let m be equal to an iteration index

1) Guess initial heads for m = 1

2) Calculate heads at m + 1 from heads at m

3) Iterate until convergence, or until the difference in hydraulic head

between two iterations is less than predetermined error criteria.

Gauss-Seidel

1) Sweep through grid in order, as if reading a book.

$$h_{i,j}^{m+1} = \frac{h_{i-1,j}^{m+1} + h_{i+1,j}^{m} + h_{i,j-1}^{m+1} + h_{i,j+1}^{m}}{4}$$

Using the newly computed heads makes the iteration more efficient.



Operator sweeps through array in this manner.

$$h_{2,2}^{m+1} = \frac{h_{1,2}^{m+1} + h_{2,1}^m + h_{3,2}^{m+1} + h_{2,3}^m}{4}$$

Successive Over Relaxation (SOR)

Residual is the change in head between iterations

$$C = h_{i,j}^{m+1} - h_{i,j}^m$$

In the Gauss-Seidel method, h^{m+1} replaces h^m after each iteration, or it *relaxes* the residuals at each site during each iteration.

In SOR

1) The residual is multiplied by a relaxation factor where 1.

2) Calculate the new $h_{i,j}^{m+1}$ with the following

$$h_{i,j}^{m+1} = h_{i,j}^m + \omega C$$

More residual is added to h_{ij}^{m} , or the head is *overrelaxed*.

if = 1, then the routine is the Gauss Seidel

if < 1, then the heads are underrelaxed

$$h_{2,2}^{m+1} = \frac{h_{1,2}^{m+1} + h_{2,1}^m + h_{3,2}^{m+1} + h_{2,3}^m}{4}$$

$$h_{i,j}^{m+1} = (1 - \omega)h_{i,j}^{m} + \omega \frac{\left(h_{i-1,j}^{m+1} + h_{i+1,j}^{m} + h_{i,j-1}^{m+1} + h_{i,j+1}^{m}\right)}{4}$$

Will need to adjust these solutions for different governing equations.

1) Unconfined aquifers.

Will need to adjust these solutions for different time steps.

1) Steady state

2) Transient

There is a little bit different formulation for finite element models. We will discuss this later.

Conceptual Model

Anderson and Woessner, Chapter 3

After establishing the purpose of a model, the second step is to design a conceptual model.

Conceptual Model

A pictorial representation of the ground-water flow system Frequently in the form of a simplified diagram or hydrogeologic cross section

The conceptual model defines

- 1) Dimensions of numerical model
- 2) How the grid is designed
- 3) How the grid is oriented

Conceptual model forces the modeler to

Simplify and Organize - all available field data But, must strike a balance between simplification and accuracy of simulating flow system.

"Everything should be made as simple as possible, but not simpler." Albert Einstein

Build a conceptual model around the area of interest that considers boundary conditions, be they natural or artificial

Three steps to constructing a conceptual model

1) Define Hydrostratigraphic Units

Assemble all available geologic and hydrogeologic information Rely on your existing geologic and hydrogeologic knowledge and intuition!!!



Facies Model 1







(c) Lodgement and basal till overlain by a supraglacial sediment complex.

Facies Model 2

Maxey (1964) and Seaber (1988) have advanced the term Hydrostratigraphic unit.

- Hydrostratigraphic units are geologic units with the same hydrogeologic properties.
- Most useful when the modeler is simulating hydrogeologic systems at a regional scale.
- Hydrostratigraphic units do not necessarily correspond with biostratigraphic units.

Dependent on variability in K and S.

Facies models are conceptual models of expected distributions of geologic materials. They are too general, they can't make specific predictions, Especially at small scales.

They are not site specific.

They are not site specific.

Need actual mathematical sedimentary models or fracture models.

Need site specific data for very small scales. Requires wells or geophysical data.

Remember that in numerical models, we must specify the parameters of all saturated units, not specifying confining layers as in the aquifer viewpoint.

Data Requirements for a ground-water flow model. Physical framework

- 1) Geologic map and cross sections showing the areal and vertical extent and boundaries of the system.
- 2) Topographic map showing surface water bodies and divides.
- 3) Contour maps showing the elevation of the base of the aquifers and confining beds.
- 4) Isopach maps showing the thickness of aquifers and confining beds.
- 5) Maps showing the extent and thickness of stream and lake sediments.



