DEPARTMENT OF ENVIRONMENTAL ENGINEERING

ENVE 404 ENVIRONMENTAL MODELING

TERM PROJECT REPORT

MIGRATION OF CONTAMINANT THROUGH COMPACTED CLAY LINER FOR A LANDFILL LEACHATE LAGOON

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1. Description of the Modeling Problem

For our term project, we have chosen to model the migration of contaminants in a liner underneath a leachate lagoon. The liner is supposed to act as a barrier against the leachate chemicals reaching the aquifer underneath the site. Without such a liner being present underneath the lagoon, the chemicals can possess an environmental risk as they can pollute the water in the aquifer By modelling the behavior of the contaminants through the clay liner, we can assess its performance based on the inhabitation of the chemicals. This assessment could be helpful in the design of such facilities in the future.

2. Modelling Objectives

The specific modeling objectives of this term paper are the following:

- Develop a conceptual model for the one-dimensional migration of pollutants through a liner.
- Develop a mathematical model for one-dimensional migration of pollutants through a liner.
- Solving the mathematical model in MATLAB using an analytical solution.
- Calibrate our model by using our simulated values and the predicted values given in the article.
- Finding the most sensitive parameters for the concentration profile in the liner.
- Validate our model to test if it can simulate the future behavior of the system.
- Simulate different scenarios using our model:
    1. Estimate when the geomembrane (part of the site's composite liner) becomes inactive
    2. Effect of biannual variation of leachate height and concentration on the concentration profile
    3. Effect of the leachate height on the concentration profile
    4. Effect of time on the concentration profile

3. System Analysis

3.1. System Processes

The migration of chemicals through the liner is governed by 2 transport processes, advection and diffusion, and 1 transfer process, adsorption. The migration is generally extremely slow, so advection doesn't play as significant as a part as diffusion in the migration. The effect of adsorption of the migration depends on the chemical being modelled.

The modelling of chemical transport is a difficult process since there are a lot of factors that should be considered. The characteristics of the soil usually vary by region so there are a lot of assumptions that need to be made to produce a usable model. We have based our migration model on the transport of chemical through saturated soil. This is the model usually used to depict situations like ours.

3.2. System Variables and Parameters

Liner Parameters

- Soil porosity, $\eta = 0.43$
- Dry density of soil, $\rho = 1.53$ g/cm^3
- Liner thickness, L = 2.9 m
- Hydraulic conductivity

- For clay, $K_h = 2\times10^{-10}$ m/s
- For geomembrane, $K_h = 1.1\times10^{-11}$ m/s (Rowe, 2003)

Chemical Parameters

- Diffusion coefficient
  - For Chlorine, $D = 7\times10^{-10}$ m^2/s
  - For Sodium, $D = 4\times10^{-10}$ m^2/s
  - For Potassium, $D = 7\times10^{-10}$ m^2/s
- Linear partitioning coefficient
  - For Chlorine, $K_d = 0$
  - For Sodium, $K_d = 0.2$ mL/g
  - For Potassium, $K_d = 7$ mL/g

Independent Variables

- H: Hydraulic Head (L)
- t: Time (T)
- z: soil height (L)

Dependent Variables

- C: Chemical concentration (ML^{-3})

3.3. Conceptional Model Description

The following figure describes our model. Our model is only concerned with the one-dimensional vertical migration of contaminants through the liner. The leachate moves downwards through the liner to reach the aquifer underneath.

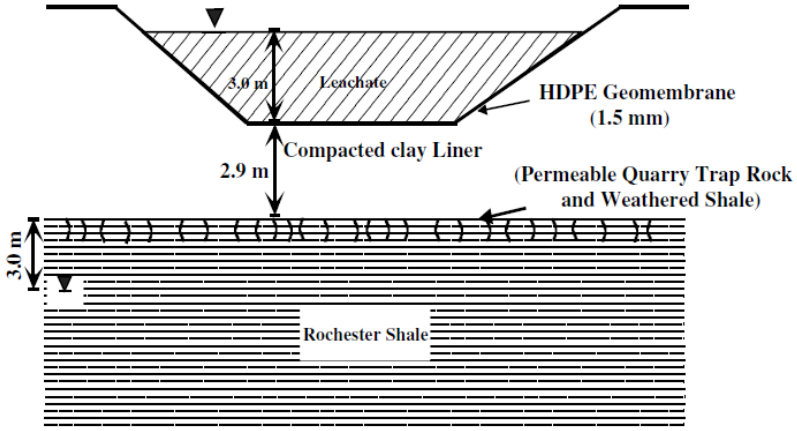


Figure 1 Diagram of the leachate lagoon liner being modelled

3.4. Mathematical Model Description

The general equation (Lake, 2005) is:

$$\eta \frac{dC}{dt} = nD \frac{d^2C}{dz^2} - \eta v \frac{dC}{dz} - \rho \frac{dS}{dt}$$

Assuming the sorption is linear, the equation can be written as:

$$R \frac{dC}{dt} = D \frac{d^2C}{dz^2} - v \frac{dC}{dz}$$

Where:

$$R = Retardation\ Factor = 1 + \left(\frac{\rho K_d}{\eta}\right)$$

The initial and boundary conditions are:

$$C(z, 0) = C_b$$

$$C(0, t) = C_0$$

$$\frac{dC}{dt}(\infty, t) = 0$$

z: Liner height (L)
t: Time (T)
C_b: Intial soil concentration of contaminant (ML^{-3})
C_0: Leachate lagoon concentration of contaminant (ML^{-3})
D: Diffusion coefficient (L^2T^{-1})
K_d: Linear partitioning coefficient (L^3M^{-1})
P: Dry density of soil (ML^{-3})
η: Soil porosity (-)
S: mass of solute removed from solution per unit mass of solute (-)

The seepage velocity is calculated Darcy's Law.

$$i = \frac{\Delta H}{\Delta z}$$

$$q = K_h(i)$$

$$v = \frac{q}{\eta}$$

K_h: Hydraulic conductivity (LT^{-1})
ΔH: Hydraulic head difference (L)
Δz: vertical distance difference (L)
i: Hydraulic gradient (-)
q: Darcy flux (LT^{-1})
v: Seepage velocity (LT^{-1})

3.5. Model Assumption

- The clay is uniform and unfractured.
- The clay is saturated.
- The porosity of the clay is constant with respect to depth.
- The dry density of the clay is constant with respect to depth.
- The leachate is in direct contact with the liner, there is no sludge at the bottom of the lagoon.
- The transport and adsorption of the contaminant being measured isn't affected by the other chemicals in the leachate.
- Sorption is linear.

