

SaltSMART Project



Internship report

Hydrology of a waterwork Transport and retardation of Chloride in groundwater

Example of Elverum

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May 2011 - July 2011 <u>Supervisor</u>: Nils-Otto Kitterød

<u>Abstract</u>

The salt is more and more used in Norway for cars security during the snowing period. But this salt infiltrates easily into groundwater and we find salt in several pumping wells. To know the potential danger of road salt, to know its propagation and to think about solutions to avoid high concentration in wells, we present a case study of the Elverum water work. The approach used to model the Elverum aquifer can be applied for other groundwater works.

We introduce two physicals laws which are the Darcy Law and the Transport Equation. The modeling is made with software called COMSOL MULTIPHYSICS. In the first part we discuss the Darcy's Law and we explain the method used to get the velocity field into the aquifer and the drawdown of the aquifer. We study the influence of some parameters like the seasons on the results. In a second part, we present the method used to model the transport of salt into the aquifer and to get the concentration of salt into the well. There is too a part about the bioretention of salt by the vegetation and by sediments. This part of the study show how the retardation factor linked to bioretention can influenced the final result. Finally, we discuss the results and indicate some areas for further work.

<u>Thanks</u>

We would like to thank Nils-Otto Kitterød, our supervisor, for all his help, his motivation in our internship, his kindness and for the trust he had on us.

We thank Camille Join too. She prepared the input data for us and explained everything in detail. Thanks also for giving us a lot of valuable advices for our study and for our stay in Norway!

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Introduction

Background:

The climate in Norway forces the authorities to put a lot of salt on roads during the snowing period (from September to April approximately) to assure cars security. This amount of salt protects people but it is also a potential hazard for the environment.

According to European's Water Directive, the water's resources shall have good ecological status in 2015. To check if this directive will be violated, the Norwegian Roads Authorities initiated a research project to study the influence of roads salt application on the chloride concentration into Norwegian fresh water resources. This project is called the SaltSMART Project.

Purpose:

The purpose of this study is to observe the influence of the arrival of salt from roads to groundwater. To estimate the salt concentration inside these resources, we use the software COMSOL MULTIPHYSICS. This software is able to solve physical problems like the Darcy's Law and the Transport Equation.

With COMSOL MULTIPHYSICS, we modeled an aquifer which is corresponding to a real water work, the Elverum groundwater work. First, we study the Darcy's Law and look how the water is flowing into this aquifer. Then we look at the roads' location and study the Transport Equation to see if the salt put on the roads is going into the pumping well.

Plan and method:

In the first part we present the method used to model the aquifer. We introduce the Darcy's Law and the Transport Equation and explain the mechanisms on a simple example. In the second part we apply the physics seen in the first part to the Elverum groundwater work. Then in the third part we discuss the results and indicate how to improve the modeling.

We explain how we get the results, where we get the data and what method we use. All the software's operations are explained in this report, and the models are available on Fronter (UMB Website).

I. Method and materials

In this part we explain how we model the aquifer and how the equations are solved numerically. We also explain where the data we used come from. Most parts of these data are from the SaltSMART Project and prepared by Camille Jouin (Bioforsk).

1. The Darcy's Law Equation

To model the groundwater, the most realistic thing we can do is to use the Darcy's Law. To explain the equations we study a stationary experiment.

1) Darcy's Experiment

In 1856 Darcy, a French scientist, made an experiment where he found that the flow rate Q in a sand filter is proportional to the hydraulic head difference (hc-ha) and the filter's area A. Q is in inverse proportion to the filter's length L.



Figure 1: Darcy's experiment

With his experiment Darcy found the relation $Q = KA\left(\frac{\Delta h}{L}\right)$, where K is the hydraulic conductivity [m/s]. K changes with the material. This relation can be simplify to $\boldsymbol{q} = -\boldsymbol{K}\left(\frac{d\boldsymbol{h}}{dx}\right)$ where K is the hydraulic conductivity , $q = \frac{Q}{A}$ is the flowrate [m/s/m2] and $\left(\frac{d\boldsymbol{h}}{dx}\right)$ is the hydraulic gradient (no unit).

2) Continuity Equation and Laplace's Equation

The continuity equation is based on the fact that the total outflow is equal to the total inflow. If there is no recharge of the aquifer, the result of this simple assumption is **the continuity equation**: $\frac{\partial qx}{\partial x} + \frac{\partial qy}{\partial y} + \frac{\partial qz}{\partial z} = 0$

If the continuity equation is combined to the Darcy's Law, **Laplace's Equation** gives us the following result: $\frac{\partial^2 \cdot h}{\partial x^2} + \frac{\partial^2 \cdot h}{\partial y^2} + \frac{\partial^2 \cdot h}{\partial z^2} = 0$

These laws will be helpful to understand the next chapter.

3) Dupuit-Forcheimer Flow

a. Dupuit-Forcheimer assumption

In reality, the water is flowing in 3 dimensions. To solve problems in 3D seems is computer demanding. In 1886 the Dupuit-Forcheimer assumption proposes that the vertical gradient is very smaller than the horizontal gradient (which means that L>>H in the following figure):



Figure 2: Dupuit-Forcheimer assumption

It means that we can say that $\frac{\partial h}{\partial z} = 0$.

b. Poisson's Equation

Now we consider a Dupuit-Forcheimer Flow with a recharge N. We are in 2 dimensions. With this hypothesis, the continuity equation is $\frac{\partial Qx}{\partial x} + \frac{\partial Qy}{\partial y} = N$.

We have Qx = hqx and Qy = hqy. Combined to Darcy's Law, it is:

$$Qx = -Kh\left(\frac{\partial h}{\partial x}\right)$$
; $Qy = -Kh\left(\frac{\partial h}{\partial y}\right)$

We use a new variable $\varphi = \left(\frac{1}{2}\right) Kh^2$ and with this new variable, we have:

$$Qx = -\frac{d\varphi}{dx}$$
; $Qy = -\frac{d\varphi}{dy}$.

In the end, if we combine the Darcy's law with the continuity equation, the result is called the **Poisson's Equation**:

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} = -N$$

c. Unconfined Flow

Here, we study an unconfined aquifer and we consider a one dimensional flow with a constant recharge N:



Figure 3: One dimensional unconfined flow

The Poisson's Equation gives us $\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} = -N$. Here we have a one dimensional flow, along the x component. In these conditions, the Poisson's Equation is:

$$\frac{\partial^2 \varphi}{\partial x^2} = -N$$

It is this equation which is involved in the groundwater model we study here. In reality, the velocity field and the flow are along the components x, y and z, but it is more simple to consider this 1D example.

4) Equations in COMSOL MULTIPHYSICS

The purpose of this chapter is to present the equations according to COMSOL MULTIPHYSICS' conventions and compare them to the equations seen in the I.1.1, I.1.2 and I.1.3.

a. Equations in COMSOL MULTIPHYSICS

To see them, go on Darcy's Law->Equation.

Then you can see:

$$\nabla . \left(\rho u \right) = Qm$$

$$u = -\left(\frac{\kappa}{\mu}\right) \nabla P$$

If we replace u in the first equation, we have:

$$\nabla \left(\rho \left(-\left(\frac{k}{\mu}\right) \nabla P \right) \right) = Qm$$

In COMSOL the variable is the pressure P. In I.1.1 we studied equations where the hydraulic head was the variable. There is a simple relation between h and P: $h = z + \frac{P}{\rho g}$. If we put z = 0, we have

 $h = \frac{P}{cr}$. If we combine this relation with the COMSOL equation, we have:

$$\nabla \cdot \left(\rho \left(-\left(\frac{k}{\mu}\right) \nabla (\rho g h) \right) \right) = Q m$$

where:

- Qm is a mass source term [kg/(m³.s)]
- k is the permeability [m²]
- ρ is the density of the fluid [kg/m³]
- µ is the dynamic viscosity [kg/(m.s)]
- g the gravity [m/s²]
- h the hydraulic head [m]

In COMSOL, we can also choose between k = permeability $[m^2]$ and K = hydraulic conductivity [m/s]. If we choose the hydraulic conductivity, we replace $\frac{k\rho g}{\mu}$ by K in the equation. It becomes:

 $\nabla . \left(-\rho K \nabla h \right) = Qm.$

To have the same equation than in I.1.3.c., we need to do a little operation. We are going to transform hydraulic conductivity into transmissivity (see I.1.5.d.). The equation becomes: $\nabla \cdot (-\rho Kh \nabla \cdot h) = Qm \cdot h$.

Now Qm units is [kg/(m².s)]. In the data we have the runoff N (precipitation-evapotranspiration) in [mm/year]. So we will put $Qm = N * \rho$ to have the consistent units. With these operations the last equation becomes:

 $\nabla (-\rho Kh \nabla h) = N\rho$ and then $\nabla (-Kh \nabla h) = N$.

If we introduce the variable $\varphi = \left(\frac{1}{2}\right) K h^2$ we have:

abla.(abla arphi)=N.Then $oldsymbol{
abla}^2 oldsymbol{arphi}=-oldsymbol{N}$

If we consider a 1D flow, along the x component for example, we have exactly what we looked for: $\partial^2 \phi$

 $\frac{\partial^2 \varphi}{\partial x^2} = -N$

We can see that COMSOLMULTIPHYSICS's equations and the 1d equations are the same.

b. Simple study in COMSOL

Building the model

We want to study a simple model in COMSOL, and check the results by compare the results get by calculation by hand.

To simplify the study, we choose to work in two dimensions (*Model Wizard->2D*). The Physic involved here is a fluid flow and more particular the Darcy's Law (*Fluid Flow-> Porous Media and Subsurface Flow -> Darcy's Law*). We choose a stationary flow, which means that the flow is not dependent from the time (*click on Next and on Stationary*).

We run this study with a geometric form, which is here a rectangle (*Geometry->Rectangle*). Choose a 100x200m rectangle. Next we have to enter information to solve the Darcy's Law. We enter into the model the density and the hydraulic conductivity (*Darcy's Law->Fluid and Matrix Properties*). Put $\rho = 1000[kg/m^3]$ and K = 1e-4[m/s]*dl.H (we use here the transmissivity, see I.1.5.d.).

To have a constant hydraulic head, add a hydraulic head (*Darcy's Law->Hydraulic Head*), then select a boundary and put $H_0 = 10m$. In Initial Values (*Darcy's Law->Initial Values*), select all domains and put an initial hydraulic head of 10m.



Figure 4: Simple model on COMSOL

Now we need an inflow term, which corresponds to the runoff. Add a mass source term (*Darcy's Law->Mass Source*), select all domains and put $Qm = 1[m/year]*1000[kg/m^3]$.