Figure 7-3. (figure 3.2, Anderson and Woessner)

Translation of geologic information into a conceptual model suitable for numerical modeling. (a) Florida aquifer system, west to east cross section for central Florida (Bush and Johnston, 1986)

Creating a conceptual model - Example 1



(c) Sand and gravel aquifer in Pensacola, Florida (Franks, 1988). (d) Glacial-drift river-valley aquifer in R hode Island (Morrisey, 1988)

Creating a conceptual model - Example 2

Hydrogeologic framework

1) Water table and potentiometric surface maps for all aquifers.

2) Hydrographs of ground-water head and surface-water levels and discharge rates.

3) Maps and cross sections showing the hydraulic conductivity and/or transmissivity distribution.

4) Maps and cross sections showing the storage properties of the aquifers and confining beds.

5) Hydraulic conductivity values and their distribution for stream and lake sediments.

6) Spatial and temporal distribution of rates of evapotranspiration, ground-water recharge,

surface water-ground water interaction, ground-water pumping, and natural ground-water discharge.

2) Preparing a Water Budget

Quantify all Sources of flow into system (In) Precipitation, snow melt Underflow across aquifer boundaries Recharge from wells or lagoons

Quantify all Sources of water out of system (Out)

Ground-water discharge (baseflow or underflow) Evaporation Transpiration Ground-water withdrawals (pumping) Springs/seeps

Construct a conceptual water budget with units to match output of numerical model

Use the conceptual water budget as a calibration target

3) Defining the Flow System

Where does water flow? How fast does water flow? How old is the water in the flow system?

How do we get this information

1) Precipitation (NWS, NOAA)

Recharge

2) Water levels (USGS, State water agencies) Ground-water flow directions Surface-water/ground-water interactions

Changes in storage

- 3) Baseflow, surface-water discharge (USGS, Bur. Rec., Army Corps) Surface-water/ground-water interactions
- 4) Evapotranspiration (USDA, USFS)

Plant water use

Shallow soil evaporation

5) Geochemical data

- a) Infer directions of ground-water flow
- b) Identify locations, rates of recharge
- c) Ground-water velocities and ages
- d) Identify mixing processes between layers



waters. (Location of map of north well field is shown in pl. 1). (Figure 10, Sources of Water in the Killbuck Creek Valley).





Identify mixing processes - Example 2

Estimating aquifer parameters

Important to define all of the data we specified in the table earlier in the lecture. Deterministic models Stochastic models Scale dependence of parameters

Grids

Anderson and Woessner, pp. 46-68

A grid forms the framework of the model.

Grid objectives should be based on

- 1) Objectives of study
- 2) Boundary conditions
- 3) Geologic framework
- 4) Changes in hydraulic gradient

In general, the grid spacing should be sufficient to enable the model to describe the greater changes in the potentiometric surface (hydraulic gradients).

Types of Grids

1) Finite difference

Can be squares or rectangles (2-D) Mesh centered or block centered flux boundaries

Block centered - on the sides of the block Easier, used in MODFLOW



Mesh centered - coincides with a node



2) Finite elements

Allow for more flexibility in model design Better at handling boundaries with complex shapes

Two Dimensional 1) Triangular elements

2) Quadrilateral elements



(finite difference is a subset of these elements)

Three dimensional elements are 1) Tetrahedrons



2) Hexahedrons



3) Prisms







AQUIFEM - linear, triangular elements FEMWATER - linear, 3-D elements (tetrahedrons, hexahedrons, or prisms)



Figure 8-1. Finite difference and finite element representations of an aquifer region. (Ander son and Woessner Fig. 1.1, Adapted from Mercer and Faust, 1980a.)

(a) Map view of an aquifer showing well field, observation wells, and boundaries.



(b) Finite grid with block centered nodes, where Δx is the spacing in the x direction, Δy is the spacing in the y directrion, and b is the aquifert hickness.

Finite-difference grid



(c) Finite difference grid with mesh centered nodes.



^Q Source*i*sink node

(d) Finite element mesh with triangular elements where bis the aquifer thickness.

