TRANSPORT OF POLLUTANTS – YEARS OR CENTURIES?

01004 Mathematics 1b - 2024

1 Purpose

Pollution is a global – and a local problem. Pollution from surrounding soil areas is transported to watercourses, e.g. via groundwater flow. The pollution can e.g. consist of pesticides sprayed on fields or, in rarer cases, non-recyclable waste located in so-called landfills. This pollution can pose a threat to the plants and animals that live in the water.

The purpose of this project is to analyse a simple model for how pollutants are transported by means of groundwater flow. Physically, such transportation is described by Darcy's law:

$$Q = -K_s \cdot A \frac{\partial h}{\partial x}$$

Darcy's law is similar to Ohm's law of electrical circuits, while K corresponds to the conductivity (resistance^{-1}) and A is a cross-sectional area. The pressure gradient $\partial h/\partial x$ drives the flow

Mathematically, the project deals with topics such as solving linear and non-linear differential equations for $h(x)$ via numerical and exact methods (e.g. via diagonalisation). In addition, it deals with the

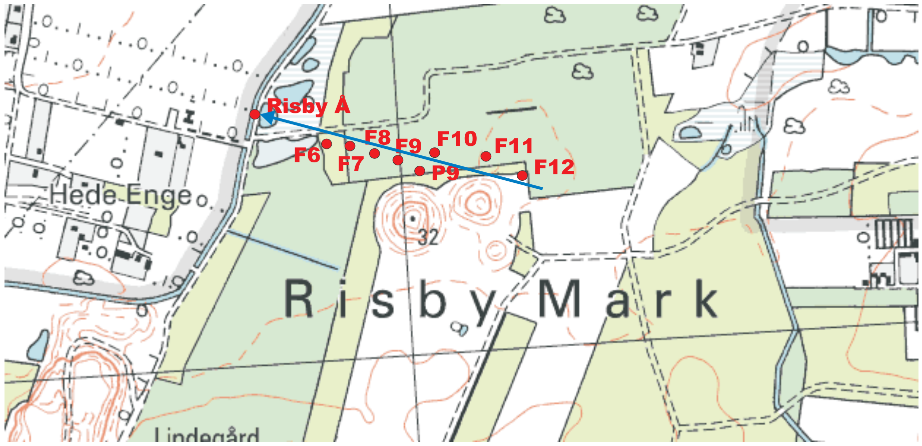

Figure 1: Map of the Vestskov landfill area. The three landfills are perceived as elevations in the landscape. Immediately north of the landfills is a transect of boreholes where the groundwater level is measured.

determination of the minimum for a function of several variables for adapting the model to measurement data.

With these results, one can answer the key question: how long does it take for the pollution to be transported down to the creek (ie. what is the removal time)?

2 Background

In the first part of the project, one has to examine how pollution is transported via groundwater flow. The example studied here is pollution to Risby Creek ("Risby å") in Vestskoven.

A map of the area by Vestskoven is shown in Figure 1 (top). In the area there are three landfills with deposits. Pollution has occurred in the area due to leakage from these landfills. In the area there are a number of boreholes where the groundwater level, or rather, the hydraulic pressure level is measured. Using these pressure levels one can outline the direction of flow of groundwater. Figure 1 thus shows the boreholes that will be used in this project. The groundwater flow is from borehole F12 past the landfills and towards Risby Creek.

Figure 2 (page 4) shows a sketch of the regional geology in the area. At the top is the area of approx. 2-4 meters of moraine sand, followed by approx. 18 meters of moraine clay. Limestone is found under this layer. A section through the local area is shown in Figure 3 (page 4). This cut is laid approximately along a streamline from F12 to Risby Creek. The figure shows the boreholes where the groundwater level (h, outlined in the figure) is measured. The figure also shows that there are two groundwater reservoirs. An upper secondary basic water reservoir (fine sand/silt), which is in contact with the nearby river (Risby), as well as a lower primary groundwater reservoir in the limestone used in the area for drinking water supply. The moraine clay separates the two groundwater reservoirs.