COMSOL calculations

Run the study (*Study->Compute*) and watch the results (*Results->2D Plot Group and then 2D Plot Group->Surface*). Select all domains and enter dl.H (hydraulic head). The result is the next:



We can also see the results in one dimension (*Results->1D Plot Group->Line Graph*). Then select the boundary at y = 0 and enter dl. H:



Figure 6: Hydraulic head on simple model along a line

Check with calculations by hand

To check the model we solve the Darcy's Law for the simple case by hand. Darcy's Law gives us:

$$\frac{d\phi}{dx} = -Nx \text{ with } \phi = \frac{1}{2}kh^2$$

So we have:
$$\phi = -\frac{Nx^2}{2} + C$$
$$\frac{1}{2}kh^2 = -\frac{Nx^2}{2} + C$$
$$h^2 = -\frac{Nx^2}{k} + \frac{2C}{k}$$
$$h(x) = \sqrt{-\frac{Nx^2}{k} + \frac{2C}{k}}$$

We know that h(200) = H (the hydraulic head called H₀ in COMSOL), so $C = \frac{kh^2}{2} + N * 20\ 000$ Therefore we get:

$$h(x) = \sqrt{-\frac{Nx^2}{k} + H^2 + \frac{200^2N}{k}}$$

We calculate two values to check if we find the same results as COMSOL MULTIPHISICS.

•
$$h(0) = \sqrt{H^2 + \frac{200^2 N}{k}} = \sqrt{100 + 200^2 * 3,17.10^{-4}}$$

h(0) = 10,615 m

• $h(100) = \sqrt{100 + 200^2 * 3,17.10^{-4} - 3,17.10^{-4} * 100^2}$

h(100) = 10,465 m



Figure 7: Hydraulic head along a line

We find the same results by hand and with COMSOL MULTIPHISICS.

c. Conclusion

In studying a simple example, we were able to show that COMSOL do exactly what we expect. This software seems very reliable and efficient. We can trust what COMSOL do, and we are always able to check if the results are logical. If a problem appears, the most efficient thing is to go back to the simple model and understand why it is not working with a more difficult problem.

5) Others parameters

a. The Mass Source term

In our case, the mass source term corresponds to the runoff. The runoff is equal to the precipitation minus the evapotranspiration. The runoff on the area is a grid where the two first columns correspond to the coordinates, and the third corresponds to the runoff in each point [mm/year].

After import the grid "grid_runoff_mm_waterwork" on COMSOL, call it run. In Darcy's Law->Mass source, put Qm = run(x,y). Now, the mass source term is equal to the runoff. We supposed that all the water infiltrates into the soil.

b. Constant Head and Outflow Boundary

In the model, we have to enter a constant head, and to show where the water is going outside. In the model we consider that the outflow points are in the river. All the other boundaries are no flow boundaries.

River's location

To find this outflow boundary, we need to locate the river. This operation can be done on ArcView, where we can look at the river's coordinates. Then this coordinates points can be entered on COMSOL: the river is now digitalize on our model. This river's digitalization is an approximation but it is the best we can do.

Now we know where the water goes out. The next step is to find the hydraulic head in the river at this point. This hydraulic head has to be a constant, and we call it H_0 . On COMSOL, we can put a constant head only on boundary lines. The river has to be a boundary line. To do that, the only way is to cut our geometry in two parts. To do that we just need to plot a second line closed to the river's location.



Figure 8: River's location

The domain which represents the river is considered as an outflow area. The physics are not applied to the river in the model.

Constant Head

Then, H_0 can be found with the topography on COMSOL (see I.2.2.). We have to be careful with the data, because the topography's interpolation corresponds to DEM points on a 25m length. COMSOL does an interpolation which is not always corresponding to the reality. For example if we are in this case, the reality is not respected:



Figure 9: Error on topography into the river

To do the minimum of error, we choose to subtract a 1m head. The topography along the river is not a constant: we have to put different constant hydraulic heads in the model.

c. The bottom of the aquifer

The waterworks we work on are unconfined aquifers, which mean there is no non-porous layer on the top of the water table:



Figure 10: Unconfined aquifer

From Camille Jouin (Bioforsk), we have grids with the depth to the bedrock from the surface (d). From the topography's grids (see I.2.2.) we have the head from the sea level to the surface (z). To have the bedrock head (bot), we just have to put bot = z-d.

To see it in COMSOL, import the two grids *grid_estimated_depth_to _bedrock_model1_waterwork* and *grid_topography_from_dtm_waterwork* and call them *d* and *topo* (Annex 2).

Then add two Coefficient Form PDE to your model (*Model->Add Physics->Mathematics->PDE* Interface->Coefficient Form PDE). To have explanations about it, see the Annex 2. In the first put u(x,y) = topo(x,y) in the second put u2(x,y) = d(x,y). Then run the two studies and in the results, plot u-u2 (Results->2D Plot Group->Surface): you can see the bedrock on your area.

It is possible too to import a new grid which gives us directly the bedrock. This grid is called *grid_bedrock_amsl_waterwork*. The two first columns are the X and Y coordinates, and the third column is the distance from the sea level to the bedrock (bot).

d. The hydraulic conductivity

> From hydraulic conductivity to transmissivity

The hydraulic conductivity (K) is a major parameter in the Darcy's Law. It represents the soil's capacity to transport water and it units is [m/s]. On COMSOL, we have to specify to which head corresponds the hydraulic conductivity. To do that, we have to multiply K by the real hydraulic head. When doing that we transform the hydraulic conductivity in **transmissivity** (T). Transmissivity unit is [m2/s].

Influence of bedrock

On COMSOL, go on *Darcy's Law->Fluid and Matrix Properties* and change K to $K^*dl.H$. If we do that, COMSOL understand that K has to be applied from the sea level to the groundwater table level:



Figure 11: Wrong transmissivity

To apply the right transmissivity, import the grid *grid_bedrock_amsl_waterworks* and call it *bot*. Then put $K = K^*(dl.H - bot(x, y))$. Then the transmissivity is applied to the real hydraulic head.



Figure 12: Right transmissivity

But if you do that, the transmissivity will be the same for all the area. However there is exposed bedrock where bedrock can be higher than topography. These areas often correspond to mountains or high places. In these places, the hydraulic head is less high than the bedrock.

To translate that into COMSOL, we use a logical operator. The logical tool we need here is the <u>if</u> tool. Indeed, if (dl.H-bedrock) >0, we have to put $T = K^*(dl.H-bot)$ like in the figure 12. If (dl.H-bedrock) <0, then we have to put another value for K, for example K'.

If we look at the Darcy's Law, we have $q = -K \frac{\partial h}{\partial x}$. If q stays constant, then K' has to be smaller than K because in the bedrock the hydraulic gradient is higher. In the bedrock the water has a very small velocity field and the water's transport is very slow. So it is reasonable to put K'<K.



Figure 13: Influence of exposed bedrock on K

To implement this in COMSOL, go on *Darcy's Law->Fluid and Matrix Properties* and change the K. Put K = if((dl.H-bot(x,y)) <= 0, K'[m/s], K[m/s]*(dl.H-bot(x,y)).

6) Pumping well and drawdown

a. How to get the drawdown

When all the parameters for the Darcy's Law are set up, it is time to add the pumping well. We have now the good velocity, the good transmissivity and the good hydraulic head. The next step is to see how the well influences the groundwater flow, to find the size of the drawdown created by the well. To do that we go back to the simple model build in I.1.4.b. We add a pumping well (*Darcy's Law->Points->Mass Flux*) and enter the value Q_w [m³/s] we want to pump. This value has to be smaller than the value Q [m³/s] = Area [m²]*Runoff [m/s] (which corresponds to the water you add into the model). Choose for example Qw = 0.1 * Q.

Then run the Darcy's Law and look in the results how the well influenced the flow:



Figure 14: Influence of the well on the flow field.

We want to know the area influenced by the well. To get this area we look at particles. We want to know which particles are coming into the well. The best thing to do is to release particles into the well and look at the reverse run.

In COMSOL, add a little circle around the well (*Geometry->Draw Circle (center*)). Then run the study and look at particles tracing (*Results->2D Plot Group->Particle Tracing*). Select the circle around the well (Particle Positioning), in Expression select -dl.u and -dl.v then plot. We can now see the run for a particle which is coming into the well. Now we know the "drawdown" i.e. the area which is influenced by the well (red points represent the arrival of particles).



W represents the width of the drawdown [m]. If the flow is uniform, it is given by the relation $w = \frac{Qw}{Q0}$

Where Qw is the pumping rate $[m^3/s]$, Q₀ is an uniform flow $[m^2/s]$ and w is the width of the capture zone [m].

b. Influence of transmissivity on the drawdown

We study now the influence of the transmissivity or hydraulic conductivity on the pumping area. On figure 15 we put $T = 10^{-4} * h$ where h is the hydraulic head. We have a width of 20.5 m for the drawdown. The purpose of this paragraph is to look at the changes in the width of the capture zone with changing K. If we put the hydraulic gradient constant, change K will change the flow field u then it will change the capture zone.

So we need a constant hydraulic gradient: we put two hydraulic heads to have a constant flow field. For example, we put one hydraulic head of 12m and another of 10m and we will have

 $\frac{dh}{dx} = -\frac{2}{200} = -10^{-2} \text{[m]}. \text{ If we choose an hydraulic conductivity of } K = 10^{-4} \text{ [m2/s]}, \text{ the Darcy's}$ Law gives us $q = -K * \frac{dh}{dx} = 10^{-6} \text{ [m/s]}.$

The next step is to change K and look at the evolution of the width of the drawdown. The pumping rate is $Qw = 6.34e-5 [m^3/s]$ and we don't change the flow. The results are:



Figure 16: Width of capture zone with hydraulic conductivity

We can see that the evolution of w with K is not linear. The choice of K could be important to determine the capture zone of the well.

7) The Darcy's Law in a time dependant study

For the moment we studied the Darcy's Law in a steady state condition. The velocity field did not change with the time. But in reality it changes with space and time. Indeed the precipitations are not the same all the year, so the mass source term is not a constant term.

a. Equations in time dependant

The equations in COMSOL in time dependant for the Darcy's Law are:

 $\frac{\partial(\rho\varepsilon)}{\partial t} + \nabla . (\rho u) = Qm \text{ where } \varepsilon \text{ is the porosity.}$

$$u = -\left(\frac{k}{\mu}\right) \nabla P$$

These equations are not the same as a stationary case. The differences are the storage term $\frac{\partial(\rho\varepsilon)}{\partial t}$, and the mass source term Qm, which is a function of time Qm = Qm(t). In this case study we neglect the storagte term, but let the infiltration be a function of time Qm(t), which means that a change in Qm has immediate impact on the pressure in the aquifer.

b. The Mass Source term

As we said the precipitations are not constant all the year. To represent the reality we cut the year in 4 seasons. For each season we have a grid of runoff and this grid is named grid_runoff_mm_season_waterwork. The sum of the 4 grids corresponds to the grid grid_runoff_mm_year_waterwork. Change the mass source in the Darcy's Law means that you

change the hydraulic gradient and the velocity field. Indeed $q = u * n = -K(\frac{\partial h}{\partial x})$ where q is the mass source term [m/s], u is the velocity [m/s] and n is the porosity [no unit]. For each point in the space, the mass source term will change four times each year.

c. Study on the simple model

We put the same simple model as I.1.4.b but we study it in time dependant conditions. So *in Model Wizard* instead of choose *Stationary* choose *Time Dependant*.