4. System Simulation

4.1. Solution of the model equations

To model our system, we used the analytical solution for the it.

The analytical solution (Van Genuchten, 1982) is:

$$C(z,t) = C_b + (C_0 - C_b)\frac{a_1 + \exp\left(\frac{vz}{D}\right)a_2}{2}$$

Where:

$$a_1(z,t) = erfc\left[\frac{Rz-vt}{2\sqrt{DRt}}\right] \;\&\; a_2(z,t) = erfc\left[\frac{Rz+vt}{2\sqrt{DRt}}\right]$$

For modelling this, we created a function called 'cfun' which took the following variables parameters as input: t, z, C_0, C_b, R, D, v. Four of these inputs (t, z, C_0, C_b) can be arrays or single values. The function loops through the length of the time array, and for each loop sets the calculated concentration values as the initial soil concentration values for the next loop. At the end, the function returns only the final calculated values. This loop is necessary to model the changes in the parameters (C_0, v, etc.) with respect to time. We have included a 'main' script file to which runs this program and returns the concentration profiles of the 3 chemicals.

The 'cfun' function:

```
function resC = cfun(t,z,C0,Cb,R,D,v)

%This is the function for simulation of the concentration profile. It
%applies the analytical solution for every z value for each loop and
%replace the intial soil concentration with the calculated value for the
%next loop.

C = zeros(length(t),length(z)); %creation of concentration matrix
C(1,:) = ones(length(z),1)'.*Cb;    %sets the row to the intial conc. entered

for i = 1:length(t) %loops through the duration values
    t(i) = t(i)*(365*24*60*60); %converts from years to sec
    %applies the formula
    a1 = erfc((R*z-v*t(i)/(2*sqrt(D*R*t(i)))));
    a2 = erfc((R*z+v*t(i)/(2*sqrt(D*R*t(i)))));
    C(i+1,:) = C(i,:)+(C0(i)-C(i,:)).*(a1+exp((v*z)/D).*a2)/2;
end

%returns only the last row of the concentration matrix since we only want
%the final concentration values.
resC = C(length(t)+1,:);
```

The 'main' script and the resulting plot:

```
clc
clear all
close all

%This is the main program file for plotting the concentration profiles of
%the 3 chemical in the compacted clay layer.

%Soil Parameters
ro = 1.53;    %avg. dry density of the soil (g/cm3)
n = 0.43;   %avg. porosity of soil (-)
Kh = 2e-10; %hydaulic conductivity (m/s)
cL = 2.9;   %clay thickness (m)
```

```
%Calculation of seepage velocity
dH = 3+cL+3; %head difference (m)
dz =3+cL;   %distance (m)
q = Kh*(dH/dz); %darcy flux (m/s)
v = q/n;    %seepage velocity (m/s)

t = [14 9.5 4.5] ; %time (years)
z = 0:0.1:cL;   %clay depth values (m)
z = sort(z,'descend');

%Chemical Parameters for Chlorine
Cb = 5; %intial soil concentration (mmol/L)
D = 7e-10;  %diffusion coefficient (m2/s)
Kd = 0; %linear partitioning coefficient (mL/g)
C0 = [251 608 510*0.8]/35.5;    %leachate concentrations(mmol/L)
R = 1+((ro*Kd)/n);  %retardation coefficient(-)

C_Cl = cfun(t,z,C0,Cb,R,D,v);   %calculating the chlorine concentration profile

%Chemical Parameters for Sodium
Cb = 3; %intial soil concentration (mmol/L)
D = 4e-10;  %diffusion coefficient (m2/s)
Kd = 0.2; %linear partitioning coefficient (mL/g)
C0 = [1425 3454 1640*0.8]/23;   %leachate concentrations(mmol/L)
R = 1+((ro*Kd)/n);  %retardation coefficient(-)

C_Na = cfun(t,z,C0,Cb,R,D,v);   %calculating the sodium concentration profile

%Chemical Parameters for Potassium
Cb = 0.3;   %intial soil concentration (mmol/L)
D = 7e-10;  %diffusion coefficient (m2/s)
Kd = 7; %linear partitioning coefficient (mL/g)
C0 = [78 252 156*0.8]/39;   %leachate concentrations(mmol/L)
R = 1+((ro*Kd)/n);  %retardation coefficient(-)

C_K = cfun(t,z,C0,Cb,R,D,v);    %calculating the potassium concentration profile

L = cL-z;
subplot(1,3,1)
plot(C_Cl,L)
title('Chlorine')
ylabel('Height (m)')
xlabel('Concentration (mmol/L)')

subplot(1,3,2)
plot(C_Na,L)
title('Sodium')
ylabel('Height (m)')
xlabel('Concentration (mmol/L)')

subplot(1,3,3)
plot(C_K,L)
title('Potassium')
ylabel('Height (m)')
xlabel('Concentration (mmol/L)'))
```

