Contents

Exercise 1: Making your own groundwater model in excel

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Objectives:

- Learn how to set up a model of an earth science process
- Learn how to constrain models with data (model calibration)
- Learn how groundwater systems function and respond to changes in recharge and pumping

Deadline: Hand in a printed or preferably digitial word document or pdf on **Friday 29 nov 2018**, plus an excel file of your model. Make sure to answer all the questions that are marked in **bold**. Add a figure of the modeled watertable for question 1, 2 and 3.

Grading: Each correctly answered question earns you 1 point. The maximum score is 10 points. Note that some of the assignments ask for your opinion. In this case there is no right or wrong answer, and any answer that is well reasoned gets the maximum amount of points.

Advice: Try to maintain a word document where you answer the questions as you go, going back to your spreadsheets later to see what answers you got is much more time consuming than answering straight away. Make frequent backups of your spreadsheet file. And dont hesitate to ask questions, it is much faster to solve problems together than to work on it by yourself.

Introduction

Solving differential equations, Euler's method

Groundwater flow and many other geological and physical processes such as heat flow, the propagation of seismic waves, etc. can be described by partial differential equations. Unfortunately partial differential equations are often difficult to solve directly. Analytical solutions of some partial differential equations do exist, but these often require strong simplifications as we will see below. We will use a numerical method to solve the groundwater flow equation, which is based on a method to approximate derivatives that was first proposed by the Swiss mathematician Leonhard Euler in the 18th century.

The definition of a derivative of a variable y over x is:

$$y'(x) = \frac{\partial y}{\partial x} = \lim_{\Delta x \to 0} \frac{y(x + \Delta x) - y(x)}{\Delta x} \tag{1}$$

For very small values of Δx the following is true:

$$\frac{\partial y}{\partial x} \approx \frac{y(x + \Delta x) - y(x)}{\Delta x} \tag{2}$$

Rearranging gives:

$$y(x + \Delta x) \approx y(x) + \frac{\partial y}{\partial x} \Delta x \tag{3}$$

Although for now this seems like a nice, but not terribly useful rearranging of equations, we will show you how to use this method to numerically solve partial differential equations. Euler's method forms the basis of finite-difference methods, which have enabled scientists to solve partial differential equations for which no analytical solutions exist and predict all kinds of physical processes. The finite difference method was first developed by Courant, Friedrichs and Lewy in Göttingen in 1928 [*Courant et al.*, 1928].

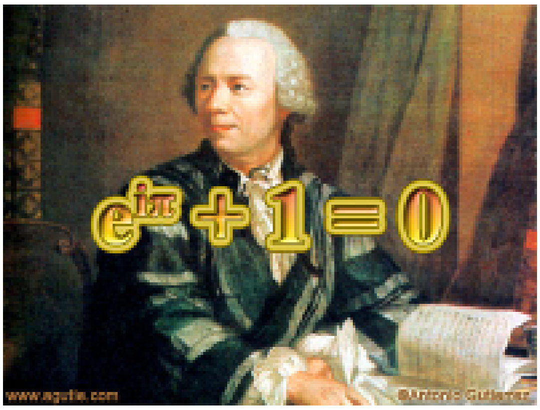

Figure 1: Leonhard Euler

Numerical solution of the groundwater flow equation

Groundwater flow is described by the following partial differential equation:

$$S_s \frac{\partial h}{\partial t} = -\nabla q + W \tag{4}$$

where S_s is specific storage (m^{-1}), h is the hydraulic head (m), t is time (sec), q is flux $(m\, s^{-1})$ and W is a term that represents external sources or sinks of water, such as groundwater recharge or pumping (s^{-1}).

For the moment we will only look at steady-state groundwater flow, which means that the hydraulic head does not change over time: $\partial h / \partial t = 0$. In addition, we consider only one spatial dimension, so $\nabla q = \partial q / \partial x$. And to simplify things a bit more we will assume that all flow is horizontal and we will calculate a vertically integrated flux over the entire depth of the geologic unit for each position x.

The vertically integrated version of Darcy's law is:

$$Q = -Kb \frac{\partial h}{\partial x} \tag{5}$$

Note that the flux (Q) represents the flux over the entire depth of the aquifer. The units are m^2 s^{-1} instead of m s^{-1}.