Figure 17: Simple model on COMSOL

On this model we try to have a Darcy's Law in time dependant conditions. As we saw we need a time dependant mass source for that. We take for example the following mass source:



Figure 18: Mass Source term in time dependant

In COMSOL we need to specify there is a time dependant mass source term. We use the logical operator (if). We decide for example to run the study on one year. The winter corresponds to the period [0-7.884e6s], the spring to the period [7.884e6s-1.5768e7s], etc... Then the expression for Qm is

if(t<7.884e6||7.884e6<=t&&t<1.5768e7||1.5768e7<=t&&t<2.3652e7,if(t<7.884e6,0.5[m/year]*1000 [kg/m^3],if(7.884e6<=t&&t<1.5768e7,1[m/year]*1000[kg/m^3],1.5[m/year]*1000[kg/m^3])),2[m/ye ar]*1000[kg/m^3]). Let the other Darcy's Law parameters as previously: = $10^{-4} * dl$. *H* ; $\rho = 1000 \left[\frac{kg}{m_3}\right]$; put a hydraulic head of 10m on one boundary.

We want to run the study on one year. So we have to change the solver's parameters. Go on *Study*->*Step1: Time dependant* and change the parameters. Start at t = 0 [s] and stop at t = 3.15e7 [s]. Choose a time step of 86400 [s]. Then run the study.

Look at the evolution of the hydraulic head at x = 0 to see if it works (*Results->1D Plot Group-> Line Graph-> hydraulic head and time*).



ingule 151 inne dependant nyaraane neda at x = 0

We can see the hydraulic head's variations in the time. Each head modification corresponds to a mass source change. Another variable which is time dependant now is the velocity field. Indeed we can have a look at the velocity field at x = 200m:



Figure 20: Time dependant velocity field at x = 200m

With this simple study we show that it is possible to study the Darcy's Law in time dependant conditions. We can have time dependant hydraulic head and velocity field and it can change the capture zone of the well for example.

d. Impact on the drawdown

As we saw the size of the capture zone of the well is impacted by the velocity field. So if we have time dependant velocity fields we will have time dependant capture zones.

To see the impact of the time dependant velocity field on the capture zone, we study the simple model. To have more workable results we add some changes. The geometry is now a rectangle of 60mx30m. In the Darcy's Law parameters we keep the same K, the same hydraulic head and the same density as I.1.7.c. The pumping rate for the well is now:

 $Qw = -6[m/year]*1000[kg/m^3]*60[m]*30[m].$

We change also the mass source term. Now it is:

if(t<7.884e6||7.884e6<=t&&t<1.5768e7||1.5768e7<=t&&t<2.3652e7,*if*(t<7.884e6,20[*m*/year]*1000 [*kg*/*m*^3],*if*(7.884e6<=t&&t<1.5768e7,25[*m*/year]*1000[*kg*/*m*^3],30[*m*/year]*1000[*kg*/*m*^3])),50[*m*/ *year*]*1000[*kg*/*m*^3]). It looks like that:



Figure 21: Mass Source term with high runoffs

We choose very high values (which are not realistic we know) because with these values the velocity fields are higher. We need high velocity fields to be able to compare the capture zone for the four seasons. We have four different velocity fields, so we will have four different capture zones.

Run the study and look at the drawdowns (*Results->2D Plot Group->Particle Tracing*, then select –*dl.u* and –*dl.v*; see I.1.6.a). Plot the drawdowns for the 4 seasons:



Figure 22: Drawdowns for the four seasons

The blue one corresponds to the winter, the black one corresponds to the spring, the red to the summer and the green to the autumn. We see that the size of the capture zone increases with the decreasing values of runoff i.e. of velocity fields.



Figure 23: Width of the capture zone with different runoffs

e. Impact on the real model

To have a real impact of a time dependant velocity field on the capture zone we used high values for the runoff. But if we use the real runoff it will not be the same. Indeed the runoff's variations between the seasons are not so high. We can quantify this difference in 1e2 [mm/year]. So **the width of the capture zone will be not so impacted**.

2. Definition of the catchment area

In this part we explain the method we used to define the catchment area of the waterworks.

1) Boundary condition on the size

The first thing to do is to be sure that the area we are going to find is big enough. Indeed, the area's boundaries do not have to be influenced by the well. In our model, the boundaries of the area are considered as a no flow condition. So if they are a no flow line, they do not have to be influenced by the well. We have to check this condition in a first part, with simple models.

In order to find it, we try simple models on COMSOL MULTIPHISICS. We use the same model as in I.1.4.b.and we add a pumping well. For symmetric reasons, the well has to be in the middle of the model.



a. Method

The purpose of the experiment is to know if the boundaries of the area we defined are influenced or not by the well. So we have to look the boundaries and watch if the streamlines along these boundaries change or not. To do that, we have to add a new bigger area around our current area, and then we could watch the streamlines along the old area.

COMMENT:

• When the streamlines are convergent to the point, it is a pumping well (this is what we have).



Figure 25: Pumping well (Reference: Class course of M.WANKO)

• When the streamlines are divergent to the point, there is an injection well.



Figure 26: Injection well (Reference: Class course of M.WANKO)

b. Influence of the pumping rate

First we study the influence of the pumping rate. With our model we try different pumping rates. We call N the runoff, A the surface, Qt = NA the total flow and Qw the pumping flow.

To input a well into the model we add a *Mass Flux* in the *Darcy's Law (Darcy's Law->Mass Flux)* which is:

 $N_0 = -\alpha^* N[m/year]^* density[kg/m^3]^* A[m^2]$

We study three cases:

> Qw = 0.01Qt (α=0.01)







> Qw = 0.1Qt (α =0.1)

Figure 28: Hydraulic Head with Qw=0.1Qt

The pumping has a little influence on the catchment area.

Qw = 0.5Qt (α=0.5)



With this pumping rate the well influenced a lot the groundwater.

c. Influence on streamlines

The next step is to increase the area. We let Qw = 0.5Qt constant and add a bigger area around our area. We choose a 400mx200m rectangle, and watch the streamline along the old area (200mx100m):



Figure 30: Streamline for Qw = 0.5Qt

We can see that the old area is influenced by the pumping well if we keep this pumping rate. Then we have two choices: change the size of the area or change the pumping rate.

Influence of the pumping rate

We decide to keep the same area and change the pumping rate. If we apply Qw = 0.1Qt, we have this streamline:



Figure 31: Streamline for Qw = 0.1Qt

The boundary is still influenced by the well, but this influence is very small in this case.

- Influence of the area
 - Area 2 = 300mx150m

Now we have to find a new area which will not be influenced by the well. This area should be bigger than the old area. For example we can choose a 300mx150m rectangle. We keep the 400mx200m area around this new area.

We can look at the streamline's deviation for Qw = 0.5Qt:



Figure 32: Streamline for Qw = 0.5Qt

The area is still influenced by the well. Indeed the streamline is not horizontal and don't follow the line.

We can look now for a smaller pumping rate if the catchment area is influenced by the well. For example we can choose Qw = 0.1Qt.

The result is:



Figure 33: Streamline for Qw = 0.1Qt

There is a minimal deviation of the streamline. For a 300mx150m area, the maximum pumping rate is almost Qw = 0.1Qt. If we increase the pumping rate, the influenced area will be bigger. If we find some different couples "pumping rate/size of the area which is influenced", we could be able to find a relation between this two data.

Area 3 = 600mx300m

We are looking for the size of the area which is influenced by a pumping rate of Qw = 0.5Qt. We take an area of 600mx300m and watch like before the evolution of the streamline:



Figure 34: Streamline for Qw = 0.5Qt

We can see that the deviation is very low. For an area of 600mx300m, the maximum pumping rate is almost Qw = 0.5Qt

For different pumping rates and different geometries we can do the same things:

$Qw = \alpha Qt$	0.01Qt	0.1Qt	0.2Qt	0.5Qt
Min area (Lxl) with L = 2l	100x50	300x150		600x300
Min area (Lxl) with L = l	75x75	200x200	400x400	500x500
Min area with L = 1.5l		300x200		525x350

Table 1: Minimum area according to the pumping rate

d. Conclusion

Now we have a relation between α and the area A. For each well we have the pumping flow Qw and the runoff. To protect the groundwater, α has not be higher than 0.1.

With the relation $Qw = \alpha RA$ we can find A. Then with the table 1, we can find the minimum area we need.

We can take the example of Elverum: $Qw = 2\ 098\ 467\ m3/year$ R = 0.520m/year $\alpha = 0.05$ The area is A = 81km2 = 9kmx9km. Ac

The area is A = 81km2 = 9kmx9km. According to the table 1, we need at least an 8.4kmx8.4km. To be sure, we take a 10kmx10km area and check the results on COMSOL. The study does not show any deviation along the boundaries: a catchment area of 10kmx10km is big enough to imitate Elverum's area on COMSOL. This area will not be influenced by the well, and the boundaries could be considered as no flow conditions.

Example of Gol: Qw = 564 651 m3/year R = 0.855m/year α = 0.05

The area is A = 13.2km2 = 3.7kmx3.7km. According to the table 1, we need at least a 5.4kmx5.4km. To be sure, we take a 7kmx7km area and check the results on COMSOL. The study does not show any deviation along the boundaries: a catchment area of 7kmx7km is big enough to imitate Gol's area on COMSOL. This area will not be influenced by the well, and the boundaries could be considered as no flow conditions.

2) Definition of the catchment area using topography

With the data collected from Camille Jouin, we could make a topography grid on ArcView (Annex 3). This grid has three columns: X (m), Y (m) and meters amsl (m). The two first columns correspond to the coordinates of a point, and the third represents the topography of this point. There is 25m between each point. For each well, there is a grid of points which are around the well. For example, the Elverum's grid size is 14800mx18725m.

On COMSOL Multiphysics, we can import this topography grid (Annex 2), and then we can have the topography in three, then in two dimensions (*Results -> 2D Plot Group -> Surface*). With the option Contour (*Results -> 2D Plot Group -> Contour*), we can see the level lines on our surface.

This result is very useful to find the catchment area. Indeed we know that the streamlines are perpendicular to the level lines. Here we just have the topography lines, but we consider that the groundwater is following the topography. After printing the level lines and find the catchment area by hand on a paper, we can digitalize it on COMSOL.

When we found this area, we have to make sure that it is big enough. We have to respect the conditions from I.2.1.
3. The Transport Equation

Thanks to the area we estimated we can study the arrival and the propagation of the salt inside the catchment area. For that we use COMSOL MULTIPHISICS to solve the Transport Equation (Equation in 1D):

$$\frac{\partial c}{\partial t} = -\frac{u}{R}\frac{\partial c}{\partial x} + \frac{\partial}{\partial x}\left(\frac{1}{R}.D.\frac{\partial c}{\partial x}\right) + \frac{\Gamma}{nA}(cin-c) - \lambda c$$

We can see that the concentration is changing in time and in space. In COMSOL we study it in 2D, but in the calculations and explanations of the equations we will study it in 1D only.