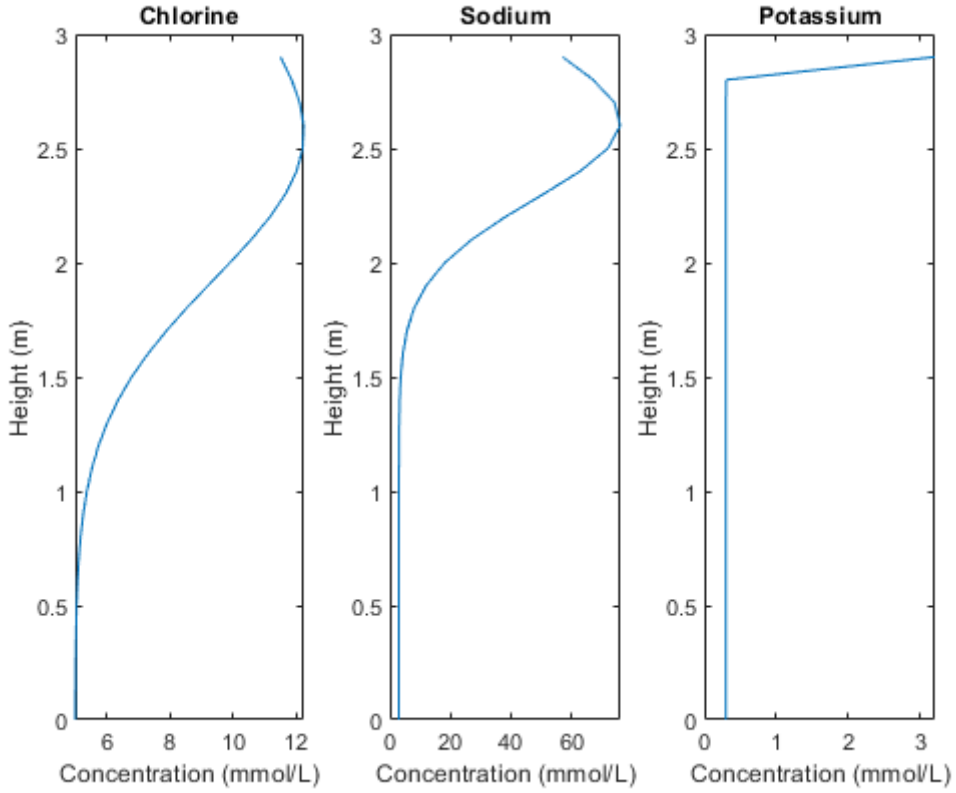


Figure 2 The 'main' script result showing our basic model

4.2. Calibration

Calibration is used to adjust the input data until computed output from the model matches with the measured output. Calibration is used to identify the values of system parameters and to test the acceptability of conceptual model. To calibrate our model, we compared our simulated values to their predicted values for geomembrane being ineffective from the beginning. We performed calibration for two parameters, hydraulic conductivity (K_h) and linear partitioning coefficient (K_d). To calibrate K_h we used the data available for Chlorine, since it is conservative ($K_d = 0$). To calibrate K_d we used the data for Sodium and Potassium.

Table 1 Predicted concentration values for geomembrane ineffective from the beginning

Clay Depth (m)	Concentration (mmol/L)		
	Chlorine	Sodium	Potassium
2.5	5	2	0.3
2.25	5	2	0.3
2	5	2	0.3
1.75	5.5	2	0.3
1.5	6	3	0.3
1.25	8	6	0.3
1	9	13	0.3
0.75	11	31	0.3
0.5	12	62	0.3
0.25	13	80	1.9
0	12	60	3.1

This is the ‘calKh’ script for calibration of K_h, similar scripts were written for the calibration of K_d. Our calibration is based on calibration error (CE) calculated using RMSE and coefficient of determination (R^2).

```
clc
clear all
close all

%Calibration of Kh using their Chlorine predicted value for no geomembrane.

t = [14 9.5 4.5] ; %time (years)

C0 = [251 608 510*0.8];    %leachate concentrations(mg/L)
C0 = C0/35.5;  %(mmol/L)

z = [2.5 2.25 2 1.75 1.5 1.25 1 0.75 0.5 0.25 0];
Cm = [5 5 5 5.5 6 8 9 11 12 13 12]; %their predicted values

cali = 0.5:0.1:1.5; %changing the value of Kh by these ratios
Kh = Kh0*cali;  %creating a row of Kh values

for i = 1:length(cali)  %loop for different Kh values

    q = Kh(i)*(delH/delz); %darcy flux (m/s)
    v = q/n;    %seepage velocity (m/s)

    C = cfun(t,z,C0,Cb,R,D,v);

    RMSE(i) = sqrt(mean((Cm-C).^2));
    deltaC = max(Cm)-min(Cm);
    CE(i) = RMSE(i)/deltaC*100; %calculating the error
    SSE = sum((Cm-C).^2);
    SSyy = sum((Cm-mean(Cm)).^2);
    R2(i) = 1-SSE/SSyy; %calculating the coeffecient of determination
end

varNames = {'Kh/Kh0','Kh','CE(%)','R2'};
T = table(cali',Kh',CE',R2','VariableNames',varNames);
disp(T)
```

The calibration result:

Kh/Kh0	Kh	CE(%)	R2
0.5	1e-10	6.1969	0.97379
0.6	1.2e-10	5.6061	0.97855
0.7	1.4e-10	5.1008	0.98224
0.8	1.6e-10	4.7146	0.98483
0.9	1.8e-10	4.4845	0.98627
1	2e-10	4.4408	0.98654
1.1	2.2e-10	4.595	0.98559
1.2	2.4e-10	4.9338	0.98338
1.3	2.6e-10	5.4278	0.97989
1.4	2.8e-10	6.0433	0.97507
1.5	3e-10	6.7512	0.96889

Based on the results of the 3 calibration studies done, we thought that there was no need to change the K_h value and the K_d value for Sodium. But the error for Potassium was higher than the expectable range, so we calibrated to the K_d value from 7 mL/g to 0.7 mL/g. This change in the K_d should be reasonable since such information is gathered experimentally. And the uncalibrated value isn't suitable probably because in the article a Langmuir sorption model is used for potassium and are assuming linear sorption for all chemicals.

4.3. Sensitivity Analysis

The aim of sensitivity analysis is to vary the values of system parameters across the range of likely values to determine the effect on the predicted output, by sensitivity analysis we can identify the most important system parameter. For sensitivity we need to first run the model for the base case using the parameter values given, and then repeat model runs by changing the values of system parameters by a certain degree one at a time. The formula for sensitivity, p is the parameter being analyzed:

$$S_p = \frac{C_p - C_{base}}{C_{base}} \times \frac{p}{\Delta p}$$

```
clc
clear all
close all
%This the file for sensitivity analysis. We have changed the parameters by
%a certian degree and compared their effect on the concentration profile of
%Sodium. To calcluate the concentration profiles the cfun.m file was used.


t = [14 9.5 4.5] ; %time (years)
z = 0:0.1:2.9;

C0 = [1425 3454 1640*0.8];    %leachate concentrations (mg/L)
C0 = C0/23;    %(mmol/L)

%Sensitivity Analysis
del = 0.2;  %20% change is parameter
fprintf("----- Sensitivity Analysis -----\n")
fprintf("The following parameters were increased by %d%%\n\n",del*100)

%Calculating sensitivity

%for soil parameters
fprintf("----- Soil Parameters -----\n")
sR = 1+(((ro*(1+del))*Kd)/n);
sensro = abs(((cfun(t,z,C0,Cb,sR,D,v)-cfun(t,z,C0,Cb,R,D,v))/...
    (cfun(t,z,C0,Cb,R,D,v))))*abs(ro/(del*ro));  %for dry density
fprintf("Sensitivity of dry density of soil: %8.2f%%\n",sensro*100)

sR = 1+(ro*Kd)/(n*(1+del));
sv = q/(n*(1+del));
sensn = abs(((cfun(t,z,C0,Cb,sR,D,sv)-cfun(t,z,C0,Cb,R,D,v))/...
    (cfun(t,z,C0,Cb,R,D,v))))*abs(ro/(del*ro));  %for porosity
fprintf("Sensitivity of porosity of soil: %8.2f%%\n",sensn*100)

sq = (Kh*(1+del))*(delH/delz);
sv = q/n;
sensKh = abs(((cfun(t,z,C0,Cb,R,D,sv)-cfun(t,z,C0,Cb,R,D,v))/...
    (cfun(t,z,C0,Cb,R,D,v))))*abs(Kh/(del*Kh));  %for conductivity
fprintf("Sensitivity of hydraulic conductivity of soil: %8.2f%%\n\n",...
    sensKh*100)

%for chemical parameters
fprintf("----- Chemical Parameters -----\n")
sensD = abs(((cfun(t,z,C0,Cb,R,D*(1+del),v)-cfun(t,z,C0,Cb,R,D,v))/...
    (cfun(t,z,C0,Cb,R,D,v))))*abs(D/(del*D));    %for diffusion coefficient
fprintf("Sensitivity of diffusion coefficient of soil: %8.2f%%\n",...
sensD*100)
```

```
sR = 1+(ro*(Kd*(1+0.2)))/n;
sensKd = abs(((cfun(t,z,C0,Cb,sR,D,v)-cfun(t,z,C0,Cb,R,D,v))/...
    (cfun(t,z,C0,Cb,R,D,v))))*abs(Kd/(del*Kd));    %for distribution coefficient
fprintf("Sensitivity of partitioning coefficient of soil: %8.2f%%\n\n",...
    sensKd*100)
```