Finite-element grid

Vertical Discretization

Must determine how many layers are needed to simulate a flow system. Rely on the conceptual model to determine how many layers (hydrostratigraphic units)

Two dimensional - one hydrostratigraphic unit in the layer Three dimensional - at least one layer for each hydrostratigraphic unit May want more than one layer in a hydrostratigraphic unit if there are large vertical hydraulic gradients. Quasi-three dimensional (we will revisit these next lecture)



Figure 8-2. Effects of grid discretization on sourses and sinks.

Discretization figure

Grid Orientation

- Align axes with principle directions of anisotropy. (x and y axes should be colinear with K_x and K_y) Not as easy to have the z axis parallel to K_z.
- 2) Minimize inactive nodes

Inactive cells are those which fall outside of boundaries, but within edge of grid. Waste memory, disk storage, and computation time. Finite element grids do a better job with irregular boundaries.

- 3) Make sure the grid falls on the boundary with finite element models or mesh-centered finite difference Make sure that flux boundaries fall on the edge of cells with block centered and head boundaries fall on the nodes.
- 4) Place boundaries sufficiently far from area of interest so as to not affect numerical solution.

Size of Grid Spacing

Make the grid spacing fine enough to describe changes in hydraulic head.

Consider the variability in aquifer parameters.

Consider variability in source/sink areas/rates. (for instance recharge vs. wells)

When using an irregular spacing, don't increase adjacent spacing more than 1.5 to 2 times the previous nodal spacing. Approximation becomes less accurate Get larger error Longer time to converge

Regular grid spacing advantages Easier to identify nodal locations Less numerical error Easier to import data into graphical packages

Irregular grid spacing advantages Fewer nodes required Fewer calculations Faster compute time

Type of Models - Estimating Parameters

Anderson and Woessner, pp. 38-46 and 68-77

Models come in many different shapes and forms.

Spatial dimensions Aquifer viewpoint ▶ 2-D areal ▶ Quasi 3-D

> System viewpoint 2-D profile Full 3-D

Temporal dimensions

Steady state

Transient







Transient conditions

2-D Areal

Can simulate Confined, Unconfined, Leaky Confined, and Mixed aquifers.

Confined aquifers

- Can simulate thickness and K changes by differing T and S (heterogeneity).
- Simulate anisotropy with different T_x and T_y .
- Generally get these values from aquifer tests (pumping and slug).

Leaky Confined Aquifers

- Use a leakage term to simulate the leaky layer and overlying source aquifer.
- Leakage term depends on K and b of leaky layer.

Unconfined aquifers

- Usually use Dupuit assumptions assume horizontal flow (no vertical changes in hydraulic head).
- Need K and S_y.
- Because the thickness changes with pumping, need a datum.
- If Dupuit assumptions are not valid must
 - 1. use a 2-D profile model
 - 2. use a full 3-D model.

Mixed Aquifers

- Combination of the above or a change during simulation between the above.
- A layer may go dry during a transient simulation.

Quasi 3-D Models

- Don't explicitly represent confining layers
- Ignore horizontal flow in confining layers.
- Don't calculate hydraulic head in the confining layers.
- Usually ignore storage in confining layer
- Need at least two orders of magnitude difference between K of
- confining layer and aquifer to use these assumptions.
- MODFLOW can use this option for some layers.



Figure 9-3 (figure 3.16, Anderson and Woessner). Representation of dipping hydrostratigraphic units in profile models.
(a) A vest-to-east finite difference model of the coastal aquifer system in Texas was developed to examine the boundary effects of the Chicot quifer and Burkeville confining layer on flow in the Evangeline auter (Grochen, 1985).
(b) The design of a finite element mesh to account for dipping beds and boundary conditions for a dam seepage problem. The detailed grid near the base of the dam is not shown (Townley and Wilson, 1980).

Profile models



Figure 9-4 (table 3.3, Anderson and Wolessner, adapted from Heath, 1983). Hydraulic conductivity of selected rocks .