As outlined in Figure 3, there is a horizontal flow from the east of the landfills down towards Risby Creek (q in Figure 3). This is because there is a pressure drop down towards the river. At the same time, there is also a downward pressure gradient and flow (q_k) between the upper and lower magazine as the pressure level in the limestone everywhere can be assumed to be $H = 13.8$ m, i.e. below the pressure level in the upper section, where h is approx. 14–17 m along the cross section (the pressure is lower as water is drained from the lower reservoir). The pollution in the area has occurred next to drilling P9 (Figure 3). The pollution will therefore move horizontally towards the river – and vertically towards the limestone reservoir.

3 Data

Data for the area in Vestskoven are shown in Tables 1 and 2 (page 5). The net infiltration into the groundwater is 200 mm/year (it rains about 700 mm per year on average, but about 500 mm drains and evaporates). The thickness of the moraine clay can be set to $m = 18$ m and the pressure level in the limestone is constant $H = 13.8$ m.

A model for the pressure, $h(x)$, in the upper groundwater reservoir is set out below for the cross section shown in Figure 3. The cross section is $L = 500$ m long and the boundary conditions are given at maintained pressure levels. At $x = 0$ m, the pressure level is $h(0) = 14.00$ m and at $x = 500$ m, the pressure level is the same as in F12, ie $h(500) = 17.09$ m.

The two unknown parameters in the model are K_s and K_m , which are the hydraulic conductivities for the upper groundwater reservoir and for the moraine clay that separates it from the lower groundwater reservoir in limestone. In practice, hydraulic conductivity is determined experimentally.

On May 14, 1999, a number of pressure levels were measured, which are shown in Table 2. The cross section in Figure 3 is almost parallel to the east-west and Table 2 therefore shows the UTM (East) coordinates for the boreholes (UTM stands for Universal Transverse Mercator).

Problem 3.1

(a) Create a plot in Python of the data points given in Table 2, e.g. of $h(x)$ as a function of the distance to the river, x. The distance is calculated using the UTM coordinates. What are the conditions on the boundary values of h?

(b) What kind of nth-degree polynomial $p_n(x)$ can approximate the data points progress? Try e.g. to experiment with $n = 1, \ldots, 4$.

4 Physical model

This section sets out a physical model for determining the pressure drop h as a function of distance, x. Liquid flow in porous media is governed by Darcy's law:

$$Q = -K_s \cdot A \frac{\partial h}{\partial x} \,, \tag{4.1}$$

where Q is the water flow (measured in m^3/s), h is the pressure level (m), A is the cross-sectional area (m^2) and K_s is the hydraulic conductivity (m/s) of the water reservoir. A K-value therefore characterizes how well "the geology conducts water". Sand has a relatively high K-value ($\sim 10^{-4} - 10^{-3}$ m/s), while clay has a lower K-value ($\sim 10^{-7} - 10^{-6}$ m/s). A pressure gradient $\partial h \partial x \neq 0$ is required to facilitate a

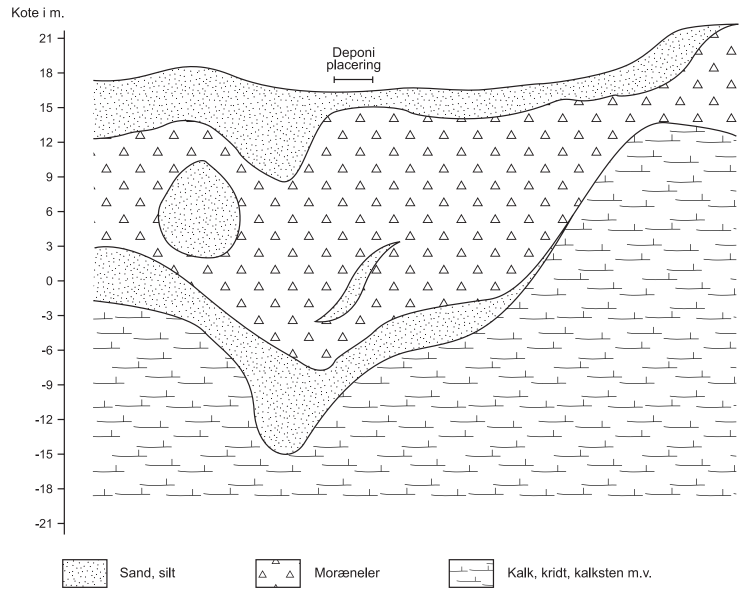

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Figure 2: Regional geology in the area. The landfill area is shown in the figure (”deponi”).