The results of the sensitivity analysis:

```
----- Sensitivity Analysis -----
The following parameters were increased by 20%

----- Soil Parameters -----
Sensitivity of dry density of soil:    23.10%
Sensitivity of porosity of soil:    12.39%
Sensitivity of hydraulic conductivity of soil:     0.00%

----- Chemical Parameters -----
Sensitivity of diffusion coefficient of chemical:     6.90%
Sensitivity of partitioning coefficient of chemical:    23.10%
```

There are 2 parameters that affect the concentration profile the most. The concentration is most sensitive to the dry density of soil and partitioning coefficient of the chemical.

4.4. Validation

Validation is used to compare the verified and calibrated model output with a different set of measured output to test if the model is capable of simulating behavior of the system. For our model we have used the predicted concentrations for geomembrane being ineffective from the start. The error between our simulation and their predicted data is calculated using the RMSE formula. The ‘validation’ script is used for this, it is similar to the ‘main’ script. The values compared are for the time period, 0 to 14 years. The results of the validation are shown below.

```
The Chlorine concentration error:    4.44%
The Sodium concentration error:    2.26%
The Potassium concentration error:    5.84%
```

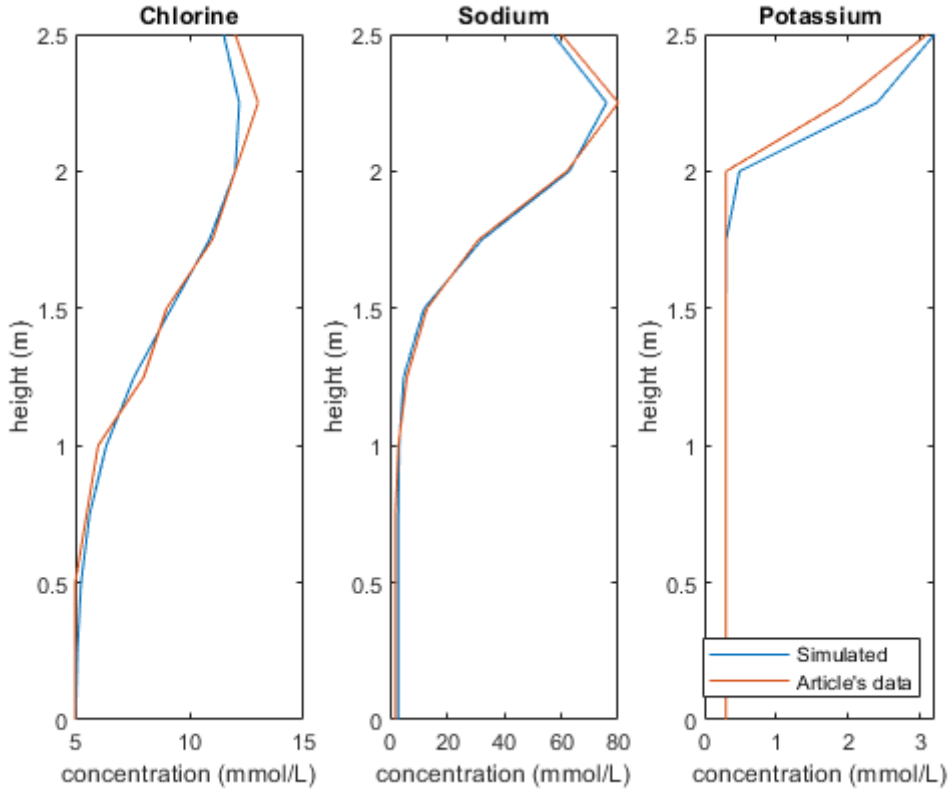


Figure 3 Our validated model

4.5. Model Application

4.5.1. Estimating the geomembrane failure time

The liner in our chosen article has a geomembrane on top of a compacted clay layer. The objective of the authors the article is to model the liner over a 14-year period for different geomembrane failure times and then comparing the plots with measured borehole values to assess with failure time fits best. We have tried to perform the same study by using the borehole measurements and determining the likely time of expiry using the coefficient of determination R^2 which can be used to determine the best fit to the data. The geomembrane K_h used in our model is the one mentioned in the complementary article written by the same authors on the performance of the geomembrane. The borehole measurements are in the following table.

Table 2 Borehole Measurements

Chlorine									
Borehole 1		**Borehole 2**		**Borehole 3**		**Borehole 4**		**Borehole 5**	
Depth (m)	**Conc (mmol/L)**	**Depth (m)**	**Conc (mmol/L)**	**Depth (m)**	**Conc (mmol/L)**	**Depth (m)**	**Conc (mmol/L)**	**Depth (m)**	**Conc (mmol/L)**
0.05	10	0.05	11	0.05	10	0.05	11.5	0.05	10.5
0.25	11.5	0.4	11.5	0.3	12	0.4	12	0.3	11
0.45	12.5	0.6	13	0.8	9	1.2	5.5	0.65	10.5
0.7	11.5	0.85	12	1.25	5.5	1.7	5	0.85	8.5
0.9	9.5	1.2	8	2	5			1.1	7
1.6	6	1.4	6						
1.7	6.5								
Sodium									
Borehole 1		**Borehole 2**		**Borehole 3**		**Borehole 4**		**Borehole 5**	

