Finite Difference Derivations for Spreadsheet Modeling

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Figure 1. Sunset with 11 swans on Little Platte Lake, Michigan.

Review of Fundamentals

The goal of this section is to teach some of the fundamental concepts of numerical methods and their limitations – without getting sidetracked too deep into applied mathematics. In numerical modeling of ground water flow and transport we break the system to be modeled into a series of discrete nodes or elements. The more finely we divide the system – the more accurate our numerical model. The easiest way to understand the basics of the modeling process is to derive and program simple finite difference models in spreadsheets. This provides an overview of modeling without a lot of complex and tedious work.

At least two methods for derivation of finite difference equations exist:

a) the flux / conservation method and

b) Taylor's series approximations

The flux method is much more powerful and very intuitive– although the Taylor's series method is easier for simple cases and thus preferred by students. If we take node i for the control volume then the continuity equation is:

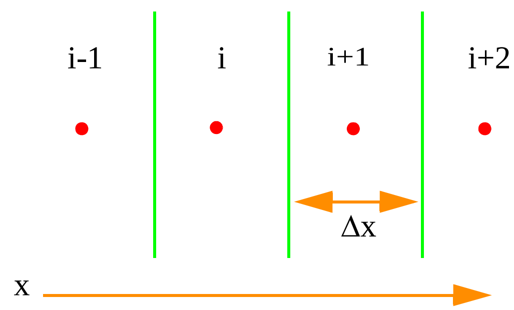

Figure 2. Example one dimensional finite difference grid.

$$VS_s\frac{\partial h_i}{\partial t} = Input - Output \mp (Source - Sink) \qquad (1)$$

$$VS_s\frac{\partial h_i}{\partial t} = \sum A_{in} q_{in} - \sum A_{out} q_{out} + \dot{Q} \qquad (2)$$

where:

$\dot{Q}$ = source of water, so a well would have a negative value (m^3/s)

V = volume of the control volume = Δx Δy Δz, note that directions not modeled are generally assumed to be of unit length (m^3)

A = surface area on relevant side of control volume (m^2)

q = flux into or out of a control volume surface, the sign of the flux depends upon the direction that is defined to be positive, fluxes in the positive direction are positive fluxes ($m^3/m^2/s$)

At this point we have not specified in the equation how many directions we will model and/or if the model will be transient or steady state. With steady state models the time derivative goes to zero.

The next step is to replace the derivatives with finite difference approximations and to replace the generic flux statements with a constitutive law, Darcy's law in this case. For the flux method we assume that the boundary between each node is half way between two nodes. Since a derivative is merely the slope, the common sense approximation of a derivative is to take the slope at small steps. The small steps can be in time and/or in space. For time this gives:

$$\frac{\partial h}{\partial t} \cong \frac{\Delta h}{\Delta t} = \frac{(h_i^{n+1} - h_i^n)}{(t^{n+1} - t^n)} \tag{3}$$

Darcy's law is used to put the fluxes in terms of hydraulic head:

$$q = -K\nabla h \tag{4}$$

We will provide a one dimensional example in the x direction. Since fluxes are at the nodal interfaces its easiest to refer to them as North, South, East, West, Top, Bottom. For a one dimensional system we have only East and West directions. The continuity equation says that the change in storage in the control volume is equal to Input - Output + Source:

$$VS_s\frac{\partial h_i}{\partial t} = -A_W K_W \frac{\partial h}{\partial x} + A_E K_E \frac{\partial h}{\partial x} + A\dot{Q} \tag{5}$$

For the one dimensional case it is more consistent to redefine $\dot{Q}$ as the source of water per unit area per unit time in the direction being modeled (m/s).

For space we get the following finite difference approximations, for output from the control volume:

$$\frac{\partial h}{\partial x} \cong \frac{\Delta h}{\Delta x} = \frac{(h_{i+1} - h_i)}{(x_{i+1} - x_i)} \tag{6}$$

and for input to the control volume:

$$\frac{\partial h}{\partial x} \cong \frac{\Delta h}{\Delta x} = \frac{(h_i - h_{i-1})}{(x_i - x_{i-1})} \tag{7}$$

where:

n = point in time, n is the current time and n+1 is one time step in the future

i = node number

What are the time steps on the hydraulic heads?

Substitution gives:

$$VS_s\frac{(h_i^{n+1}-h_i^n)}{(t^{n+1}-t^n)} = -A_W K_W\frac{(h_i-h_{i-1})}{(x_i-x_{i-1})} + A_E K_E\frac{(h_{i+1}-h_i)}{(x_{i+1}-x_i)} + A\dot{Q} \tag{8}$$