Hydraulic conductivity ranges

Profile Models

Used for flow systems with well defined flow lines

Estimating aquifer parameters

- Important to define all of the data we specified in the table earlier in the lecture.
- Estimate from published values when to start modeling and refine during project.
- Deterministic models.
- Stochastic models.
- Scale dependence of parameters

Hydraulic conductivity

- Varies 12 or more orders of magnitude
- Usually varies one order of magnitude within a homogeneous unit
- When anisotropy has been measured, usually $K_h:K_v$ is at least 3:1
- Horizontal anisotropy can be as high as 50:1 in sand and gravel with clay
- Vertical anisotropy is usually between 1 and 1000
- Vertical anisotropy is usually much greater than horizontal
- Fractures may affect anisotropy
- Hydraulic conductivity is *log normally* distributed Geometric mean is an unbiased estimator of average
- Hydraulic conductivity varies with scale of measurement Small values at small scales

2 to 3 orders of magnitude greater at larger scales



Figure 9-5 (after EOS, Jan. 7, 1997).

Relationship of hydraulic conductivity (K) to scale measurement in three carbonate aquifer units. The scale of measurement used was the volume of rock tested (V). Horizontal distance (such as radius of influence) was not used because the volume of rock measured is a more accurate measure of scale, especially for small scale tests. Geometric means are plotted on each scale of measurement. Regression lines and equations are based on all available data points (n). The 95% confidence intervals on the exponents (slopes of log-log line) are Thiensville Formation 0.54±0.06, Romeo Beds 0.54±0.21, and Mayville Formation 0.55±0.10. Regression lines are near parallel with an upper bound located at a tested rock volume of approximately 10,000 m⁻³.

Hydraulic conductivity measurements with relation to scale



Figure 9-6 (after EOS, Jan. 7, 1997).

Relation ship of longitudinal dispersivity to scale of measurement in various carbonate aquifers (solid line). The 95% confidence interval on the exponent of the relationship is 1.07 ± 0.15 . The extrapolated relationship was determined using the Mayville tracer test (bold triangle at a scale of 80m) and is shown as the dashed line. Scale of measurement is horizontal flow distance (L) because has the dimensions of (L) in the direction of flowonly. The upper bound is located at a horizontal flow distance of approximately 100m.

Dispersivity measurements with relation to scale

Storativity

- Specific storage confined
- Specific yield unconfined
- Specific storage varies over 4 orders of magnitude
- Specific yield varies within 1 order of magnitude
- Approximates porosity with specific yield Porosity needed for velocity calculations

Table 9.1. (Table 3.4, Anderson and Woessner, adapted from Domenico, 1972). Ranges of Values of Specific Storage (S_s)

Material	Specific Storage (S _s) (m ⁻¹)
Plastic clay	$2.0 \times 10^{-2} - 2.6 \times 10^{-3}$
stiff clay	$2.6 \times 10^{-3} - 1.3 \times 10^{-3}$
medium-hard clay	$1.3 \times 10^{-3} - 9.2 \times 10^{-4}$
loose sand	$1.0 \times 10^{-3} - 4.9 \times 10^{-4}$
dense sand	$2.0 \times 10^{-4} - 1.3 \times 10^{-4}$
dense sandy gravel	$1.0 \times 10^{-4} - 4.9 \times 10^{-5}$
rock, fissured jointed	$6.9 \times 10^{-5} - 3.3 \times 10^{-6}$
rock, sound	less than 3.3×10^{-6}

Can try to describe spatial variability with Geostatistics

- Try to determine spatial correlation of randomly distributed variables.
- Need a variogram to quantify the structure in the aquifer caused by the arrangement of heterogeneities. Semiovariogram describes the rate of change of the variable in a specific direction. Plot semivariance and separation distance. Variability increased with distance. Spherical, exponential, Gaussian, power (linear and others).
- Find the *Sill*, the distance at which points are no longer related.
- Find the *Range*, the distance at which the sill is attained or the distance at which all points are related.

Use Kriging to estimate the value of a variable at any unsampled location

Kriging produces

- 1. Estimates that on average have the smallest possible error.
- 2. Explicit statement of magnitude of error.

Stochastic Simulation

- 1. Process of drawing alternative, equally probable joint realizations of a variable from a random function model
- 2. Generate multiple realizations of random function model for variable (K)
- 3. Different from kriging in that we create many alternative solutions

Boundary Conditions

Anderson & Woessner, pp. 97-106

Boundary conditions are necessary to define how the site specific model interacts with entire flow system.