Depth (m)	Conc (mmol/L)	Depth (m)	Conc (mmol/L)	Depth (m)	Conc (mmol/L)	Depth (m)	Conc (mmol/L)	Depth (m)	Conc (mmol/L)
0.05	62	0.05	64	0.05	64	0.05	62	0.05	55
0.25	62	0.35	70	0.2	70	0.4	45	0.4	57
0.4	45	0.55	55	0.45	50	1.2	10	0.6	18
0.7	20	0.8	20	0.8	25	1.7	5	0.85	7
0.9	7	1.1	5	1.25	6			1.1	4
1.6	5	1.4	5	1.6	5				
1.8	5			2	5				

Potassium									
Borehole 1		Borehole 2		Borehole 3		Borehole 4		Borehole 5	
Depth(m)	Conc (mmol/L)	Depth(m)	Conc (mmol/L)	Depth(m)	Conc (mmol/L)	Depth(m)	Conc (mmol/L)	Depth(m)	Conc (mmol/L)
0.05	1.5	0.05	1.1	0.05	0.9	0.05	1.3	0.05	0.9
0.25	0.3	0.35	0.7	0.25	0.5	0.4	0.5	0.3	0.8
0.4	0.5	0.5	0.7	0.4	0.3	1.2	0.3	0.6	0.5
0.7	0.2	0.8	0.6	0.7	0.4	1.45	0.3	0.85	0.3
0.9	0.3	1.2	0.3	1.3	0.3	1.75	0.25	1.1	0.2
1.6	0.2	1.4	0.3	1.6	0.3				
1.7	0.3			1.95	0.2				

The following 'geoCl_bor' script is used to compare the borehole values with our simulated Cl concentration profile for different failure times. In the script the composite liner's hydraulic conductivity is calculated using a geometric mean of the clay's and the geomembrane's hydraulic conductivity.

```
clc
clear all
close all

%This program will estimate the geomembrane failure time.

gKh = 1.1e-11;  %geomembrane hydaulic conductivity (m/s)

%Calculation of seepage velocity
delH = 3+3+2.9; %head difference (m)
delz =3+2.9;   %distance (m)
qC = cKh*(delH/delz); %darcyflux (m/s)
vC = qC/n;    %seepage velocity (m/s)

compKh = sqrt(cKh*gKh);
compq = compKh*(delH/delz);
compv = compq/n;    %composite liner velocity using geometric mean
%compv = 1.1e-11/n;

%Chemical Parameters
D = 7e-10;  %diffusion coefficient (m2/s)
Kd = 0; %linear partitioning coefficient (mL/g)

R = 1+((ro*Kd)/n);  %retardation coefficient(-)

z = [2 1.7 1.7 1.6 1.4 1.25 1.2 1.2 1.1 0.9 0.85 0.85 0.8 0.7 0.65 0.6 ...
    0.45 0.4 0.4 0.3 0.3 0.25 0.05 0.05 0.05 0.05 0.05];
CB = [5 6.5 5 6 6 5.5 8 5.5 7 9.5 12 8.5 9 11.5 10.5 13 12.5 11.5 12 12 ...
    11 11.5 10 11 10 11.5 10.5];     %Borehole Values
```

```
t = [14 9.5 4.5];   %inactive after 0 years
C0 = [251 608 510*0.8]/35.5;
C(1,:)= cfun(t,z,C0,Cb,R,D,vC);

t = [14 10 9.5 4.5];  %inactive after 4 years
C0 = [251 251 608 510*0.8]/35.5;
C(2,:)= cfun(t(1),z,C0(1),Cb,R,D,compv);
C(2,:)= cfun(t(2:end),z,C0(2:end),C(2,:),R,D,vC);

t = [14 9.5 8 4.5]; %inactive after 6 years
C0 = [251 608 608 510*0.8]/35.5;
C(3,:)= cfun(t(1:2),z,C0(1:2),Cb,R,D,compv);
C(3,:)= cfun(t(3:end),z,C0(3:end),C(3,:),R,D,vC);

t = [14 9.5 6 4.5]; %inactive after 8 years
C0 = [251 608 608 510*0.8]/35.5;
C(4,:)= cfun(t(1:2),z,C0(1:2),Cb,R,D,compv);
C(4,:)= cfun(t(3:end),z,C0(3:end),C(4,:),R,D,vC);

for i = 1:length(C(:,1))
    SSE = sum((CB-(C(i,:))).^2);
    SSyy = sum((CB-mean(CB)).^2);
    R2(i) = 1-SSE/SSyy;
end
```

The results for Chlorine:

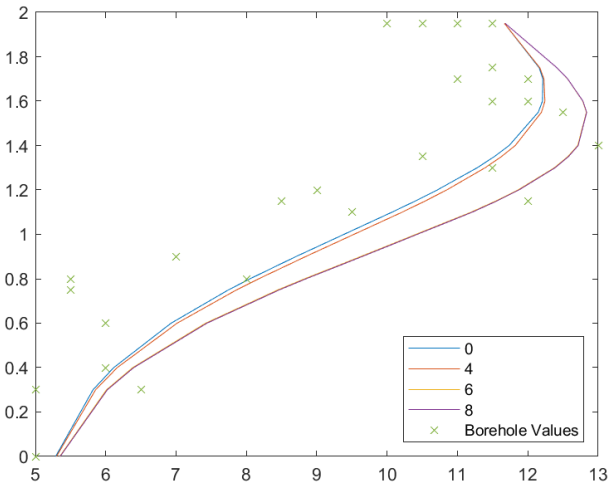
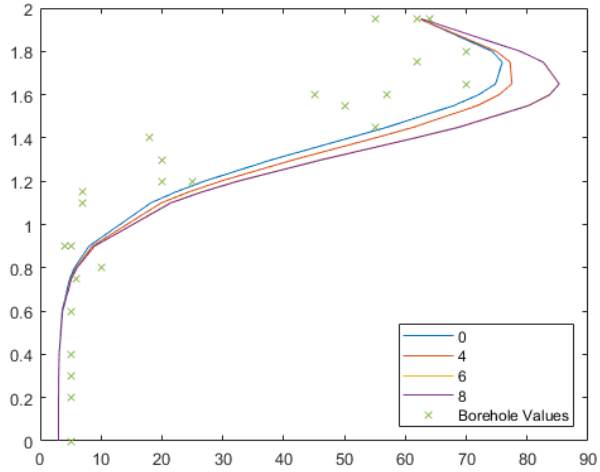


Figure 4 Chlorine concentration profile for geomembrane failure estimation

Inactive after	R2
0 yrs	0.78272
4 yrs	0.76737
6 yrs	0.60698
8 yrs	0.60265

The same was done for Sodium and Potassium. The results for Sodium are presents below. For potassium, the results weren't suitable as difference in the borehole values and our simulated values were too large.