By combining eq. 4 with Darcy's law we end up with the steady-state groundwater flow equation:

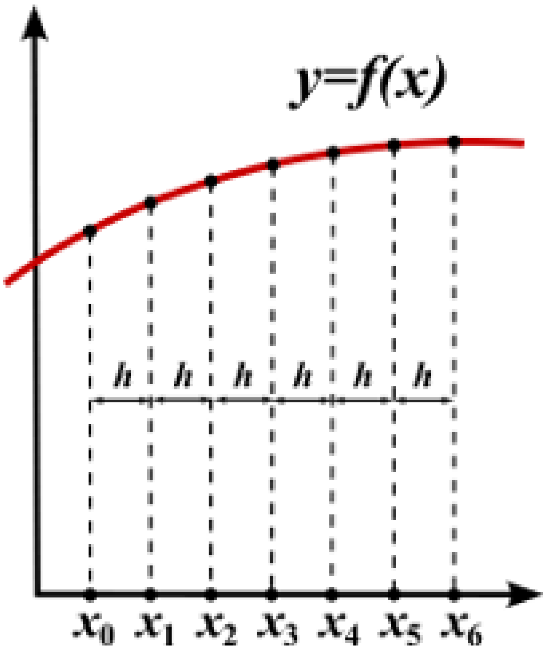

Figure 2: Approximating derivatives using finite difference methods. A potentially complex variable (ie, temperature, hydraulic head, etc) is only evaluated at discrete elements (x1, x2, etc...). In these elements the values are assumed to be constant.

$$Kb\frac{\partial^2 h}{\partial x^2} + Wb = 0 \tag{6}$$

Where K is hydraulic conductivity (ms^{-1}). Note that we have taken K out of the derivative, which is only valid if we assume that K is constant.

For the numerical solution of this equation we need Euler's method. The first order derivative of h follows from equation 3:

$$\frac{\partial h}{\partial x} = \frac{h(x + \Delta x) - h(x)}{\Delta x} \tag{7}$$

The 2nd order derivative can be found by repeating Euler's method:

$$\frac{\partial^2 h}{\partial x^2} = \frac{h(x + \Delta x) + h(x - \Delta x) - 2h(x)}{\Delta x^2} \tag{8}$$

Inserting our new formulation of the 2nd order derivative in eq. 6 results in:

$$\frac{h(x + \Delta x) + h(x - \Delta x) - 2h(x)}{\Delta x^2} = -\frac{Wb}{Kb} \tag{9}$$

Rearranging this equation shows how we can find hydraulic head at any point in space ($h(x)$) as a function of the hydraulic head at two adjacent points in space $h(x - \Delta x)$ and $h(x + \Delta x)$:

$$h(x) = \frac{1}{2}\left(\frac{Wb\Delta x^2}{Kb} + h(x + \Delta x) + h(x - \Delta x)\right) \tag{10}$$

Groundwater flow to a stream

Now lets apply this solution to a groundwater flow problem. Below is a conceptual model of groundwater flow in an permeable rock unit that is bounded by stream on the left, and is fed by groundwater recharge (shown by R). The hydraulic head is a function of the amount of recharge that enters the system, the frictional resistance that the porous rocks exert on the groundwater and the level of the stream. We would like to calculate the elevation of the watertable in this particular system. Below we will first try to calculate this by directly solving the groundwater flow equation for any point x in the geologic unit (=analytical solution) and then we will find an approximate (numerical) solution of the groundwater flow equation using Euler's method.