Occur at the edges of the active model area.

Make a piece of computer code a site specific model.

Boundaries are largely responsible for how flow occurs in the system.

The most **likely** source of error in the modeling process.

Physical boundaries

- Model boundaries correspond with actual physical boundaries.
- Faults, facies changes, surface water bodies

Hydraulic boundaries

- Model boundaries corresponding with hydrologic conditions.
- Ground-water divides
 At recharge or discharge areas
 Topographically high or low areas
- Streamlines If steady-state, separate the aquifer If transient, need to simulate how boundary changes position Can represent Toth's concepts of local, intermediate or regional flow systems

Specified head boundaries (Dirichlet conditions)

Hydraulic head is given for the boundary

Specified flow boundaries (Neumann conditions)

- Flux (derivation of head) across the boundary is given.
- A no-flow boundary has a flux of zero

Head-dependent flow boundaries (Cauchy or mixed conditions)

- Flux is dependent on the hydraulic head
- The general-head boundary in MODFLOW



Typical head boundaries



Designing the boundaries in the Conceptual and Numerical Model

- Use physical boundaries whenever possible.
- Tend to be more stable with time.
 Try to use a lower impermeable hydrostratigraphic unit as the lower boundary. Usually a 2 order of magnitude difference in K.
 - If the flux out of the lower unit is known use it instead.
 - Deep fluxes are rarely know.
- Can estimate fluxes using Darcy's Law.
- When using hydraulic boundaries
 Try to find regional ground-water divides.
 Be sure to determine how the boundary changes with time.
 Divides for local and intermediate flow systems likely to be transient.
 If simulating short times, local and regional divides may be sufficient.
- Most models are a mix of all types of boundaries.
- Can't use all specified flux boundaries.
 Must have a specified head for initial difference calculation.
 Needs a specified head for reference.
- Specified head boundaries supply unlimited flux.
- May want to use specified head first, then change to specified flux. Determine influence of head on flux.
 - If there is no difference then the model is insensitive



Figure 10-4. Boundary conditions for a groundwater basin (Anderson and Woessner Fig. 4.3).

(a) A groundwater basin with no-flow boundaries along its perimeter, EABCD, and a specified flow boundary along ED that represents underflow from the basin. A constant-head boundary node might be specified at point x to represent the head of the river.

(b) Representation of the river system in a two-dimensional profile or full three-dimensional model by representing the river as anode within the grid. The head of the river node is specified to be equal to the stream stage.

(c) The use of leakage conditions to simulate the partially penetrating river system. The river is not represented within the grid but leakage is simulated as a head-dependent condition. River stages and the vertical hydraulic conductivity and thickness of riverbed stages are assigned. The head in the aquifer below the stream is calculated by the model based on leakance of the riverbed sediments and the head difference between the stream and the aquifer.



Figure 10-5. Block-centered finite difference grid (After Anderson and Woessner Fig. 4.6).

(a) Flux boundaries correspond to the edges of the boundary cells and constant-head boundaries pass through the nodes (adapted from McDonald and Harbaugh, 1988).

(b) Representation of fluxes. Volumes of water are placed into the block or extracted from the block using wells (Q), areal recharge, or leakage ($R\Delta x\Delta y$ or $U\Delta y\Delta z$).

Locating non-physical boundaries

1. Distant boundaries

Simply locate the boundary far from the area of interest so as to minimally affect solution.

Large stresses can impact near boundaries.

Cone of depression may extend to boundary

- Well removes too much water too close to boundary

- Cone of depression not big enough

Stream recharge may extend to boundary

May want to use variable grid spacing for distant boundaries

2. Hydraulic boundaries

"Artifical" boundaries

May have the ground-water flow system defined by the streamlines of a contaminant plume. Can derive from water table or potentiometric surface maps

Typically used to define profile model boundaries.

Telescopic mesh refinement

A process of defining boundaries for successively smaller active model areas.

- 1) Use a coarse grid to simulate a regional aquifer
- 2) Refine grid size and spacing for smaller area
- 3) Use fluxes calculated from regional model as boundary conditions for smaller area.
- 4) Repeat steps 1 to 3 as necessary.