Inactive after	R2
0 yrs	0.77754
4 yrs	0.70388
6 yrs	0.52012
8 yrs	0.51585

Figure 5 Sodium concentration profile for geomembrane failure estimation

Based on these 2 graphs and the R^2 values calculated, we can observe that the geomembrane probably became ineffective during the first 4 years. We can also observe that as the duration of the geomembrane's effective time increases from 0 to 8 years, higher concentration is observed towards the top of the liner. We can also see that for the inactive at 6 years and inactive at 8 years, the difference in concentration profile isn't visible, the difference between the concentration profile isn't visible. Our graphs don't completely imitate the plots in the article, this can be attributed to several reasons: our borehole values were measured from the graphs using a naked eye, we have assumed the porosity and dry density are constant (the authors of our main article haven't), and we've used a geometric mean to find the conductivity of the composite liner.

4.5.2. Effect of Biannual Variation of Leachate Height and Concentration

The leachate lagoon site is in Ontario, Canada. The leachate received by this site comes from a landfill. We have collected annual precipitation for where the site is. The data is shown in the table below. We observed that the precipitation is high for 6 months and low for the other 6 months. So, we are going to simulate the affect of the precipitation on the concentration profile and compare it to the simulated data in which we do not consider the biannual variation. To simulate the variation, we assume that the amount of waste in the landfill is constant. So, when precipitation is high, the volume (hence the leachate height will increase) and the concentration will decrease inversely because there will be less contaminants per volume of leachate. The average leachate concentration will be constant during both cases. And we are assuming that the geomembrane fails after 4 years.

Table 3 Precipitation data for our site (Climate-data.org, 2019)

Precipitation Data				**Leachate Concentration (mg/L)**		
Month	**Precipitation (mm)**	**6-Month Average Precipitation (mm)**	**Leachate Height values (m)**	**Chlorine**	**Sodium**	**Potassium**
10	124					
11	193					
12	238					
1	267					
2	217					
3	189	204.67	4.57	289.09	1642.31	119.82
4	107	63.83	1.43	926.91	5265.69	384.18

5	81					
6	40					
7	31					
8	47					
9	77					
Average	134.25		3	608	3454	252

The ‘scenario1_Cl’script for modelling the chlorine concentration profiles is given below. The scripts for Sodium and Potassium are like this one.

```
clc
clear all
close all

%This file shows how a variable head would effect the chlorine
%%concentration profile.

t = [14 10];
C0 = 608/35.5;
Cog = cfun(t(1),z,C0,Cb,R,D,compv);
Cog = cfun(t(2),z,C0,Cog,R,D,vC);


t = 0.5:0.5:14;
t = sort(t,'descend');
lh = [4.57 1.43];
hvals = [lh lh lh lh lh lh lh lh lh lh lh lh lh lh];
lC0 = [289.09 926.91]/35.5;
C0vals = [lC0 lC0 lC0 lC0 lC0 lC0 lC0 lC0 lC0 lC0 lC0 lC0 lC0 lC0];

%Calculation of seepage velocity
delH = hvals+3+2.9; %head difference (m)
delz = 3+2.9;   %distance (m)
qC = cKh*(delH/delz); %darcy flux (m/s)
vC = qC/n;    %seepage velocity (m/s)
compq = compKh*(delH/delz);
compv = compq/n;    %composite liner velocity using geometric mean

for i = 1:length(t)
    if t(i) > 10
        Cprec(i,:)= cfun(t(i),z,C0vals(i),Cb,R,D,compv(i));
    else
        Cprec(i,:)= cfun(t(i),z,C0vals(i),Cb,R,D,vC(i));
    end
    Cb = Cprec(i,:);

end
Cprec = Cprec(end,:);

L = max(z)-z;
plot(Cprec, L,Cog, L)
ylabel('Liner Height (m)')
xlabel('Concentration (mmol/L)')
legend('Using Biannual Variation','Using Average','location','southeast')
```

The resulting graphs for Chlorine and Sodium are shown below.

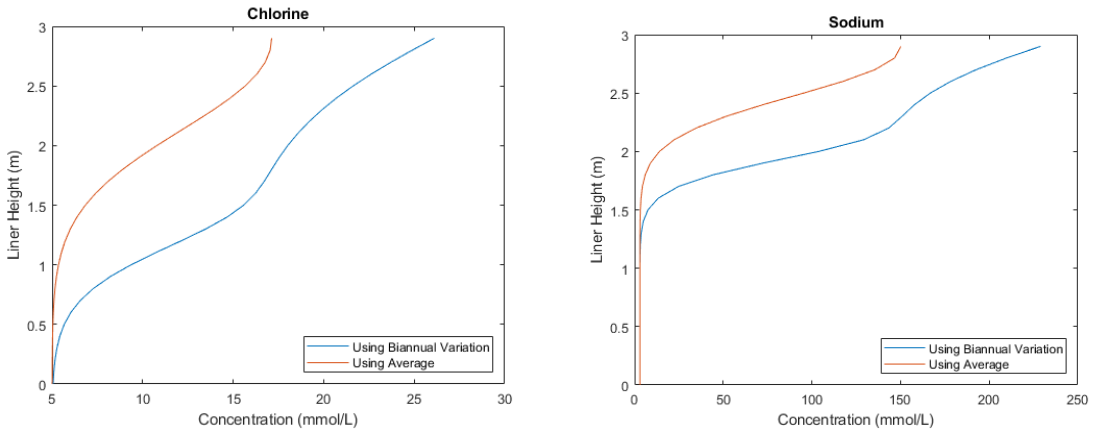


Figure 6 Biannual variation vs. average concentration profiles for Chlorine and Sodium

From the graphs, we can see that in both cases taking the biannual variation into account greatly affects our simulations. Because of taking the variation into account, the chlorine values through out the liner are higher that the ones simulated using an average value. But the variation doesn't affect the extent of the contamination by the chemical, in both graphs the concentration reaches the initial soil concentration at almost the same depth. From this, we can see that without taking the variation into account the concentration profile may be over simplified.