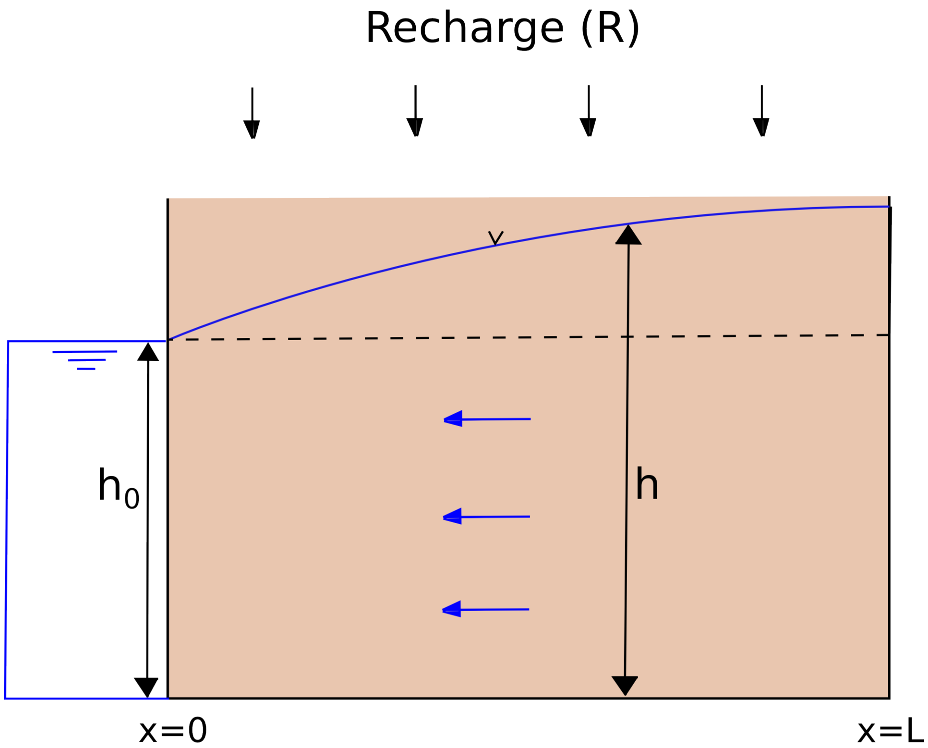

Figure 3: Groundwater flow to a stream with uniform recharge

Analytical solution

The conceptual model shown in Fig. 3 can be solved analytically, although we do need to make some simplifying assumptions to find the solutions.

The first assumption is that flow is only horizontal ($q_z = 0$). This is of course somewhat unphysical, but for systems where the overall hydraulic gradient is low flow is nearly horizontal and the error by neglecting the vertical term in the flow equation is small.

Rewriting Darcy's equation for horizontal flow in an unconfined aquifer results in:

$$q = -Kb\frac{\partial h}{\partial x} \tag{11}$$

Where q is the groundwater flux in $m^2 s^{-1}$.

b is the saturated thickness of the aquifer. b is equal to the watertable elevation above the base of the model, which is equal to the hydraulic head h. Therefore the correct equation would be:

$$q = -Kh\frac{\partial h}{\partial x} \tag{12}$$

To keep things simple, we also assume that the saturated thickness of the aquifer is constant and is independent of the watertable elevation. This is somewhat unrealistic for a unconfined aquifer as shown in Figure 1, but is a reasonable assumption provided that the elevation of the watertable is small compared to the total thickness of the aquifer (($\Delta h << b$).

The analytical solution for the flow system shown in Fig. 3 can be found by combining the simplified version of Darcy's law with a mass-balance equation. The depth integrated form of Darcy's law for an aquifer with constant thickness b (m) is:

$$q = -Kb\frac{\partial h}{\partial x} \tag{13}$$

The mass balance for the aquifer is:

$$q(x) = -R(L - x) \tag{14}$$

Which simply states that the steady-state groundwater flux at any point x in the aquifer is equal to the recharge flux multiplied by the area. R is recharge (ms^{-1}) and L is the length of the aquifer (m).

Combining Darcy's law and the mass balance equation results in:

$$-Kb\frac{\partial h}{\partial x} = -R(L - x) \tag{15}$$

One way to solve partial differential equations like these is by integration. For this we need to bring any x variable to one side of the equation and any h variable to the other side.

$$-R(L - x)\partial x = -Kb\partial h \tag{16}$$

Integrating this:

$$\int -R(L - x)\partial x = \int -Kb\partial h \tag{17}$$

Results in:

$$-R(Lx - \frac{1}{2}x^2) = -Kbh + C \tag{18}$$

where C is an unknown constant. We can find C if we have a point where we know both x and h. For the conceptual model shown in Fig. 3 the hydraulic head at the left-hand side of the model $x = 0$ is fixed at a value of h_0. If we insert $h = h_0$ and $x = 0$ we get:

$$-R(L \times 0 - \frac{1}{2} \times 0^2) = -Kbh_0 + C \tag{19}$$

which reduces to:

$$C = Kbh_0 \tag{20}$$

Now that we have found C we can insert this back into our flow equation:

$$-R(Lx - \frac{1}{2}x^2) = -Kbh + Kbh_0 \tag{21}$$

Rearranging this in a more convenient form gives us an equation that predicts hydraulic head h at any distance x in the aquifer:

$$h = h_0 + \frac{R}{Kb}(Lx - \frac{1}{2}x^2) \tag{22}$$

Assignments

Set up a numerical model in a spreadsheet

We will make a numerical model that represents a simplified version of the typical global watershed. Construct a simple numerical model to calculate the hydraulic head (h) for the conceptual model shown in Fig. 3. Use the 1-dimensional form of the groundwater flow equation (eq. 10) and the following parameters:

Table 1: Model parameters

L (m)	b (m)	h0 (m)	R (m/yr)	K (m/s)	Δx (m)
5000	250	250	0.25	10^{-5}	250

The dimensions of our model aquifer represent the median value of a global compilation of watershed dimensions [*Gleeson et al.*, 2016] (Fig. 4), which is based on global stream network data by Lehner [2006]. The thickness is approximately equal to the thickness of the active groundwater flow zone derived from a global compilation of tritium isotope data from the same publication (Fig. 5). Tritium (^{3}H) is a radioactive isotope that was added to the atmosphere during nuclear testing in the 1950s and 1960s. Finding tritium in groundwater means that this groundwater is derived from precipitation that has infiltrated at some stage during the last 50 years. The value of recharge that we use is equal to the global mean recharge of approximately 0.25 m/yr [*Wada et al.*, 2014].