This looks complicated but is not. First consider that if the system is homogeneous then $K_E=K_W=K$ If the non-modeled directions are assumed to be of length 1 and Δx is constant then the areas and volumes simplify to: A=1 m^2 and V=Δx m^2. Simplifying gives:

$$\frac{S_s}{K}\frac{(h_i^{n+1}-h_i^n)}{\Delta t} = \frac{-(h_i-h_{i-1})}{\Delta x^2} + \frac{(h_{i+1}-h_i)}{\Delta x^2} + \frac{\dot{Q}}{\Delta x} \tag{9}$$

or:

$$\frac{S_s}{K}\frac{(h_i^{n+1}-h_i^n)}{\Delta t} = \frac{(h_{i-1}-2h_i+h_{i+1})}{\Delta x^2} + \frac{\dot{Q}}{K\Delta x} \tag{10}$$

or:

$$h_i^{n+1} = \frac{\Delta t K}{\Delta x^2 S_s}\left[(h_{i-1}-2h_i+h_{i+1}) + \frac{\Delta x\dot{Q}}{K}\right] + h_i^n \tag{11}$$

The time step on the hydraulic heads depend upon the numerical method chosen for advancing the equations in time. Explicit methods assume that the value of h at the current (i.e., known) time step are used. The *explicit* method makes solution of the equations very simple: Just solve the equation for the only unknown – h at time step n+1.

The *implicit* method assumes that the value of h is taken at a future time step. Thus a series of equations (i.e., a matrix) must be solved to advance the solution in time.

The explicit method is easier to program but is less powerful because it is less stable. The maximum time step for the explicit method is:

$$\frac{K\Delta t}{S_s(\Delta x^2)} \le \frac{1}{2} \tag{12}$$

Finite Difference by Taylor's Series

The equation for two dimensional horizontal flow in a homogeneous isotropic medium is:

$$T_x \frac{\partial^2 h}{\partial x^2} + T_y \frac{\partial^2 h}{\partial y^2} + R - L = S\frac{\partial h}{\partial t} \tag{13}$$

We will show a one dimensional example but the same derivation applies to multiple dimensions. The Taylor's series approximation to a function, in this case hydraulic head is:

$$h(x + \Delta x) = h(x) + \Delta x\frac{\partial h}{\partial x} + \frac{(\Delta x)^2}{2!}\frac{\partial^2 h}{\partial x^2} + \frac{(\Delta x)^3}{3!}\frac{\partial^3 h}{\partial x^3} + \frac{(\Delta x)^4}{4!}\frac{\partial^4 h}{\partial x^4} + Error \tag{14}$$

In terms of our finite difference grid where we have nodes:

$$h_{i+1} = h_i + \Delta x\frac{\partial h}{\partial x} + \frac{(\Delta x)^2}{2!}\frac{\partial^2 h}{\partial x^2} + \frac{(\Delta x)^3}{3!}\frac{\partial^3 h}{\partial x^3} + \frac{(\Delta x)^4}{4!}\frac{\partial^4 h}{\partial x^4} + Error \tag{15}$$

and

$$h_{i-1} = h_i - \Delta x\frac{\partial h}{\partial x} + \frac{(\Delta x)^2}{2!}\frac{\partial^2 h}{\partial x^2} - \frac{(\Delta x)^3}{3!}\frac{\partial^3 h}{\partial x^3} + \frac{(\Delta x)^4}{4!}\frac{\partial^4 h}{\partial x^4} + E(\Delta x^4) \tag{16}$$

These are fourth order accurate. If we can accept second order accuracy then they can be truncated after the first two terms:

$$h_{i+1} = h_i + \Delta x\frac{\partial h}{\partial x} + \frac{(\Delta x)^2}{2!}\frac{\partial^2 h}{\partial x^2} + E(\Delta x^2) \tag{17}$$

and

$$h_{i-1} = h_i - \Delta x\frac{\partial h}{\partial x} + \frac{(\Delta x)^2}{2!}\frac{\partial^2 h}{\partial x^2} + E(\Delta x^2) \tag{18}$$

to get second order accurate equations. If we add the above two equations we get:

$$\frac{\partial^2 h}{\partial x^2} = \frac{h_{i-1} - 2h_i + h_{i+1}}{(\Delta x)^2} + E(\Delta x^2) \tag{19}$$

Or we could get even more crude and just truncate the above equations to first order accuracy:

$$\frac{\partial h}{\partial x} = \frac{h_{i+1} - h_i}{\Delta x} + E\Delta x \tag{20}$$

$$\frac{\partial h}{\partial x} = \frac{h_i - h_{i-1}}{\Delta x} + E\Delta x \tag{21}$$

Steady State Simulation Example

Let's apply our newly found finite difference equations to the two dimensional flow in a confined aquifer situation given above. But, since I'm tired, only to the steady state situation with no sources or sinks. At steady state this becomes:

$$T_x \frac{\partial^2 h}{\partial x^2} + T_y \frac{\partial^2 h}{\partial y^2} = 0 \tag{22}$$

Plugging and chugging we finally get:

$$h_{i,j} = \frac{h_{(i-1,j)} + h_{(i+1,j)} + h_{(i,j-1)} + h_{(i,j+1)}}{4} \tag{23}$$

Notice that this equation has a circular logic when applied to multiple nodes.

How do we solve such an equation?

1. Put in boundary conditions. For fixed heads this is just the value of the head at the node. For no flux boundary conditions consider that there is no flux if the head is the same on both sides of the node. Make an imaginary node and assume it has the same head as the node on the opposite side (show example spreadsheet).

2. Put in the basic equation on all interior nodes.

3. Set the spreadsheet to iterate to convergence.