4.5.3. Effect of leachate height on the concentration profile

In this scenario, we simulate the concentration profiles using different values of leachate height to check the effect of the leachate height on the concentration profile. The leachate height values used are 1 m, 3 m, 6 m, 20 m. These concentration profiles have been prepared for all three contaminants. The 'scenario2a_Cl'script for Chlorine is shown below. The scripts for the other two chemicals are similar.

```
clc
clear all
close all

%This file shows how an increase or decrease in head would affect the
%concetration profile of chlorine.

z = 0:0.1:cL;

L = max(z)-z;

lhvals = [1 3 6 20];
for i = 1:length(lhvals)

    lh = lhvals(i);
    %Calculation of seepage velocity
    delH = 3+cL+lh; %head difference (m)
    delz = 3+cL;   %distance (m)
    q = cKh*(delH/delz); %darcyflux (m/s)
    vC = q/n;    %seepage velocity (m/s)
    compq = compKh*(delH/delz);
    compv = compq/n;    %composite liner velocity using geometric mean

    t = [14 9.5 4.5];
    C0 = [251 608 510*0.8];
    C_ng(i,:) = cfun(t,z,C0,Cb,R,D,vC);
```

```
    C_nf(i,:) = cfun(t,z,C0,Cb,R,D,compv);

    t = [14 10 9.5 4.5];
    C0 = [251 251 608 510*0.8];
    C_f(i,:)= cfun(t(1),z,C0(1),Cb,R,D,compv);
    C_f(i,:)= cfun(t(2:end),z,C0(2:end),C_f(i,:),R,D,vC);

end
subplot(1,3,1)
plot(C_ng,L)
hold on
plot(Cl_L*ones(length(z),1)',L,':','LineWidth',1.5)
xlabel('Conc. (mg/L)')
ylabel('Liner Height (m)')
title('No Geomembrane')

subplot(1,3,2)
plot(C_f,L)
hold on
plot(Cl_L*ones(length(z),1)',L,':','LineWidth',1.5)
xlabel('Conc. (mg/L)')
ylabel('Liner Height (m)')
title('Fails after 4 yrs')

subplot(1,3,3)
plot(C_nf,L)
hold on
plot(Cl_L*ones(length(z),1)',L,':','LineWidth',1.5)
xlabel('Conc. (mg/L)')
ylabel('Liner Height (m)')
title('Never fails')
legend('1 m','3 m','6 m','20 m','Limit','location','southeast')
```

The Chlorine result is shown on the next page. The plots for sodium and potassium follow similar trends.

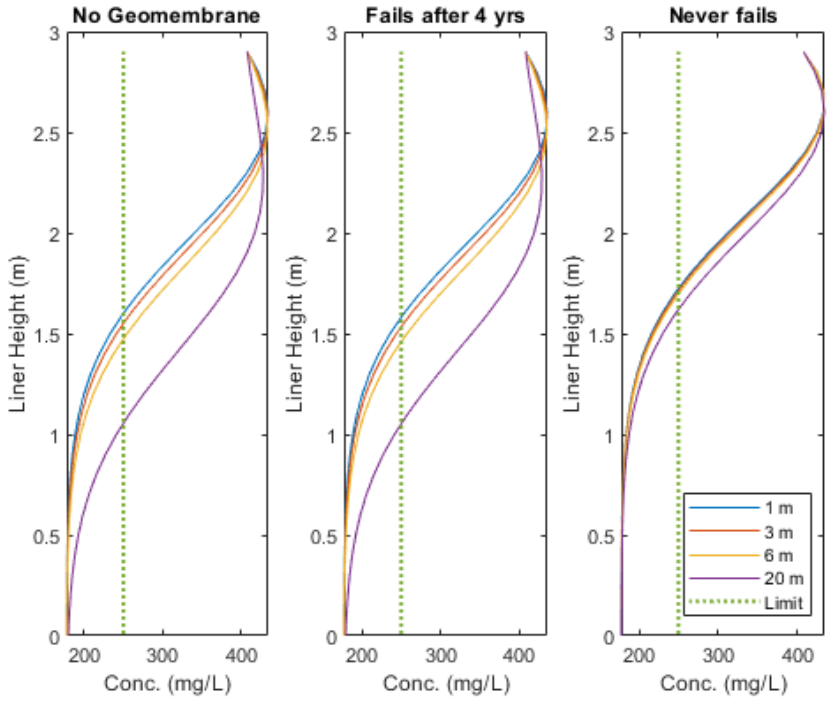


Figure 7 Effect of leachate heights on 3 different liner setups

In the second part of the scenario, we have calculated the maximum leachate height possible before the concentration at the bottom exceeds the concentration standards mentioned in the article. For this purpose, only chlorine was considered since it is a conservative contaminant and it does not sorb, so it would always be the first to reach the bottom. The 'scenario2b' script for it is like the script for the first part, the only difference is a while loop into which checks when the limit is exceeded. Also, the leachate concentration was kept constant at the maximum value mentioned in the article. To keep this report concise, I will only report the results for the second part.

The results are:

```
In case of no geomembrane, the maximum leachate height is   64.90 m.
In case of the geomembrane failing after 4 years, the maximum leachate height is   66.20 m.
In case of the geomembrane never failing, the maximum leachate height is  295.70 m.
```

By looking at the plots for the first part, we can see that by increasing the leachate height the concentration profile shifts downwards. That means that the concentration travels more with an increase in the leachate height. The graphs for no geomembrane and the geomembrane failing after 4 years is similar, the concentration profiles follow a similar trend. But considering that the geomembrane is intact for the complete 14 years the graph is different, the increase or decrease in the concentration profile is relatively small. In none of these cases the concentration exceeded the limits at the bottom of the liner. The second part's results show that even in the case without a geomembrane the maximum leachate height allowed before the limit is crossed is unreasonably high. And in that case the geomembrane which fails after 4 years doesn't change the result significantly.

4.5.4. Effect of time on the concentration profile

In this scenario, we simulate the concentration profiles using different values of duration for which the lagoon is operational to check the effect of the time on the concentration profile. The concentration profiles were simulated for durations of 10 years, 14 years, 30 years and 100 years. These concentration profiles have been prepared for all three contaminants. The 'scenario3_Cl'script for Chlorine is shown below. The scripts for the other to chemicals is similar.

```
clc
clear all
close all

%This file compares how an increase of decrease in the operation of the
%lagoon will affect the concentration profile.

L = max(z)-z;

tdes = [10 14 30 100];
for i = 1:length(tdes)
    t = [tdes(i) tdes(i)-4.5 tdes(i)-9.5];
    C0 = [251 608 510*0.8];
    C_ng(i,:) = cfun(t,z,C0,Cb,R,D,vC);
    C_nf(i,:) = cfun(t,z,C0,Cb,R,D,compv);

    t = [tdes(i) tdes(i)-4 tdes(i)-4.5 tdes(i)-9.5];
    C0 = [251 251 608 510*0.8];
    C_f(i,:)= cfun(t(1),z,C0(1),Cb,R,D,compv);
    C_f(i,:)= cfun(t(2:end),z,C0(2:end),C_f(i,:),R,D,vC);

end
```