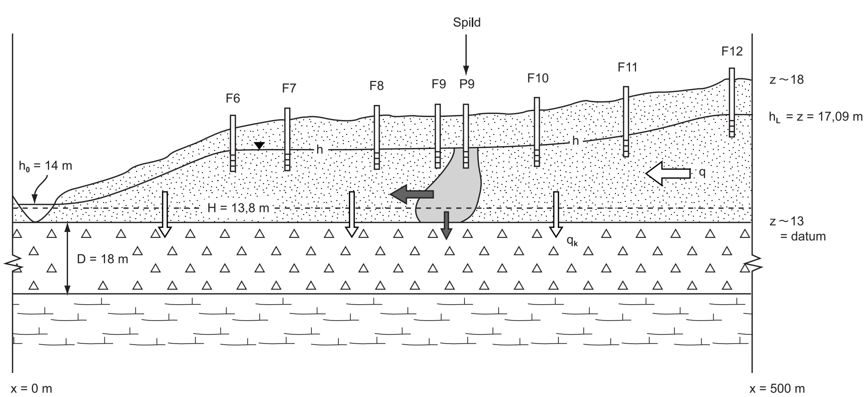

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Figure 3: Transect with local geology, boreholes and pressure levels in upper and lower groundwater reservoir.

Table 1: Data from Vestskoven

Parameter	Value	Unit
Net infiltration, N	0.2	m/yr
Datum, z_0	13	m
Thickness of moraine clays, m	18	m
Pressure level in limestone, H	13.8	m
Porosity in upper magazine, θ	0.21	-
Length of cross section, L	500	m
Fixed pressure, h_0	17.09	m
Fixed pressure (creek), h_L	14.00	m

Table 2: Observed pressure levels, h, and UTM-east coordinates.

Borehole	UTM-East (m)	Pressure level (m)
F12	333147	17.09
F11	333068	16.38
F10	333008	16.38
P9	332961	16.14
F9	332938	16.11
F8	332883	16.09
F7	332836	16.05
F6	332788	16.06
Risby Creek	332647	14.00

current, analogous to the fact that a potential difference is necessary to create a current in an electrical circuit

In principle, the area A is a function of three variables $A = A(x, y, z)$, ie it can change in horizontal and vertical direction. In the following, we only need to look at a one-dimensional model. Here we define the area to be $A = (1m \cdot d)$, where $d = h - z_0$ is the saturated layer thickness (m) in the sand, see Figure 3 (z_0 is datum, ie. reference point). In other words, everything is calculated in "per meter width". The cross-sectional area is therefore changed with the distance depending on whether the groundwater level changes. Hereby (4.1) is rewritten to

$$Q = -K_s \cdot (h - z_0)\frac{dh}{dx}\,. \tag{4.2}$$

The water flow Q is therefore non-linear with respect to h as there is a non-linear term $h\frac{dh}{dx}$ on the rhs. In the following, it is used that the Darcy velocity is defined as flow per total area, ie

$$q = \frac{Q}{A} = -K_s\frac{dh}{dx}\,. \tag{4.3}$$

A flow balance (total flow in = total flow out) can also be established for the control volume in Figure 4 (next page) which states that no liquid accumulates in the control volume,

$$-\frac{dQ}{dx}dx + Ndx - q_k dx = 0\,. \tag{4.4}$$

Here, N corresponds to the net infiltration on an annual basis (ie precipitation minus current evaporation, ie the part of the precipitation reaching down to the groundwater). The quantity N can be assumed to