1) The transport equation

The transport equation works with different terms such as the convection term, the diffusion term, the source term and a degradation term:



Where:

- u is the velocity field [m/s].
- R is the retardation factor (due to the adsorption in the main part)(no unit). We will study this parameter in a specific part (see I.3.4 and I.3.5).
- D is the hydrodynamic dispersion $[m^2/s]$. D = Dm + Dl where Dm is the molecular diffusion and Dl is the longitudinal dispersion. In general Dm<<Dl.
- Γ is the infiltration intensity $[m^3/s/m^2]$ which is approximate by the runoff [m/s].
- Cin is the initial concentration of the groundwater (in salt here) [kg/m³]
- λ is the decay [s⁻¹]. It is often due to chemical reactions. Here we consider that we have not any reactions into our model. We put $\lambda = 0$.

We will try to solve it by hand on a simple model and after compare it to COMSOL results, like we did on the Darcy's Law.

2) Equation and checking in COMSOL

We want to check the COMSOL's equations. In COMSOL, the module which corresponds to the transport equation is the *Transport of Diluted Species Module*. If you look at the equation on COMSOL, there is:

 $\frac{\partial c}{\partial t} + u\nabla c = \nabla (D\nabla c) + R$

It is exactly the same equation as previously. The mass source is R $[mol/(m^3.s)]$, D is the coefficient diffusion $[m^2/s]$ and u is the velocity field [m/s].

a. Analytical solution "by hand"

In 1 dimension, the general solution to the transport equation is:

$$c(x,t) = \frac{\Delta M}{(4\pi)^{\frac{1}{2}} * nbm * (\alpha L * u * t)^{\frac{1}{2}}} * \exp(-\frac{(x-ut)^2}{4 \alpha L * ut})$$

Where:

- c(x,t) is the concentration of salt [kg/m³] or [mol/m³]
- ΔM is the quantity of salt introduce into the model in one point [kg] or [mol]
- m is the hydraulic head [m]
- u is the velocity field [m/s]
- n is the porosity
- b is the length of the line we look at [m]
- αL is the longitudinal dispersion [m]

We apply this solution on a simple model. We are in 2D and we have a rectangle of 100mx200m. We consider a velocity field only along the x-component. The parameters are:

- n = 1
- b = 100 [m]
- m = 1 [m]
- αL = 1 [m]
- ΔM = 4372 [mol]

We add salt in x = 0 [m] and we monitor what happen in x = 100 [m]. We start our study at t = 0 [s] and we stop it at t = 2e7 [s]. The time step is $\Delta t = 1e6$ [s]. We supposed there is no salt into the model at the beginning (c(x,0) = 0 [mol/m3]).



Figure 35: Transport equation on a simple model

For each time step, we calculate with an Excel function the concentration c(100,t). Then we "accumulate" the results which means we put c(100,t_i) = $\sum_{j=0}^{i} c(100, t_j)$. We called this graph "cumul":



Figure 36: Concentration with time by hand

The red curve represents the "accumulate" function. The value which is reach is $C_0 = 0.219 \text{ [mol/m}^3\text{]}$.

b. Calculations in COMSOL

Building the model

The Darcy's Law

We want now check if COMSOL is doing the same calculations. To do that we build the same model as in I.1.4.b. We choose the same geometry.

We add a Darcy's Law to our model and we enter the following parameter:

- K = 1e-3 [m²/s]
- $\rho = 1000[kg/m^3]$
- We add an hydraulic head on the first boundary H1 = 12m
- We add a second hydraulic head on the second boundary H2 = 10m

We add two different hydraulic heads to have a constant velocity field. Indeed thanks to the Darcy's

Law, we have: $q = -K\left(\frac{dh}{dx}\right)$.

We know that q = u * n where n is the porosity and u the velocity field [m/s]. With our parameters, we have: $u * n = -0.001 * (\frac{2}{-200})$. If n = 1 we have $u = 1 * 10^{-5}$ [m/s] exactly as we want.

Then run the study and look at the results (*Results->2D Plot Group->Surface->dl.u*). You can see that the velocity field is constant to 1e-5 [m/s] everywhere.

The transport equation

The next step is to add the transport equation. To do that we add the correspondent physics (*Model*->*Add Physics->Chemical Species Transport->Transport of Diluted Species*) and choose a time dependent study.

Now we have two studies: one stationary for the Darcy's Law and one time dependant for the Transport Equation. We have to specify to COMSOL this characteristic.

To do that go on the solver's parameters (*Study->Step1*) and select only the dependant variables you want to be solve. For the stationary study, select only the Darcy's Law. For the time dependant study select only Transport of Diluted Species.

To solve the Transport Equation we need the velocity field from the Darcy's Law. To specify it to COMSOL go on the time dependant solver's parameters (*Study->Solver Configurations->Solver1->Dependant Variables*) and for Values of Variables Not Solved For select Solution in the Method node. Then select the solver corresponding to the stationary study (Solver1 normally). The software will understand that the velocity field will come from the Darcy's Law with this operation.

The last thing to do is to set the Transport of Diluted Species parameters (*Transport of Diluted Species->Convection and Diffusion*). Put u = velocity fields (dl1/dm) and Dc = 1e-5 [m²/s]. Then add an Inflow (*Transport of Diluted Species->Inflow*) and put C₀ = 0.2185 [mol/m³]. Choose C = 0 as initial value (*transport of Diluted Species->Initial Values*) on all the domains.

To compare the results with the hand calculations, we have to put the same time step. Go on the Time dependant solver (*Study->Step1: Time Dependant->*Study Settings) and choose to start at t = 0 [s] and to stop at t = 2e7 [s]. Select a time step $\Delta t = 1e6$ [s].

Results in COMSOL

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Then compute the time dependant study and look at the results. Plot the concentration with time along the line corresponding to x = 100m (*Results->1D Plot Group->Line Graph->concentration*).



Comparison between hand calculations and COMSOL results

We can now compare the two results. We export the data from COMSOL in a grid (see Annex 4) and we open it with Excel. We can now plot the two graphs on a same figure:



Figure 38: Comparison between hand calculation and COMSOL results

We can see that the two curves are closed. The difference between these two graphs can be explained by the numerical dispersion.

Advective part

The advective part in the transport equation is due to the term $-u * \frac{\partial c}{\partial x}$. If we consider just the advection, we have $-u * \frac{\partial c}{\partial x} = \frac{\partial c}{\partial t}$. If we look at the concentration at the point $t = \frac{x}{u}$ we will have normally $c\left(x, \frac{x}{u}\right) = \frac{c0}{2}$ if C₀ is the concentration added at x = 0. In our case, C₀ = 0.2185 [mol/m3] and the point $t = \frac{x}{u}$ corresponds to $t = \frac{100}{1 \times 10^{-5}} = 1 \times 10^{7}$ [s]. In the hand calculations, we find c(100,1e7) = 0.13 [mol/m3] and in the COMSOL results, c(100,1e7) = 0.108 [mol/m3]. We should find c(100,1e7) = 0.109 [mol/m3]. The both results are closed to the good value, and the COMSOL results seem better than the hand calculations!

Numerical dispersion

The numerical dispersion is due to the calculations in a model; indeed we can have more or less precision in a calculation. In COMSOL MULTIPHYSICS this precision is linked to the mesh which corresponds to the precision of the space step. We can have an extremely coarse mesh with a very big space for each calculation or at this opposite a very small mesh. The difference between these two meshes is the numerical dispersion:



Figure 39: Numerical dispersion in COMSOL MULTIPHYSICS

To minimize this numerical dispersion we change the mesh. Δx is the size of the mesh and thanks to the Gridpeclet number, we know that $\Delta x \leq 2\alpha L$. In our case we know that $\alpha L = 1$ so the Δx has to be smaller than 2 meter. It is corresponding to the finest mesh (extremely fine mesh).

Conclusion

Exactly like with the Darcy's Law, the software COMSOL MULTIPHYSICS is solving the Transport Equation as we want. Simple tests on simple models allow us to be sure of that and we are confident that we are using the software according to our intentions.

3) Building the real model

We can now start to build the real problem and try to solve the Transport equation with more complicated water works. For that open the previous file with the Darcy's Law and adds the transport equation node (*Model->Add Physics->Chemical Species Transport->Transport of Diluted Species*).

a. Convection and Diffusion

This part refers to the parameters for the advection (or convection) and diffusion. In COMSOL it is in *Transport of Diluted Species->Convection and Diffusion*. You have two main parameters to adjust in this node.

The first parameter is the velocity field. We have to specify to COMSOL that we want to take the velocity field from the Darcy's Law (look at I.3.2.b.).

The second parameter is the Diffusion Coefficient which gives the importance of the diffusion in our model. For the testing model, we consider $D_L = \alpha L^* u$. where D_L is the longitudinal dispersivity. So we had $D_L = 1e-5 \text{ m}^2/\text{s}$. We can compare the previous result with different values of the diffusion coefficient Dc:



Figure 40: Influence of the diffusion coefficient in COMOSOL MULTTIPHYSICS

The diffusion coefficient has a big influence on the result and the value of 1e-5 seems to be adapted for this test.

Nevertheless in the real case, this previous value is no more adapted because we are working is a bigger area and a Dc of 1e-5 will give negative values of concentration. So to have good results we need to increase the diffusion coefficient. Therefore we study the curve of concentration with time for different Dc. The best result is obtain for $Dc = 1e-3 [m^2/s]$, so we will use this value for the real case of Elverum.

b. Salt application

We need now to import the salt into the model. In reality the Road Salt Authorities are putting salt on the road. So the roads have to be digitalized. For that we use the same method as we did for the river: look at the coordinates of the roads which are closed to the well on ArcView and enter these coordinates on COMSOL.

When the roads are added to the model the next step is to add salt on these roads. From the Road Salt Authorities we have the mass of salt put on the road per kilometer. Thanks to Camille Jouin (Bioforsk) we have too a grid of salt for each water work. This grid gives us the tons of salt per year put on each 25[m]x25[m] grid and is called *grid_roadsalt_ton_per_year_waterwork*.

This grid does not give a constant salt application along the road. For example if we import a grid of salt for Elverum's water work into COMSOL (Annex 2) and if we plot the salt along a road, we can see big variances:



Figure 41: Salt application along a road for Elverum

If the capture zone of the well intersects the road on the area 1, the salt will be overestimated. If it intersects the road on the area 2, it will be underestimated.

To avoid these mistakes we decide to take an average value of salt per kilometer. On Excel open the grid *grid_roadsalt_ton_per_year_waterwork* and sum all the values. The result is the total salt applies on the roads, we call it M [t/year]. On COMSOL measure the total length of the roads for the area and call the result L [km]. Then do $dM = \frac{M}{L}$. dM unit is [t/year/km] and it represents the amount of salt per kilometer of road for the water work.