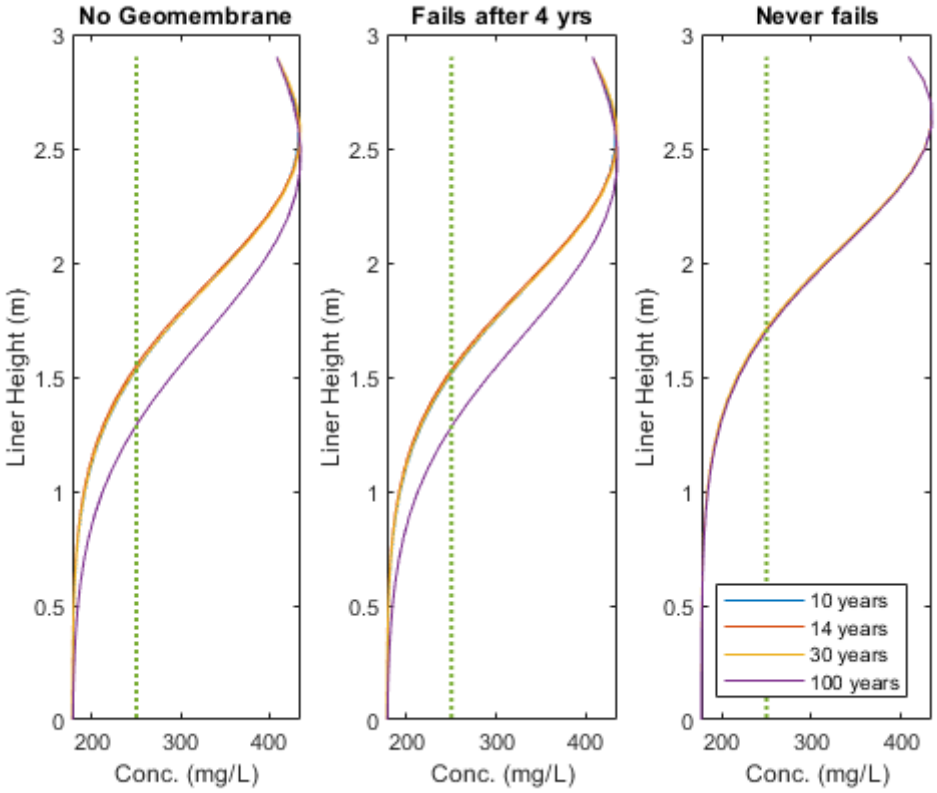


Figure 8 Effect of Operational duration on the concentration profile

By looking at the plots, we can see that by increasing the duration of operation of the lagoon the concentration profile shifts downwards. That means that the concentration travels more with an increase in time. The graphs for 10, 14 and 30 years don't vary much in all the plots, only if we increase the duration to 100 years, we see a difference in the concentration profile. In the case of geomembrane never failing, even for 100 years the concentration profile is the same. From these plots we can conclude that varying the duration of operation of the lagoon wont much of a difference unless the duration is unrealistically long. Most lagoons for landfill leachate and tailing waste are designed for 30 years so for all practical purposes the duration doesn't affect the concentration profile significantly.

4.6. Discussion of Modelling Results

In this modelling study of the performance of a leachate lagoon line, we found the following results:

- In order to make it simple to model the liner performance, the changes of the clay with depth were ignored, leading to differences between our model and the article's predicted values
- In the calibration of our model we expected the results for the predicted values for geomembrane failing from the start and simulated data to be compatible. Our simulations were accurate except the one for potassium, the linear partitioning coefficient had to be calibrated to fit better.
- In the sensitivity analysis, the dry density and linear partitioning coefficient were found to the most sensitive parameters.
- In the validation of our model, we validated our model using the article's predicted values for 14 years. Our calibrated model was found to be appropriate having a low error.
- In our scenarios:
    - Our geomembrane failure time study wasn't like the one done by the authors of the article. There were a few simplifications that could've led to the difference. Our model still correctly predicted the geomembrane failure time.

- Biannual variation of chemical leachate concentration and leachate head due to precipitation leads to higher chemical concentrations throughout the liner depth.
- The leachate height is had a considerable effect on the concentration profile, an increase in leachate height increase the concentration at every depth.
- The duration of operation of the lagoon doesn't have a substantial effect on the concentration profile.

5. Summary and Conclusion

The leachate lagoon liner we modeled based was based on the one in our main article 'The 14-year performance of a compacted clay liner used as part of a composite liner system for a leachate lagoon'. We focused on the compacted clay part of the liner. Instead of using different dry densities and porosities, we used average values through the liner. For potassium, we used a linear partitioning coefficient instead of a Langmuir sorption model to make the modelling easier. This led to problem's in its modelling even after calibration. An issue we encountered was that there is a discrepancy between the initial soil concentration for chlorine reported(4 mmol/L) in the article and the value shown in the graphs (5 mmol/L), we chose to use the latter value for our model.

To stop the chemicals from reaching the underlying aquifer, the most effective way would be to keep the amount of water or the liner as low as possible. And if data is available for such sites, a more accurate and descriptive model would be obtained if the seasonal or biannual variation is considered. An increase in operation duration wouldn't affect the chemical profile.

NOTE: Some of the m. file scripts provided were cropped to keep the length of the report short.

6. References

Climate-data.org. (2019, December 27). *Climate Canada: Weather by Month*. Retrieved from Climate Data: https://en.climate-data.org/north-america/canada-116/

Lake, C. R. (2005). The 14-year Performance of a Compacted Clay Liner used as Part of a Composite Liner System for a Leachate Lagoon. *Geotech Geol Eng 23*, 657–678 .

Rowe, R. K. (2003). Evaluation of an HDPE geomembrane after 14 years as a leachate lagoon liner. . *Canadian Geotechnical Journal*, 536-550.

Van Genuchten, M. T. (1982). Analytical Solutions of the One-Dimensional Convective-Dispersive Solute Transport Equation.

TASK DIVISION

We all participated in each part of the term project and the preparation of this report. The following table shows who was the main person for each step.

Team Member	**Duties**	**Expected contribution (%)**
Erdem Arslan	Was responsible for coming up with the scenarios and running the simulation.	25
Yunus Duruk	Was responsible for writing the report and debugging the code.	25
Amin Ghaderikia	Was responsible for the calibration, validation, verification.	25
Waqas Bin Hamed	Was responsible for the conceptual and mathematical model and wrote the MATLAB files for the basic function	25