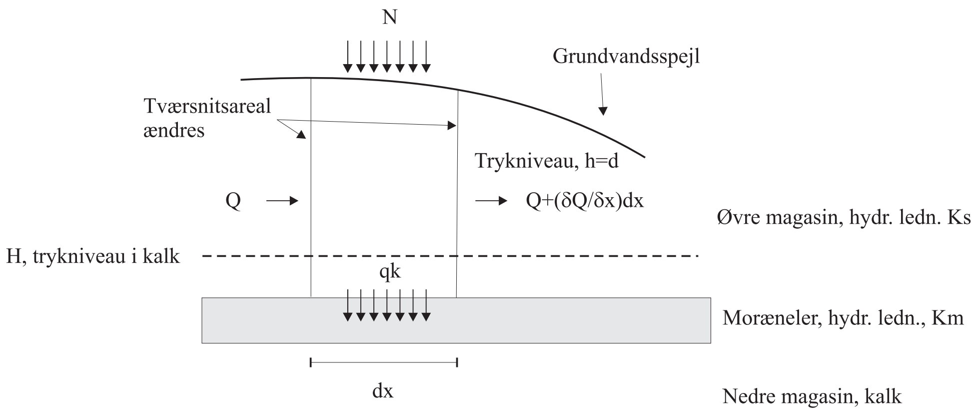

Figure 4: Control volume for setting up flow balance. The section is shown from the other side in relation to Figure 3.

be constant corresponding to a mean infiltration over a year, and q_k is the amount of water lost from the upper groundwater reservoir due too a gradient down towards the limestone. This amount of water is not necessarily constant. The pressure level in the limestone (H, see Figure 3) can be considered constant, but since the upper pressure level (h) varies, q_k will also vary, according to Darcy's law written in the vertical direction:

$$q_k = -K_m \cdot \frac{H-h}{m} \tag{4.5}$$

where K_m and m, are the hydraulic conductivity and the thickness of the moraine clay, respectively

5 Solving the differential equations

Problem 5.1

(a) Using the formulas from section 4, derive that the pressure drop $h(x)$ is determined by the differential equation

$$\frac{d^2\left((h-z_0)^2\right)}{dx^2} + \frac{2K_m}{K_s}\frac{H-h}{m} + \frac{2N}{K_s} = 0\,. \tag{5.6}$$

(b) What is the order of this differential equation? Why is it a non-linear differential equation? Consider what other conditions h must meet. It may be, for example, that h has specific values at the endpoints of the interval where we seek to determine h (called boundary conditions)

Problem 5.2

The differential equation (5.6) can not be solved analytically. Although one can not solve (5.6) directly, one can say something about what a possible solution would look like.

(a) Define $y(x) = h(x) - z_0$ and find an equation for $y(x)$ using equation (5.6). Specifically, one must show that $y(x)$ satisfies an equation of the form

$$y'(x) = \frac{1}{6y(x)}\sqrt{12Ay(x)^3 - 18By(x)^2 + 36C}\,. \tag{5.7}$$

Can Python solve this equation for $y(x)$?

(Hint: Write (5.6) in the form $(y^2(x))'' - Ay(x) + B = 0$, multiply the left side of (5.6) by $y(x)y'(x)$ and integrate on both sides)

Problem 5.3

One way to approach (5.6) is to look at different limits, where the solution is of a relatively simple form.

(a) First, assume that the solution to the differential equation (5.6) is a constant function $h(x) = h_K$ (even if it is contrary to the boundary conditions). Derive an expression for h_K in terms of the given constants.

(b) Assume that the solution is a linear function, ie. $h(x) = \alpha x + \beta$. Is there a solution $h(x)$ for equation (5.6) with $\alpha \neq 0$?

(Hint: insert the two different solutions in equation (5.6))

Problem 5.4

We now know that the desired function, $h(x)$, can not be a linear function, ie. a straight line, but must have a more complicated shape.

(a) Set the hydraulic conductivities to $K_m = 5 \cdot 10^{-8}$ m/s and $K_s = 3 \cdot 10^{-6}$ m/s and determine from this an approximate value for h_K in problem 5.3 given data in Table 1 (**in the table N is calculated in m/year, it should be converted to m/sec)**.

(b) Consider why the second term of the differential equation (5.6) must be small whenever $h \simeq H$. Solve the differential equation (5.6) in the case where the second term (proportional to K_m/K_s) is ignored, ie. find an exact solution in this case without the use of Python.