Now if we want to know how many salt we applied on a road section, we just have to pick up the length of the road l and do m = dM * l. We will have the mass of salt apply on the road.

c. Mass flux

According to the capture zone defined above (I.1.6.a.), we can estimate the mass flux which arrives on the well and compare it to the mass flux from the road. We digitalize the drawdown on COMSOL MULTIPHYSICS and we calculate its area thanks to the software (*Results -> Derived Values -> Surface Integration*). We also estimate an average of the runoff and of the background (atmosphere) concentration in this area. We have:

Area of the capture zone	А	m2
Average of the runoff	\overline{N}	m/s
Average of the background concentration	(Cback)	g/m3

We have the mass flux from the atmosphere:

Mf (Atmosphere) = $\overline{Cback} * A * \overline{N}$

We know that we have dM [t/year/km] in our catchment area (I.3.3.b.). Next we observe that the part of the road which can impact the well has a length of l [m] (part of the road which crosses the drawdown), so we calculate the massflux of salt from the road:

$$Mf(Road) = dM * l$$

Then we have to compare the two mass fluxes to see if it is the road or the atmosphere that bring the most part of the salt into the well. The results for Elverum are presented on II.3.1.a.

d. Inflow

In the node *Transport of Diluted Species*, we choose the velocity from the Darcy's Law (we work on the same model as I.1.4.b) and a diffusion coefficient of 1e-3 $[m^2/s]$ like we saw in I.3.3.a. We use the mass flux from the road m = dM * l and the velocity on this part of the aquifer to have an inflow in $[mol/m^3]$. The velocity is obtain on COMSOL by integrate the velocity on the line which is corresponding to the road (see annex 5). The result is u $[m^2/s]$ but we work with the transmissivity in the Darcy's Law (see I.1.5.d) so the result is already multiply by the hydraulic head and it is equivalent

to a flow in [m³/s]. So we enter:
$$Inflow = \frac{m \left\lfloor \frac{v}{y} \right\rfloor}{58 \left\lfloor \frac{g}{mol} \right\rfloor * u \left\lfloor \frac{m^3}{s} \right\rfloor}$$
.

We know the concentrations into the well measured between 1984 and 2010. We compute the model during several years to observe the concentration with the time and to compare it with the real measures. To specify that we add the salt only during the winter (three months) we use again the <u>lf</u> tool. For example for 10 years of adding salt, enter the following expression: $if(t<=7.88e6||3.15e7<=t\&&t<=3.94e7||6.31e7<=t\&&t<=7.1e7||9.46e7<=t\&&t<=1.02e8||1.26e8<=t\&&t<=1.34e8||1.58e8<=t&&t<=1.66e8||1.89e8<=t&&t<=1.97e8||2.21e8<=t&&t<=2.29e8||2.52e8<=t&&t<=2.6e8||2.84e8<=t&&t<=2.92e8,m[t/year]/58[g/mol]/u[m^3/s],0).$

4) <u>Retardation factor by sediments</u>

In the Transport Equation we didn't include a retardation factor which represents the adsorption of salt in the area. This salt can be catch by sediments or by plants and release later, so we will have decay in the flux of salt. In this part we present thinking with data from Elverum's waterwork. This data can be taken as example.

a. Type of soil

The aquifer of Elverum is for a main part constituted of sand and gravels. The following graph allowed us to estimate the porosity of the area:



Figure 42: Estimation of the porosity

Source: Class course of M. WANKO

So we choose a **porosity of 0.37** and the density is estimated like the average of the sand density (1600 kg/m3) and the gravel density (1450 kg/m3). So we choose a **density of 1525 kg/m3**. The salt content of the soil can be estimated with the electrical conductivity, the pH and the Sodium Absorption Ratio (SAR). The SAR is given by the ratio of sodium and calcium plus magnesium.

Some samples were made in the Elverum's well and all the chemical parameters were studied. We make an average of parameters we are concerned on:

рН	Electrical conductivity (mS/cm)	Cl (mg/L)	Mg(mg/L)	Na (mg/L)	Ca (mg/L)
6.89	4.52	2.66	1.12	1.78	4.55

Table 2: Average of the chemical parameters in Elverum's well

So the SAR of the soil is : $SAR = \frac{Na}{(Ca+Mg)} = 0.31$.

According to the following table, all the parameters from these samples show that we are working with a **saline soil**.

Electrical Conductivity* (mmhos/cm)		рн	Sodium Adsorption Ratio* (SAR)
Saline soil	greater than 4	less than 8.5	less than 13
Sodic soil	less than 4	8.5 to 10	greater than 13
Saline-Sodic soil	greater than 4	less than 8.5	greater than 13

 Soil chemistry measurements used to classify saline, sodic and saline-sodic soils,

 Source: http://www.ag.ndsu.edu

b. Partitioning coefficient

The partitioning coefficient Kp is the ratio between the salt adsorbs by the sediments and the salt which is added. So in our case we can define Kp like:

$$Kp = \frac{Kilo \ of \ salt \ adsorbs \ by \ kilo \ of \ sediments}{Kilo \ of \ salt \ add \ by \ m3 \ of \ sediments} = \frac{Ca}{C}$$

≻ Ca

In our study we are looking for the salt from the road which arrives on the well. So we can consider that here the sediments impacted by the salt are only the sediments closed to the well. We can consider the following approximation.

The hydraulic head of 180m is given by the Darcy's Law in COMSOL. We are considering only the part of the road which is impacted by the well. We estimate a width of 100m for the area of sediments impacted by the runoff coming from the road.

We calculate Ca like the ratio of the mass of salt by mass of sediments: $Ca = \frac{Msalt}{Msediments}$



Figure 43: Estimation of the volume of sediments impacted by the road salt

So we can estimate the volume of sediments impacted by the salt: Vrocks = (1 - n) * h * L * lVsediments= 9.072e7 m³

The density in this aquifer is approximately 1525 kg/m 3 , so the mass of sediments is:

Msediments= 1525*9.072e7

Msediments= 1.37e8 t

We know that on one year there is 13.52 tons of salt which are spread on the road (see II.3.1.a). So we have Msalt = 13.52 tons and Msediments = 1,37e8 t.

Therefore Ca= 9.85e-8 kg/kg

➤ C

We can consider C like the concentration of salt in the water. According to the data from the samples in the Elverum's catchment, we find an average of chloride at 2.66 g/m3. So we estimate C = 2.66e-3 kg/m3

≻ Кр

So we get $Kp = \frac{Ca}{c}$ Kp = 3.79e-5 m³/kg

c. Formula

According to the literature, we can calculate the retardation factor with:

$$R = 1 + Kp * \frac{1-n}{n} * \rho s$$

All the data are now known.

5) Retardation factor by bioretention

Now we will study the retardation phenomenon with the decay create by the salt's adsorption in trees along the road where the salt is applied. In Norway we can find Maple along the roads, so our study will be based on this tree and especially on the salt coming from the deicing of roads.

a. Impact of salt in trees

According to *Bedunah and Trlica (1979)* the mortality of a leaf occurred at a concentration of 350 ppm of chloride. But the tolerance to chloride is dependent on species, season and age of leaves (*J. Fuhrer and K.H. Erismann, 1980*) and the Norway Maple has a low injuring rate (1/5) according to fields work (*Canadian Environmental Protecting Act, 2001*).

The salt can arrive and go out in the tree by different ways (INRA, 2003):



Figure 44: Ways for the salt in a tree

➢ The exclusion

The tree stops the salt before it coming to the leaves. A first fence appears on the roots thanks to some intern cells of the roots. Other mechanisms are playing a role in this stop but there are unknown for the moment.

The inclusion

The tree pumps the salt with the water and leads it to the leaves. Here the salt is separated from the important cell's constituents by isolation in the vacuole, closed unit, of the leaf.

Crossing process

A new process has been found by searchers (*INRA, 2003*), we choose to call him the "crossing process". Indeed this process is a mix of the two processes previously introduced. The salt is leading to the leaves but it is immediately pumps to the roots which can exclude it from the tree.

So we think that these three processes are mix in a tree exposed to salt. A lot of fields work and lab works are necessary to have more information on these exchanges between trees and salt.

Splash phenomenon

We are interesting on the splash phenomenon amongst all theses following exchanges:



Figure 45: Exchanges of salt with the soil and the atmosphere

But amongst all the salt spreading on the road a very few part will arrive on the tree by splashes from cars. The main part will arrive by the soil or by evaporation. So we are not going to study only the splash phenomenon on leaves but we take the entire tree in consideration knowing that exchanges are for the main part with the soil thanks to the roots. We consider that exchanges with leaves are also with the atmosphere (evaporation, precipitations).

Then we can notice exchanges between:

- The biomass and the soil
- The biomass and leaves
- The leaves and the soil
- Leaves and atmosphere

All these exchanges are hard to quantify, they answer to kinetic laws which are for a main part unknown or in study. That is why we will based our study on a result from J.Fuhrer and K.H. Erismann (*1980*) which is "Areas of leaf necrosis were directly proportional to accumulations of chloride in the range 10 to 16 mg/g dry weight". So we consider that **a leaf dies when the ratio weight of Cl- into the leaf and weight of a dry leaf reach 1.3%.**

The mechanism of the death is explain in *Flowers and Yeo* (1986): "Salt accumulating in transpiring leaves to excessive levels, exceeding the ability of the cells to compartmentalize salts in the vacuole [...] Salt build up in the cytoplasm and inhibit enzyme activity or they build up in the cell walls and dehydrate the cell".

b. Area of road and trees

We are always working on the Elverum's case. So we consider this approximation for the road's dimension:



Figure 46: Schema for Elverum's area

So we have an area of road which is 1.45e6 m². The Leaf Index Area (LAI) is approximately 0.3 in Norway (*Guang Zheng and L. Monika Moskal, 2009*). So 30% of the area of the road is vegetation. We consider a Maple of 30m high and the salt on the road is able to reach the entire tree. But we are working in space with area of road (m²) and m² of leaves. So we have to consider the high of the tree which can be impacted. Indeed one m² of road contain several m² of leaves. In our mind a tree is composed with 1/3 of leaves and 2/3 of air. Therefore for a 30m tree we have 10m² of leaves (by spreading all the leaves on the floor) in one m² of road. So we choose a coefficient of 10 to illustrate this idea. Therefore we obtain an **impacted area of leaves of 4 350 000 m²**.

c. Biomass

Our aim is now to know the weight of biomass in our area. For that we always consider the Maple and its leaves. The Maple's leaf is about $0.0225m^2$:



Figure 47: Schema of a Maple's leaf

And we estimate the weight of a dry leaf at 0.005kg. So we can calculate the weight of biomass:

Number of leaves/m2	1/0,0225 = 44	1/m2
Kilo Biomass/m2 of leaves ŋ	0,005/44 = 0,22	kg/m2
Kilo biomass in the area	0,22*4 350 000 = 966 667	kg

Table 3. Calculation of the weight of biomass

d. Other exchanges

If we consider an exclusive exclusion, the salt concentration into leaves will be equal to the salt in atmosphere.