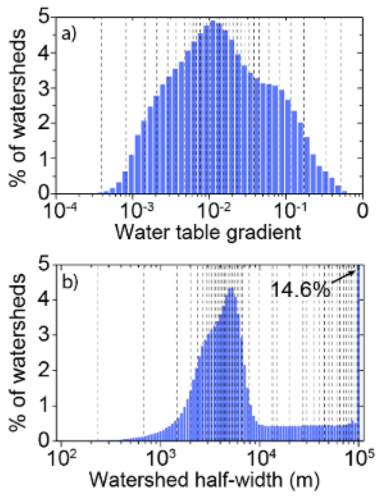

Figure 4: Global distribution of (a) watertable gradients, based on watertable data by Fan et al. [2013] and global elevation data [*Danielson and Gesch*, 2011], and (b) watershed dimensions

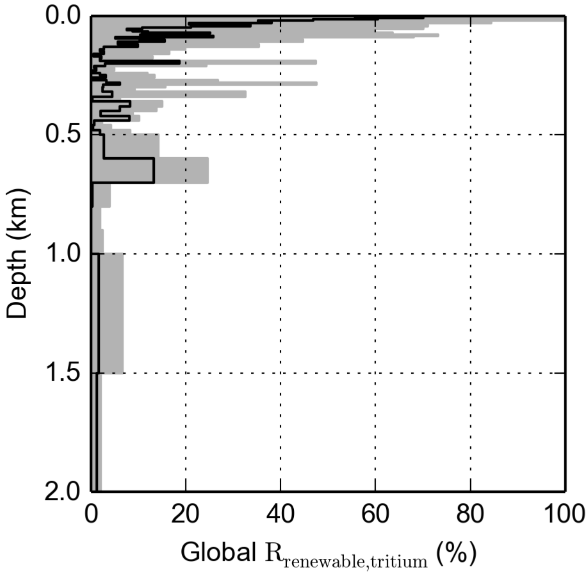

Figure 5: Distribution of renewable groundwater with depth, based on a global compilation of 3H data in groundwater [*Gleeson et al.*, 2016]

Calculate the dimensionless value of the source term

A slightly counterintuitive thing in the groundwater flow equation is that the units of the source term W are (s^{-1}); ie, the source term has no spatial dimensions. However, we would like to use the source term to model the effects of groundwater recharge, which is given in m/yr. To calculate the value of W for each grid cell we need to multiply the recharge by the width of each grid cell and then divide this by the area of a single grid cell: $W = \dfrac{R \Delta x}{\Delta x b}$.

Setting up a numerical grid

Start by setting up the x-coordinates of your numerical 'grid' as a column of numbers in a spreadsheet. For example, with a grid size (Δx) of 250 m this would be a column of numbers starting with 0, 250, 500, 750 m etc.. Now add a column for the numerical solution of the groundwater flow equation (eq. 10). The convenient way to do this is to add one column with the value of W, one column next to it with the value of $\frac{W b \Delta x^2}{K b}$ and another column with the calculated value of h (using equation 10). Note that $h(x)$ stands for the value of h at location x (and not h multiplied by x or something like this).

Boundary conditions

Your numerical solution is not complete yet. You have a solution for how the hydraulic head depends on the hydraulic head in each adjacent cell. However, we still need to tell the model what happens at the model boundaries. The next step is to add so-called boundary conditions. We will use two different boundary conditions at the left and right hand side of the model domain. At the left side of the domain we will maintain a specified hydraulic head that is equal to the waterlevel of the stream. We can add this condition by simply deleting equation 10 from the first row, and adding a fixed value of h in the first row.

For the right hand boundary we assume a no-flow boundary condition, ie. there is no groundwater flow accross it. Following Darcy's law, no flow (q=0) equals no change in hydraulic head: $\dfrac{\Delta h}{\Delta x} = 0$. We can implement this by simply assuming that the hydraulic head in the node to the right of the last node (outside the model domain) has an equal hydraulic head to the last node of our numerical grid. In excel we can do this by adding a new value below the last row that is always equal to the value at the last row.

For instance, the last row in your excel grid is in row 10, and your equations are in columnn D, then enter =D10 in cell D11. This will assure that the values in both rows are always the same.