(Hint: If $(y(x)^2)'' =$ constant, $y^2(x)$ must be a quadratic polynomial)

Problem 5.5

One can simplify (5.6) by assuming that the cross-sectional area A in equation (4.1) is constant, ie. that (4.1) is modified to

$$Q = -K_s \cdot d_0 \frac{dh}{dx}\,, \tag{5.8}$$

where d_0 is a constant that e.g. is an average of $h - z_0$ along the transect of boreholes.

(a) Use equations (4.4) and (4.5) to derive that the resulting differential equation corresponding to (5.6), in this case is *

$$\frac{d^2(h-H)}{dx^2} - \frac{K_m}{d_0 \cdot K_s \cdot m}(h-H) + \frac{N}{d_0 \cdot K_s} = 0\,, \tag{5.9}$$

and that this is therefore a linear differential equation.

(b) What kind of differential equation is (5.9)? Solve (5.9) directly, using the known theory from Mathematics 1.

(Hint: first solve the corresponding homogeneous equation, then the inhomogeneous).

*Note that (5.6) is a differential equation for $h - z_0$, while (5.9) is a differential equation for $h - H$.

6 The model as a system of differential equations

As an alternative to solving a 2nd order differential equation (5.9), one can set up the model as a system of 1st order equations. The idea is to use the variables h and Q to write up a system of first-order differential equations, which is a model for the system, see equations (4.1) and (4.4). Note that these two equations express the horizontal flow and the vertical flow respectively. We assume that A is constant equal to d_0, thus replacing (4.1) by (5.8)

Problem 6.1

(a) Show that the system of differential equations (5.8) and (4.4) can be written in matrix form (you will also need equation (4.5)). Set up a set of equations of the following form,

$$\mathbf{y}'(x) = \mathbf{A}\mathbf{y}(x) + \mathbf{B}\,, \tag{6.10}$$

where $\mathbf{y}(x) = (h(x), Q(x))^T$, $\mathbf{y}'(x) = (h'(x), Q'(x))^T$ and $\mathbf{A}$ is a 2×2 matrix while $\mathbf{B}$ is a column-vector.

(b) What kind of system of differential equations is this, and what does the complete solution look like according to the theory?

Problem 6.2

Determine the solution to the corresponding homogeneous equation by diagonalizing $\mathbf{A}$, ie. $\mathbf{D} = \mathbf{P}^{-1}\mathbf{A}\mathbf{P}$, where $\mathbf{D}$ is a diagonal matrix and $\mathbf{P}$ is a square matrix determined by the eigenvectors of $\mathbf{A}$.

(a) Find the eigenvalues and the eigenvectors of $\mathbf{A}$. Start by showing that the eigenvalues are given by $\lambda_\pm = \pm\sqrt{\frac{K_m}{md_0K_s}}$.

(b) Then write the complete solution to (6.10) by determining a constant solution to $\mathbf{y}'(x) = 0$. The complete solution depends on $\lambda_\pm$ and on two unknown constants, which we call c_1 and c_2 .

Problem 6.3

We do not yet know the values of the hydraulic parameters from the given data. Therefore set $K_m = 5 \cdot 10^{-8}$ m/s and $K_s = 3 \cdot 10^{-6}$ m/s to begin with. Furthermore, set d_0 equal to the average of $h - z_0$ along the boreholes.

(a) Insert these values for K_m, K_s in the solution found and use Python to determine the two unknown constants c_1, c_2 using the boundary conditions for $h(x)$.

(b) Plot $h(x)$ and compare, if necessary, with the plot in problem 3.1.

(c) Try changing K_m and K_s by up to $\pm 10\%$ and see if this gives a visibly better approximation to the data points.

7 Determination of the hydraulic parameters

On the basis of data, it should be possible to find the values of the unknown hydraulic conductivities K_s and K_m by comparison with the model. When you have to "calibrate" a given model, you employ a measure of the error between model (function h) and measured data on the form

$$ERR = \left[\sum_{i=1}^{N} |h(x_i) - h_{\text{meas}}(x_i)|^p \right]^{1/p} \quad . \tag{7.11}$$

Here $h_{meas}(x_i)$ are the measured pressures in the positions $x_i, i = 1, \ldots, N$ (N is the number of data points). The power p is chosen depending on what you want to achieve; different choices of p correspond to different "sensitivities" to model deviations from data. In the following $p = 2$ is used.