The exchanges with the atmosphere are very low, only 7g of Cl per ton of biomass is transformed in CH_3Cl each day (*H. Deep Saini*, 2009). The weight of biomass is 0.97t, so 6.8 g of Cl are transformed each day; it is a very small quantity. So we can neglect exchanges with atmosphere or consider these exchanges as balance.

e. Inclusion's rate

Now we consider only the salt includes in the tree from the roots. This inclusion can take water with all the salt contains in the soil or only a part of this concentration. We called the percentage of salt adsorbs by roots the inclusion's rate (IR).

We study the time to the death for a leaf which is impacted by salt with different inclusion's rates. We consider that a leaf dies when (see I.3.5.a):

 $\frac{\text{Weight of Cl in leaf}}{(\text{Weight of a dryleaf})} > 1.3 \%$

For that we consider that the concentration on the leaf is IR multiply by the concentration on the soil. We just take in consideration the salt applied each day (5 200 000 g/day) and the quantity adsorbed by the entire biomass (about 193 millions of leaves) from the soil. The mass of salt in a leaf is taken as the concentration on the leaf multiply by the volume of the vacuole. Indeed we saw previously that the salt is stock into the vacuole. We estimate its volume like 80% of the leaf's volume and a thickness of 0.1 mm. So the new concentration on the soil is the previous concentration plus the new input of salt minus the salt taken by the biomass. We make the hypothesis that exchanges with

the atmosphere are balanced (see I.3.5.d.) and all the salt from road infiltrates on the soil (no runoff to the river).

f. Salt

We know the amount of salt spread in one year (476 813 kg), so we can calculate the amount of salt spread each day: 5 200 000 g/d.

Like with sediments we need to estimate a partitioning coefficient. In our case, we can easily compare this coefficient with the weight of salt adsorbed by plants compared to the weight of salt applied. So we have:

$$Kd = \frac{\frac{Weight \ of \ chlore \ in \ biomass}{Weight \ of \ biomass}}{\frac{Cl \ add}{Aroad \ * \ LAI}} = \frac{Ca}{C}$$

The weight of chloride in biomass increases each day, so we consider it only when the leaf dies (fall) which means when the salt returns to the floor and can be take away to the river or infiltrated directly to the aquifer. So we have also to consider the amount of salt add during the life of the leaf. So we have:

Days to death	D	
Kilos of salt in the area/d	5 200 000	g/d
Kilos of salt spread in the area K	D * 5 200 000	g
Kilo of salt add/m2 of Biomass C	K/4.35e6 (Area of leaves)	g/m ² biomass
Weight of salt in Biomass at the death W	Give by IR calculations	g
Kilo of salt adsorbed/kilo of biomass Ca	W/966 667	g/kg
К	Ca/C	m²/kg

Table 4: Calculation of the partitioning coefficient

g. Formula

To estimate the retardation factor we use a comparison with sediments. The retardation factor is calculated in sediments with the following formula: $R = 1 + Kd * \frac{1-n}{n} * \rho$

- We already estimate the Kd calculation
- The porosity n gives the idea of the available area for the contaminant. (1-n) correspond to the area where the contaminant can go.

We compare (1-n) with LAI which is the area where the salt can go from the road. So:

$$\frac{(1-n)}{n} = \frac{LAI}{1-LAI}$$

• ρ is the density of the material so it is the mass of material per unit of volume.

We can compare it with the weight of biomass per m² of impacted biomass; this rapport is the η previously calculated. So: $\rho = \eta = 0.22 \text{ kg/m}^2$.

Therefore we suggest the following formula to estimate the retardation factor with a biomass:

$$R = 1 + Kd * \frac{LAI}{(1-LAI)} * \eta$$

6) Retardation factor in COMSOL MULTIPHYSICS

a. Species Transport in Porous Media

The retardation factor is added in COMSOL MULTIPHYSICS thanks to the *Species Transport in Porous Media* module. This one works exactly as the same as the Diluted Transport module (velocity with the Darcy Law, diffusion, inflow) but you can add a partitioning coefficient K for the adsorption. We can also define the dispersion (which we let null).

Thanks to the values of K previously define we can test the influence of a retardation factor on the well's concentration.

b. Checking In COMSOL

Exactly as we did previously we assure our self that we can have reliable results with COMSOL. For that we use the same model as I.1.4.b and we add a retardation factor in the hand calculation (the velocity is divided by R). This test is made for the case of the retardation creates by sediments. We obtain the following result for a fine mesh in the software:



Figure 48: Concentration with a retardation factor by hand calculations and by COMSOL MULTIPHYSICS

The mesh chooses has a big influence on the result, so the little difference we observe is still due to the numerical dispersion (see I.3.1.b.).

II. Results for Elverum

Here are the results for the water work Elverum. This part contains just the results there is no interpretation of it.

1. Definition of the catchment area



When we import the topography grid for Elverum the result is:

With that we can have the catchment area (I.2.2):



Figure 50: Geometry of the catchment area for Elverum

When we found this area, we have to make sure that it is big enough. We have to respect the conditions from I.2.1. For Elverum, we need at least a 10kmx10km area. The area we find is almost 11kmx14km: it is big enough; the boundaries will not be influenced by the well.

2. The Darcy's Law

1) River location

We are looking for the location of the river. After look at the coordinates on Arcview, we can digitalize the river on COMSOL. To enter a constant hydraulic head we need the river to be a boundary. Then the river has to be cut in two parts:



Figure 51: Elverum's catchment area with the river

2) <u>Bedrock</u>

We can see the bedrock on Elverum's area. It is corresponding to the distance from the bedrock to the sea level. We will use this parameter to define the hydraulic conductivity.



3) Hydraulic head and hydraulic conductivity

On the model we add the Darcy's Law and we run the study:



Figure 53: Hydraulic head for Elverum

It corresponds to the hydraulic head from the sea level for the groundwater table. We specify to COMSOL that the hydraulic conductivity is now the transmissivity with the logical tool "if" (see I.1.5.d). After that we can have look on the water table. For example, along the river:



Figure 54: Hydraulic head in the river

On this figure, the blue line represents the hydraulic head in the river, the green line represents the topography and the red line represents the bedrock. We add different constant heads in the river to be the most realistic. Indeed the head in the river has to be smaller than the topography and higher than the bedrock.



We can now have a look on a "cutline" on the model, to see if our conditions are respected.

Figure 55: Hydraulic head along a cut section

On this graph the colors are the same: green for topography, red for bedrock and blue for groundwater head. We can see that the "if" expression we enter on K (see I.1.5.d.) works. Indeed when bedrock is higher than hydraulic head we have a different K, and we can see it on the slope's modification for the hydraulic head.

4) Pumping well and drawdown

a. Drawdown

For Elverum we know that the pumping rate is $Qw = 2\ 098\ 467\ \left[\frac{m3}{year}\right]$. After adding the well on the model we are looking for the capture zone of the well (see I.1.6.a).



Figure 56 illustrate the result of back-tracking of particles from the well to the boundaries. There are probably some minor numerical artifacts (as crossing of streamlines in fig. 57), but if the input parameters reflect reality, this image illustrate the zone of influence (or capture zone) to the pumping well. We can "zoom" and have look on what happened near to the well.



We can see that there is water which is come from the river and is going into the well.

b. How much water is coming from the river into the well?

We want to know how much water is coming from the river into the well. We know that Qw = Qaq + Qr where:

- Qw is the pumping rate $[m^3/s]$. For Elverum we know that Qw = 2 098 467 $[m^3/year]$.

- Qaq is the flow from the aquifer coming into the well.
- Qr is the flow from the river coming into the well



Figure 58: Repartition of the pumping rate

To find Qr we look on the segment of the river where the velocity field is negative. We integrate the velocity field (see Annex 5) along this segment and we will find Qr. Indeed the well is located in the left part of the river and negative values of velocity field are corresponding to a flow <u>from</u> the river to the well. Positive values are corresponding to a flow <u>to</u> the river from the aquifer.

We find that $Qr = 0.009 \left[\frac{m^3}{s}\right]$ and we know that $Qw = 0.067 \left[\frac{m^3}{s}\right]$ so we can conclude that

Qr = 0.13Qw

c. Time dependent study

We run a time dependent Darcy's Law. We want to add the four grids of runoff into the mass source term. For that we need to import the four grids with the interpolation function (*Definitions-Function-Interpolation*). Call each grid by the name of the season it represents. Then enter this expression into the mass source term:

if(t<7.884e6||7.884e6<=t&&t<1.5768e7||1.57687e7<=t&&t<=2.3652e7,if(t<=7.884e6,vinter(x,y)[m m/year]*1000[kg/m^3],if(7.884e6<=t&&t<1.5768e7,var(x,y)[mm/year]*1000[kg/m^3],sommer(x,y)[mm/year]*1000[kg/m^3])),host(x,y)[mm/year]*1000[kg/m^3]).

We want to see the changes in the hydraulic head and in the velocity fields.

Hydraulic head

First the changes on hydraulic head: we look at the hydraulic head along a cut line for each season.



Figure 59: Hydraulic head season by season

Green line: hydraulic head for spring Red line: hydraulic head for summer and autumn (same value) Blue line: hydraulic head for winter

> Velocity field

Second the changes on the velocity fields. We look at the integration of the velocity field along the road's segment just closed to the well (see Annex 5).



Figure 60: Velocity field integration along a road's segment

We can see that hydraulic head and velocity are both higher in spring, when the precipitations are higher. We can see too that summer and autumn data seem to be approximately the same.

3. The transport equation

1) Concentration on salt in the pumping well

We study the concentration on salt in the well. The salt is coming from the road (part which is crossing the drawdown) and the atmosphere (background). The outflow is the river closed to the pumping well.



Figure 61: Location of the pumping well in COMSOL

a. Mass Flux

As explain in I.3.3.c. we want to compare the two mass fluxes to see if the most part of the salt is coming from the road or from the atmosphere. With Elverum's water work we obtain:

Area (Capture zone)	8.07e6	m²
Average of the runoff	8.24e-9	m/s
Average of the background concentration	0.6126	g/m³

So we can have the mass flux from the atmosphere:

 $Mf(Atmosphere) = \overline{Cback} * A(Drawdown) * \overline{Runoff}$

M_f (Atmosphere) = 0.041 g/s

We know that we have **16.9** [t/km/year] in our catchment area. Next we observe that the part of the road which can impact the well (*I*) has a length of 800m. So we calculate the mass flux of salt from the road:

Mf(Road) = 16.9 * L

M_f (road) = 13.52 tons/year

M_f (road) = 0.43 g/s

Therefore the impact of the salt from the road is **ten times** more important that the salt from the background.

b. Inflow

As explain in I.3.3.d. we have to specify the influx of salt on roads. For Elverum, the inflow is: $13,53\left[\frac{t}{-}\right]$

 $Inflow = \frac{13,53\left[\frac{t}{y}\right]}{58\left[\frac{g}{mol}\right]*0.05\left[\frac{m3}{s}\right]}.$ We want to add salt only on winter and we want to run the study on

several years. To respect these conditions we add an inflow (*Transport of Diluted Species->Inflow*) and we select the road's segments which cross the capture zone of the well. Then we enter the following expression:

if(t<=7.88e6||3.15e7<=t&&t<=3.94e7||6.31e7<=t&&t<=7.1e7||9.46e7<=t&&t<=1.02e8||1.26e8<=t &&t<=1.34e8||1.58e8<=t&&t<=1.66e8||1.89e8<=t&&t<=1.97e8||2.21e8<=t&&t<=2.29e8||2.52e8< =t&&t<=2.6e8||2.84e8<=t&&t<=2.92e8||3.15e8<=t&&t<=3.23e8||3.47e8<=t&&t<=3.55e8,13.52[t/ year]/58[g/mol]/0.05[m^3/s],0)

It corresponds to an inflow of twelve years.

c. Concentration with road salt

Thanks to the model "comsol_model_elverum_transport_salt" in COMSOL which uses the Darcy Law previously established we obtain the concentration of salt for 12 years of input. The calculations are made every month (time step of 2.63e6 seconds).