Simulating Boundaries

Anderson & Woessner, pp. 106-121

Specified Head Boundaries

Set the head at the boundary = to a known head Remember the rule of

Head on boundary - Finite element and mesh-centered finite diff Head on node - Block centered finite diff

In 2-D areal models

Heads represent fully penetrating surface water bodies or Vertically averaged head in aquifer at the boundary



Figure 11-1. Block-centered finite difference grid (Anderson and Woessner Fig. 4.6).

(a) Flux boundaries correspond to the edges of the boundary cells and constant-head boundaries pass through the nodes (adapted from McDonald and Harbaugh, 1988).

(b) Representation of fluxes. Volumes of water are placed into the block or extracted from the block using wells (Q), areal recharge, or leakage ($R\Delta x\Delta y$ or $U\Delta y\Delta z$).

In 3-D models

- Specified head usually represents water table or water body in layer 1.
- Examine the example shown in Figure 11.1.
- In figure 11-2 specified heads are used to represent a surface water body.
- In figures 11-3 through 11-5 specified heads are used to represent a bay.
- The boundary location varies with layer in Figures 11-3 through 11-5.

Note

- A specified head represents an unlimited supply of water
- You can get recharge or discharge across the boundary without changing the head
- Might need to use some type of mixed boundary condition
- Let flux be dependent on the head at the boundary, or, change the heads on
- the boundaries during the simulation

Specified Flux

Used to describe flow across a boundary

Surface water bodies

- Springs/seeps
- Underflow figure 11-6
- Leakage out of bottom of model figure 11-7

Remember example of telescopic mesh refinement

Often times, you may need to use the specified flows for calibration

- Stream gain/loss (baseflow)
- Spring discharge
- Tile drainage

Land surface	;
Watertable before tile ⊽	
Water table after tile	

Tile drainage figure

Sometimes, a finer grid spacing is needed around a specified head Especially can be a problem with rivers in a large, coarse regional model.

In MODFLOW and FLOWPATH and other models

Simulate a specified flux with a "well" either discharging or recharging water Must assume that the flow is evenly distributed throughout the model cell/element

Typically, models allow areal, surface recharge to be input as a rate (L/T)

$$\frac{L}{T}L^2 = \frac{L^3}{T}$$

Head-Dependent Flow

These boundaries are used when the head across the boundary is dependent on head on each side of the boundary.

Typically, you specify the head on one side of boundary and the model calculates the head on the other side dependent on a conductance term

For instance, the leakage out of a stream is dependent on Hydraulic conductivity of stream Thickness of streambed Head difference between stream and aquifer *Darcy's Law!!!*

Application of FDM Method to Ground-Water Flow Problems

Two-dimensional steady-state confined flow problem

As an example of a groundwater model involving Laplace's equation and suitable boundary conditions, we present a regional groundwater problem described by **Toth** (1962). He was able to draw conclusions about the configuration of regional groundwater systems by using a mathematical model.

Figure (##) represents a cross section through a small watershed bounded on one side by a topographic high, which marks a regional groundwater divide, and on the other side by a major stream, which is a groundwater discharge area and marks another regional groundwater divide. The aquifer is assumed to consist of homogeneous, isotropic, porous material underlain by impermeable rock.

We first consider the boundary conditions. The left and right groundwater divides can be represented mathematically as impermeable, no-flow boundaries. Although no physical barrier exists, a groundwater divide <u>has the same effect as an impermeable barrier</u> because no groundwater crosses it. Groundwater to the right of the valley bottom discharges at point A, and groundwater on either side of the topographic high flows away from point B. The lower boundary is also a no-flow boundary because the impermeable basement rock forms a physical barrier to flow. The upper boundary of the mathematical model is the horizontal line AB' even though the water table of the physical system lies above AB'.