Problem 7.1

(a) Determine values of K_s and K_m that make the error ERR as small as possible for the data listed in Table 2. For $h(x)$ the type of solution determined in problem 6.2 is used, ie K_m, K_s are varied slightly away from the original values and new values for c_1 and c_2 can then be determined by using the boundary conditions.

For example, one can calculate the error ERR at five points in the (K_m, K_s)–plane: first with the values in problem 6.3. Then change K_m by $\pm 10\%$ while maintaining K_s, and vice versa. One can also examine ERR as a function of K_m (maintain the value of K_s as $3 \cdot 10^{-6}$ m/s).

Problem 7.2

(a) Use Python to determine the nth degree polynomial $p_n(x)$ that best matches the data. Try with $n = 1, 2, ..., 8$.

(b) Calculate the error ERR for each of the eight polynomials in question (a).

Problem 7.3

There is a unique "Lagrange polynomial", which is the polynomial of degree $\leq n$ that goes through $n + 1$ given points (x_i, y_i).

(a) The data points in Table 2 consist of nine points. Determine the Lagrange polynomial that goes exactly through all points. Plot the Lagrange polynomial together with the data points, and calculate ERR.

8 Transport of pollutants

In the last part of the project, one must examine how quickly pollution is transported via groundwater flow.

Darcy's law (4.1) expresses the flow per total cross-sectional area, A. Since the area is made up of the grains of sand and pore space (the area between sand grains) the pore water velocity is defined as

$$v = \frac{q}{\theta}\,, \tag{8.12}$$

where θ is the porosity. The porosity is defined as the number of cubic meters of pore space per cubic meter totalvolume and is therefore less than 1. The pore water velocity is therefore greater than the Darcy velocity, q.

The average removal time in a piece of soil of a particle transported with the groundwater is found by expressing velocity as a derivative

$$v = \frac{dx}{dt}\,, \tag{8.13}$$

where x is the position of a particle after a given time, t. The removal time T of the particle over the interval $[x_1, x_2]$ is calculated as

$$T = \int_0^T dt = \int_{x_1}^{x_2} \frac{1}{v} dx\,. \tag{8.14}$$

If the pore water velocity is constant, it is especially obtained that the removal time in an interval of length l is

$$T = \frac{l}{v}\,. \tag{8.15}$$

This gives the simple result that the removal time is the length divided by the speed. In the case where v is not constant, the calculation becomes a little more complicated. It is possible to give an estimate of the removal time in the following way: the velocity between P9 and the creek can approximately be calculated using Darcy's law as,

$$|v| = \frac{K_s}{\theta}\frac{\Delta h}{\Delta x} = \frac{3\cdot 10^{-6}}{0.21}\frac{16.14-14}{314} = 9.7\cdot 10^{-8}\,m/s \simeq 3.1\,m/yr \tag{8.16}$$

This means that the removal time can be estimated at,

$$T = l/|v| = \frac{314}{3.1}\,yr = 101\,yr\,. \tag{8.17}$$

With proper integration, one will find that time becomes something else as the pore water velocity increases dramatically down towards the river due to the less saturated layer thickness, just as it is almost zero in the middle of the transect. To make this more precise, one finds $v(x)$ by differentiating the expression for $h(x)$, cf. equation (8.16), where $\Delta h/\Delta x$ is an approximation to the derivative. Then T is found by integration, cf. equation (8.14).

Problem 8.1

(a) Find the pore water velocity, $v(x)$, and thus the removal time T in the upper groundwater reservoir to the river, if the particle is "released" at landfill 3, corresponding to borehole P9. For $h(x)$ the solution used is determined in problem 6.3.

(b) What happens to the removal time if the particle "begins its journey" at borehole F6? For $h(x)$ choose the solution determined in problem 6.3.

Problem 8.2

(a) Consider whether these results are sensitive to the estimates of K_s and K_m. What happens to the removal times if the two parameters change independently with e.g. $\pm 10\%$?

Problem 8.3

(a) What happens to the removal time if you use the simple model from problem 7.2 (eg a cubic polynomial)? Is this model realistic?