Figure 62: Road salt concentration (without background)

d. Concentration with road salt and background





Figure 63: Concentration with road salt and background

After 12 years we can observe that a part of the pollution is already on the river (the outflow) but there is still salt on the area of the well:



Figure 64: Concentration of salt in the area's well for t=12 years

2) <u>Retardation factor by sediments</u>

The formula gives us: R = 1.098

3) <u>Retardation factor by biorentation</u>

We present in this part some results on the retardation factor, like the influence of some parameters on it.

a. Inclusion's rate

We study the days before the death for different inclusion's rate:

Rate of inclusion	Days before death
5 %	201
10 %	101
20 %	51
30 %	34
40 %	26
50 %	21
60 %	17
80 %	13
100 %	11

Table 5: Days before death with different inclusion's rates



We can have a relation between the days before death and the inclusion's factor:

Figure 65: Influence of the inclusion's rate on the death

b. Influence of the LAI on the retardation factor

The Leaf Area Index (LAI) corresponds to the percentage of vegetation on the area. We study here the consequences of a bigger vegetative area comparing the retardation factor for a LAI of 0.3 and a LAI of 0.7 (70% of the area is cover by vegetation).



Figure 66: Influence of the LAI on the retardation factor

The number of leaves change the repartition of the salt in a tree for example. So a bigger LAI will influence the adsorption of each leaf, which is estimate by the partitioning coefficient Kd.



Figure 67: Influence of the LAI on the adsorption (Kd)

c. Concentration on salt in the pumping well with a retardation factor

Retardation factor due to sediments

The sediments around the well can adsorb some salt and release it later. So it can create decay in the concentration on the well. We use the circle draw for the particle tracing like the zone of adsorption by sediments. The study is for 7 years:



Figure 68: Impact of sediments in the well's concentration

We can observe a little decay in some part of the curve but it is very low and quite negligible.

Retardation factor due to plants

Thanks to the module *Species Transport in a Porous Media*, we enter a retardation factor (which is represented by the partitioning coefficient in the software). We test if there is any influence of the vegetation on the concentration of salt in the well. This study is made for a LAI of 0.3 and 0.7 (more vegetation in the area). We only give the result with an inclusion's rate of 100% which is the more relevant.



Figure 69: Concentration in the well with a retardation factor and LAI = 0.3



Figure 70: Concentration in the well with a retardation factor and LAI = 0.7

<u>Comment</u>: The little difference between the two figures is due to a change of the time step between LAI 0.3 and 0.7 to have reliable results.

III. Discussion

In this part we will discuss the results and the relevance of its.

1. Catchment area

In the part II we found a relation between the pumping rate, the infiltration velocities¹ and the size of the catchment area. We saw too that this condition is respected for Elverum. The catchment area we found was a bit bigger than necessary, but that is far better than having a catchment area that is too small. The method we used to delimit the catchment area (I.2.2) was based on the assumption that the flow field was perpendicular to the topography. This hypothesis can be controlled by doing long term pumping tests. If the drawdown is circular (or semi-circular) in the horizontal plane around the well, the assumption of approximate isotropy in the horizontal direction is valid.

2. The Darcy's Law

1) Discussion on the time dependant study

We studied the Darcy's Law both in steady state and in time dependant conditions. The results for Elverum are presented in the paragraph II.2.4.c. A time dependant study may be considered as more realistic because we know that infiltration velocities change during the seasons. However, the changes in averages from season to season do not have a significant influence on the salt concentration into the well. Indeed as explain in I.1.7.e the size of the capture zone of the well in the real model is not very impacted by the changes in the velocity field. We did not have time to prove that but it is based on the fact that the precipitations' differences during the year for Elverum for example are not very big. There is just more precipitations in the spring time (see II.2.4.c).

2) Discussion on the hydraulic head and the transmissivity

The simulated hydraulic head for Elverum groundwater work (II.2.3) is in large located between the surface (topography) and the bedrock, which is a plausible result. The exceptions are areas with exposed bedrocks (see explanations in I.1.5.d). In these areas we expect lower hydraulic conductivities than in the sediments, which resulted in steeper gradients in the groundwater head.

It is possible to subdivide the catchment into sub-domains with different hydraulic conductivities (K) (c.f. Sellevold, 2011). However, adding domains with different K-values will complicate the model. We think it is important to keep the model as simple as possible, thus we chose only two different transmissivities (see I.1.5.d).

¹ Note that for steady state flow, specific runoff is equivalent to infiltration velocities into the groundwater.

3) Discussion on the capture zone of the well

The final result we look for when we solve the Darcy's Law in this problem is the area of the capture zone for the well. The method used to find this area is explained in I.1.6.a. The results for Elverum are available in II.2.4.a. We see that with infinite time the area of the capture zone is just a little part of the catchment area we defined (5% only).

3. Transport Equation

The values measured on the well give a concentration of salt between 2.4 mg/L and 4mg/L. These values have been measured between 1984 and 2010 but there is no clear indication of an increasing trend in salt concentration in the production wells.



Figure 71: Concentrations measured into the well

We obtain a concentration maximum equal to 2.43 mg/L which is not incoherent with the values measured on the well ([2.4; 4 mg/L]).

But we don't know the climatic conditions for the year we are studying (data of salt for one year). The result is dependant of the appliance of salt. Maybe this year was almost like 1990 or 2004 with a low amount of salt. Nevertheless variations of salt in one year are possible like we see for the year 1984 and there can be storage of salt and accumulation in the groundwater like we saw with our modeling (the amount of salt is always increasing with the time).

Nevertheless we have to be careful with our result because we made a lot of simplifications, but the amount of salt is not supposed to increase all the time. Indeed we saw with measurements that the amount of salt is not always increasing with the time but contrary it can change a lot.

4. Retardation factor

1) <u>Sediments</u>

The sediments have minor impact on the chloride concentration in groundwater according to our result. Nevertheless it could be interesting to look at the real area of sediments which is impacted by the salt. Besides the calculation of the retardation factor is made with a lot of approximations, so lab works are necessary to know the relations between a soil of sand and gravels and salt. Therefore a better result for the retardation factor could be found and another impact can be show with COMSOL MULTIPHYSICS.

2) Splash phenomenon

In the case of a splash phenomenon an inclusion's rate of 5% (or less) can be expected. So the retardation factor will be very low and the impact on the concentration in the aquifer will be negligible. So it is better to consider the arrival of salt in the entire tree, including the roots.

3) **Bioretention**

The results show that whatever the vegetation, the impact of this one is also quite negligible on the concentration on the well.

4) Conclusion on the retardation factor

According to our results the influence of the vegetation in the transport of salt is negligible. Nevertheless this study has to be completed by lab works to determine more precisely the kinetic of the different exchanges between the biomass, the soil and the atmosphere.
Conclusion

This study presents results from numerical modeling of the Elverum groundwater work. We indicate a quantitative approach to delimit the flow domain for calculation of capture zone of a groundwater work. By using public information on water balance and topography, and combining this information with estimates of depth to bedrock, we calculate the capture zone of the water work. The capture zone is essential for the water quality of the groundwater work. The numerical simulations of salt concentration are consistent to observations (~2.4 mg/L). Validation of the capture zone can be done by tracer tests.

Figure 72 summarize our mains results and indicate the most important parameter in Elverum's area:



Figure 72: Processes explanations

Bibliography

BLONDEL T. INERIS, Projet TRANSPOL – Programme 2000. Cabinet Conseil Blondel, Septembre
2001. Volet 2, Pollution souterraine: Paramètres et paramétrages des Modèles en écoulement et en transport de polluants, p. 5-43.

CALU G. Effet du stress salin sur les plantes. Comparaison entre deux plantes modèles : *Arabidopsis thaliana* et *Thellungiella halophila*. Mater 1 Recherches Biotechnologiques : du gène a la molécule, 2004-2006. 14 p.

CANADA ENVIRONMENTAL PROTECTION ACT. Priority Substances List Assessment Report, Road Salts. PSL Assessment Report, Minister of Publics Works and Government Services, 2001. 170p.

FRANKLIN W.S. and HUBAO Z. Fundamentals of groundwater. The Ohio State University, John Wiley& Sons Edition, 2003. 583p. ISBN 0-471-13785-5

FUHRER J. Environmental Pollution Series A, Ecological and Biological. Institute of Plant Physiology, University of Berne, Switzerland, Science Publishers Ltd, April 1980. Volume 21, Tolerance of Aesculus hippocastanum L. to foliar accumulation of chloride affected by air pollution, p. 249-254.

HAITJEMA H.M. Analytic element modeling of groundwater flow. School of Public and Environmental Affairs, Indiana University, Bloomington, India, Academic Press, 1995. 394p. ISBN 0-12-316550-4

INRA. Découverte d'un nouveau mécanisme de tolérance des plantes au sel. Embo Journal [on line] 1th may 2003, [look on the 10/06/2011]

<<u>http://www.inra.fr</u>>

JOIN C. Data preparation for salt transport modeling in groundwater. Bioforsk, Ås, Norway, 2011. 15p.

KITTERØD N.O. Lectures 9-10-11-12, University of Oslo, Norway, 2003.

MUNNS R. Salinity: Environment-Plants- Molecules. CSIRO Plants Industry, Canberra, Australia, Kluwer Academic Publisher, 2002. Chapter 13, Salinity, Growth and Phytohormones, p. 271-290.

PRESCOTT James. The Journal of Agricultural Science. Cambridge University Press, September 1916. Volume 8, Part I, The phenomenon of absorption in its relation to soils: A résumé of the subject, p. 111-130.

SELLEVOLD, J., 2011, Modelling of Øvre Eiker groundwater work, NTNU, (pers. med)

SAINI H. Chloride-Plant interactions: Implications for vegetation as an effective BMP for salt removal. University of Waterloo, United-States. 2009.