Fig (), Schematic representation of the boundaries of a two-dimensional regional groundwater system, after Wang.

$$q_x = -K \frac{\partial h}{\partial x} = 0 \qquad \Rightarrow \frac{\partial h}{\partial x} = 0$$
$$q_y = -K \frac{\partial h}{\partial y} = 0 \qquad \Rightarrow \frac{\partial h}{\partial y} = 0$$
$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = 0$$

Thus the rectangular problem domain of the mathematical model is an approximation to the actual shape of the saturated flow region. Along the boundary AB', the head is taken to be equal to the height of the water table, and the water table configuration is considered to be a straight line.

Toth (1962, 1963) finds that this mathematical model is a realistic representation of the general configuration of the flow system where the topography is subdued and the water table slope is gentle. **Toth** (1963) also uses a more general expression for the configuration of the water table in a region of gently rolling topography.

We must express the boundary conditions shown in Figure (##) in mathematical terms. The coordinate system is defined in Figure (##).



An equation is required for each boundary. Consider the upper boundary first. The boundary is located at $y = y_0$ for x ranging from θ to s. The distribution of head along this boundary is assumed to be linear.

The equation for a linear variation such that $h(0, y_o) = y_o$ is $h(x, y_o) = cx + y_o$ for $0 \le x \le s$, where *c* is the slope of the water table. The specification of head along the upper boundary makes it a <u>Dirichlet</u> boundary condition.

The other three boundary conditions are for no-flow boundaries. Darcy's law relates flow to gradient of head. Along a vertical, no-flow boundary, $q_x = 0$ implies $\frac{\partial h}{\partial x} = 0$, and along a horizontal, no-flow boundary, $q_y = 0$, implies $\frac{\partial h}{\partial y} = 0$.

First, we discretize the domain using evenly-spaced nodes in both directions so that:



at real nodes, (h) is known or calculated. Fictitious nodes are used to specify no-flow boundary condition. Write the FD approximation to the PDE for an interior node i,j (blue).

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial x^2} = 0$$
$$\frac{h_{i-1,j} - 2h_{i,j} + h_{i+1,j}}{\Delta x^2} + \frac{h_{i,j-1} - 2h_{i,j} + h_{i,j+1}}{\Delta x^2} = 0$$

for $\Delta x = \Delta y$, $h_{i-1,j} + h_{i+1,j} + h_{i,j-1} + h_{i,j+1} - 4h_{i,j} = 0$

Write the FD approximation to the PDE for a no-flow boundary node (red).

FORTRAN Example (Point Iterative Solution)

- Dimension Statement H(i, j) \rightarrow H(13, 7), and it can be more than those values, but not less.
- Read or Set Input Parameters NX = 13 DX = 20.0

.....

• Initialize all H(i, j) Values to be 100

DO J=2,NY-1

```
DO I=2,NX-1
H(I,J) = 100.0
ENDDO
```

ENDDO

• Set Constant-Head Boundary:

H(I, 1) = 100 + 0.02*DX*(I-2)

- Set Left, Right and Bottom No-Flow Boundary
- Solve for Unknown Nodes and Calculate Error

```
DO J=2,NY-1

DO I=2,NX-1

.....

H(I,J) = (H(I-1,J) + H(I+1,J) + H(I,J-1) + H(I,J+1))/4

.....

ENDDO

ENDDO
```

• Determine if Maximum Error is Acceptable If YES, then end program If NO, revise estimates for *h* and repeat solution procedure

One-dimensional, transient, confined groundwater flow

```
FORTRAN Example (Direct Solution using Thomas Algorithm):
· Dimension Statement
· Read or Set Input Parameters
NX = 11
DX = 10.0
DT = 5.0
. . . . . . . . .
N = NX - 2
\cdot Set initial conditions for all H(I) to be 11
DO I=2,NX-1
HOLD(I) = 11.0
ENDDO
· Set constant-head boundary values
· Define matrix constants: a, b, c
· Begin Time Steps
DO N=1,NT
DO I=2,NX-1
D(I-1) = .....
ENDO
CALL TRIDIA(N)
DO I=2,NX-1
HNEW(I) = X(I-1)
ENDO
. . . . . . .
DO I=2,NX-1
HOLD(I) = HNEW(I)
ENDDO
ENDDO
```

The Main program "calls" the Subroutine TRIDIA, passing the variable "N" (N = number of unknown nodes). The variables A, B, C, X, and F are calculated in the Main program and are passed using the COMMON command.

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