Iterative solution

The solution has to be calculated iteratively in excel or any other spreadsheet software that you are using. To do so we first have to enable iteration in Excel or Libreoffice.

For Excel: Go to Options/Optionen -> Formeln -> Iterative berechnung aktivieren.

For Libreofffice: Go to Tools -> Options -> Libreoffice Calc -> Calculate and enable iterations.

Set the number of iterations to 10000 or higher if possible.

In most versions of Excel or Libreoffice pressing F9 triggers the recalculation of all formulas, try CMD + = on a Mac.

Your first model results

If all went well you should have a numerical solution of the hydraulic head at each point in your numerical grid. Now try to answer the following questions:

Question 1a: What is the hydraulic head at the right hand side of the model domain? Make sure you have the correct answer by comparing your numerical solution to the analytical solution.

Question 1b: Try to run your model with two more values for grid size (Δx) of 100 m and 50 m. In your opinion, which grid size would be sufficient for an accurate but also fast model of groundwater flow in this case?

Question 1c: What is the water flux Q to the stream? And what is this flux halfway the model domain?

Question 1d: What is the shape of the watertable? Why is the watertable not linear? Hints: try to think about how the flux (Q) changes over the model domain? Is it constant? And what is the relation between flux and hydraulic gradient in Darcy's law?

Question 1e Recalculate the hydraulic head using the global mean permeability of $10^{-13.5}$ m^2 [*Gleeson et al.*, 2011]. To do this, first convert permeability (k) to hydraulic conductivity (K) using the hydraulic conductivity equation: $K = \frac{\rho g k}{\mu}$. Look up typical values for the viscosity (μ) and density (ρ) of fresh water online (Wikipedia), or if you want to be more exact look up values in Batzle and Wang [1992] (see the literature list on stud.ip). Is the modeled value of hydraulic gradient in accordance with the hydraulic gradient data shown in Figure 4?

Simulate the effect of pumping

One major advantage of numerical solutions over analytical solutions is that parameters such as hydraulic conductivity or recharge do not have to be constant but can be varied over the model domain. We will use this flexibility to adjuist the source term (W) to simulate the effect of pumping on water levels. Add a pump at 1000 m distance to the stream. Use a well discharge that is exactly equal to the total amount of recharge that the aquifer receives (ie the recharge times the total length of the watershed). Note that the pumping rate in this case has the unit $m^2 s^{-1}$ because we are working in two dimensions, instead of three.

You can add a pumping well by modifying the column with the source term (W). For the grid cell (=row in your spreadsheet) that contains the pumping well (at x=1000 m) change the source term W to a value that is equal to recharge minus pumping at the location of the well. Again make sure to convert the units of pumping from $m^2 s^{-1}$ to s^{-1} by dividing the number by the area of one grid cell ($\delta x * b$).

Note that for this question you can use the original model parameters again (Table 1), instead of the hydraulic conductivity value of 1e.

Question 2a: What is the hydraulic head at the pumping node? And what is the hydraulic head at the watershed divide?

Question 2b: Is this value higher or lower than the level of the stream? What would be the long term consequence of pumping at this rate?

Model calibration

In many cases the exact value of model parameters such as hydraulic conductivity or recharge in a particular aquifer or geologic unit are unknown. One way to get around this is to first guess these parameters and then keep on adjusting the value of these parameters until the simulated hydraulic head are close to those observed in the field. This is called model calibration or inverse modeling.

Now assume that we have installed a borehole exactly at the watershed boundary at 5000 m distance of the stream. We measured the hydraulic head, which is found to be exactly 100.0 m above the level of the stream. Use this new information to estimate a new value of recharge, by calibrating your numerical groundwater model. Use the hydraulic conductivity value from Table 1 and vary the recharge to match hydraulic head in our observation borehole with an accuracy of 1.0 m or less. Also make sure you remove the pumping well that you have added for question 2.

Question 3a: What is the calibrated value of recharge?

In most cases the hydraulic conductivity and permeability are by far the most uncertain parameters, which can easily vary several orders of magnitude even in single geologic units. Now assume that the recharge value of 0.25 $m\,yr^{-1}$ provided earlier was correct and calibrate the hydraulic conductivity instead.

Question 3b: What is the calibrated value of hydraulic conductivity? Given this value, what type of material could the geologic unit consist of? Look up typical values for permeability in Gleeson et al. [2011].

Question 3c: Assume we only have information on the hydraulic head at one or more locations and no information on recharge and hydraulic conductivity. Can we estimate both parameters using our numerical model? Hint: Compare the shape of the watertable for questions 3a and 3b.

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