SHERER T., SEELIG B., FRANZEN D. Soil, Water and Plant Characteristics Important to Irrigation. EB-66 [on line] February 1996, [look the 04/07/2011]

<<u>http://www.ag.ndsu.edu</u>>

WANKO A. Lecture of Hydrogeology. ENGEES, Strasbourg, France, 2011.

WARREN VIESSMAN Jr. and GARY L. Introduction to hydrology. University of Florida, Harper Collins College Publishers, 4th ed., 1996, 760p. ISBN 0-673-99165-2

ZHENG G. and MOSKAL M. Retrieving Leaf Area Index (LAI) Using Remote Sensing: Theories, Methods and Sensors. Sensors 9 [on line] 2009, no. 4: 2719-2745 [Published the 17 April 2009] <http://www.mdpi.com/1424-8220/9/4/2719/pdf>

Annexes

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<u>Annex 1</u>: How to calculate the real area

On COMSOL, enter a new variable (*Definition->Variables*). In the expression of the variable put the value 1. Then compute and in the results plot your new variable on the surface. Then add a surface integration (Results->Derived values->Surface Integration) and select the area. Push Evaluate and the result will appear in the results box.

For Elverum, the catchment area is estimated to $1.5576e^8m^2 = 155km^2$

<u>Annex 2</u>: How to import a grid in COMSOL

To import the grid on a model: Definitions->Functions->Interpolation and then you browse the grid you want to import. Plot it to have a view in 3D, COMSOL recognize X and Y as coordinates.



Figure 73: 3D view of Elverum's topography

If you want to have a 2D view, you need to use a tool called the *coefficient form equation*. You can find this tool in *Mathematics->PDE Interface->Coefficient Form PDE*. The general equation solve by the computer is:

$$ea\frac{\partial^{2}u}{\partial t^{2}} + da\frac{\partial u}{\partial t} + \nabla (-c\nabla u - \alpha u + \gamma) + \beta \nabla u + au = f$$

If you choose a stationary study, this equation becomes:

 $\nabla (-c\nabla u - \alpha u + \gamma) + \beta \nabla u + au = f$

We want to see the topography on a 2D surface. So the final equation we want is topo(x,y) = h, where h is the elevation. If we consider that u = h in our equation, we have to put α , β , γ , c = 0 and a = 1; and put f = topo(x,y).

After that we just need to add a geometry which is intersecting the coordinates of the grid (here the topography). For Elverum's topography we choose a square equal to the grid's size. Then click on *Study->Compute* and watch the result:



The coefficient form equation could be used to see a grid on a 2D surface. The grid you import has to have three columns: X, Y, and the parameter you want to see.

<u>Annex 3</u>: How make the topography grid

This annex will explain the procedure to obtain grids of topography. In this goal we use the software ARCVIEW with two extensions: 3D Analyst and Spatial Analyst.

<u>Comment</u>: Be careful with the names of your fields because ArcView can't understand some characters like spaces.

Extensions:

- 3D Analyst
- Spatial Analyst
- Geoprocessing

Files: You need files in .DEM

Import files

You have to import data from USGS (*file => Import data source => USGS*) and choose all the .DEM files (expect if you know which one you need). We advise you to let the files in C:/TEMP because ArcView don't find them if you change the way.

Next you have to import the grid which contains data of topography of the point you study (here it is a well). And you localize the point on one of the .DEM file.

Decomposition of the grid in shapefiles

You have to select the Get grid value extension (*File=> Extension*). We advise you to do a copy of the grid and to work with it. With the select button choose a part of the grid (<10 000 points) and transform this part in a New Shapefile. Next click on the G button, the first enter is your new

shapefile, the second the .DEM file in which you work and choose a name for the column (always enter the same, for example: metres_amsl). After delete the features which are selected to see which part of the grid you have already did (*Theme => Start editing, Edit => Delete features, Theme => Stop editing*). And repeat this operation while the grid is finish.

<u>Comment</u>: If you have a message like "Segmentation violation" during the running, take fewer points in your selection.

➢ The grid

Merge all the "New shapefiles" together (*View => Geoprocessing Wizard*) and export the grid in .txt. You can after open it in Excel, you have just to choose coma like column separation. To work with the grid in software (like Matlab) put a % before the first line.

<u>Comment</u>: If you can't work with the values on Excel is probably because the separation with decimals is the dot (.) in the grid but it is the coma (,) in the computer. We can easily check that in Excel: take a value and divide it by 2 for example. If #NUMBER appears in the cell, it means that Excel doesn't recognize the value like a number. To solve this problem go on the Control Panel, pick language and regional options, in regional options click on Customize, put a dot (.) in Decimal symbol and apply.

Annex 4: How export data from COMSOL MULTIPHYSICS

You can export data like grids after calculation in COMSOL MULTIPHYSICS. For that you have to go on *Results* and to right click on *Reports*, then go on *Data*. Here you can choose the data you want export (for example the velocity field) and the place you want register these data.

To open easily the data on Excel we advice you to choose 2 in *Dimension* on the Data window. Then in Excel, in the *Open window* you have to select *All the files* and after choose your file if it doesn't open, you have to select the second option in the first window which appears.

<u>**Comment</u>**: Don't forget to save your work as Excel file and no like Text.file to conserve all your modifications in Excel.</u>

<u>Annex 5</u>: How to integrate the velocity field along a segment

When we want to integrate the velocity field along a segment or a section, we just want to have the perpendicular velocity. To be sure to take only the perpendicular part of the velocity field we use the normal vector.



Figure 75: Velocity field

The velocity vector has two components: the x-component called u and the y-component called v. The normal vector is a vector perpendicular to the segment and its x-component is nx and its ycomponent is ny.

We want to put $U \cdot n = 1$. If we talk with coordinates it is u * nx + u * ny = 1.



Figure 76: Velocity field and normal vector

In COMSOL: *Results->Derived Values->Line Integration*. In Selection select the segment you want to integrate along. In Expression enter dl.u * dl.nx + dl.v * dl.ny then compute. The result will appear in the result field. With that we take only the perpendicular part of the velocity flow.

<u>Annex 6</u>: How obtain a velocity field with the topography and the runoff

We do the following approximation: the velocity of the water is very close to the runoff, so we estimate the velocity field \underline{u} like the mass source, which means that $/\underline{\vec{u}}/=R$ (m/s). And we consider that the hydraulic head follows the topography, so the main flow is given by the topography. We can also choose the topography like the direction of the velocity vector.

In the followed picture we have the result of the Darcy law with the topography (in color) and the arrows (in green) represent the velocity field:



Figure 77: Topography and velocity in Elverum's area

In COMSOL MULTIPHYSICS we import the grid of topography (cf. Annex 2) and thanks to the Darcy Law we observe and export (see Annex 4) the X (dl.u) and Y (dl.v) coordinates from the velocity field. Next we draw the graph dl.v=f(dl.u) and we obtain:



Figure 78: Graph of the velocity field

We are looking for the angle α between the axe of dl.u and the main flow. To determinate this main flow we use the trendline in Excel (black line in the figure 78). Now some trigonometry allowed us to find the velocity field (u_x and u_y). We work with the following triangle obtain from the graph above:



Figure 79: Triangle obtain thanks to figure 78

\succ α calculation

In a first time we are looking for the value of α . We calculate α with: $\cos(\alpha) = \frac{a}{b}$

We have $a=3.10^{-3}$

Thanks to Pythagore's theorem we can have b: $b^2 = a^2 + c^2$ So b=3.04.10⁻³

And $\cos(\alpha) = \frac{3.10^{-3}}{3.04.10^{-3}} = 0.9868$

So **α = 9.30°**

\succ u_x and u_y calculation

We know that the average's runoff is $9,25.10^{-9}$ m/s, so we define b'= $9,25.10^{-9} \ll b=3,04.10^{-3}$ and we have the new triangle (in red):



Figure 80: New triangle with the runoff

We know α and b', so we have:

a'=b'*cos(α) a'=9,25.10⁻⁹*cos(9.3)

a'=9,13.10⁻⁹ m/s = u_x

c'= b'*sin(α) c'=9,25.10⁻⁹*sin(9.3) c'=**1.49.10⁻⁹ m/s = u**_y

So this approximation give us the velocity filed in Elverum's area, we can use this result to solve the transport equation if we don't use the Darcy law's velocity. But be careful with the results obtained.

A test is made on the Elverum's catchment during one year with an inflow of 1 mol/m3. We compute the model with the velocity from the Darcy Law, the previous velocity and a velocity of 1e-5 m/s on x component and 0 m/s on y component.



Figure 81: Concentration with time for different velocity fields

The result is quite interesting because the two first curves are very similar contrary to the third one with a hazardous velocity. So we can conclude that the velocity field find previously can be adapted at the Elverum's catchment.

Annex 7: Discussion on the main mechanisms

The different studies are made in the same model (*comsol_model_test_massbalance*) in COMSOL MULTIPHYSICS with these initial parameters:

Study	Time dependant	
Hydraulic conductivity	k= 1.10-3	m/s
Porosity	1	

H1	10	m
H2	12	m
Velocity field	From the Darcy law = 1e-5	m/s
Diffusion coefficient	1e-5	m2/s
Pumping rate	Qw = 0	kg/s
		14.5
Inflow	0.2186	mol/m3

The inflow is added on the west boundary and the concentration with the time is studied in the east boundary of the model.

> Diffusion coefficient (Dc) Cf. paragraph 3.3.a) in the report.

The diffusion coefficient has a big influence on the result, we need to adapt it with the size of the area.

> Numerical dispersion *Cf. paragraph 3.2.b) in the report.*

The difference obtained between two different meshes corresponds to the numerical dispersion which is an imprecision in the calculation. We work with a normal mesh.

Convection/Diffusion

The paragraph "Advective part" (3.2.b) in the report explains the influence of the advective part in the Transport Equation. Here we are going to see the role and the influence of the diffusive flux and the convective flux in the concentration.

We study these two fluxes on the x component and for the same time step (5e6 seconds). For the convective flux, we obtain:



Figure 82: Convective flux, x component, t=5e6s

The diffusive flux is symmetric and the values are lower than the convective flux:



On the result for the concentration we can see the influence of the two fluxes; the black arrows represent the convective flux ad the magenta represent the diffusive one:



Figure 84: Concentration and arrows of the diffusive and convective fluxes, t=5e6s

We can observed that the convective part is more important than the diffusive part; indeed there are more black arrows and they are bigger than the magenta one. Besides the dispersion of the concentration is closer to the convective flux (figure 82) than the diffusive flux (figure 83).

Peclet number

The Peclet number is a measure of the relative importance of advection to diffusion. It can be defined like the following ratio:

$$Pe = \frac{Tadv}{Tdiff} = \frac{u * L}{Dm}$$

The molecular diffusion is hard here to estimate. But we know that $Dc = D_L + Dm = 1e-5 \text{ m}^2/\text{s}$. So the maximum value of Dm is 1e-5 m²/s.

$$Pe \ge \frac{1e - 5 * 200}{1e - 5}$$

 $Pe \geq 200$

Therefore the advective/convective part is the main mechanism before the diffusion.