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Machine Problem 1:

ONE-DIMENSIONAL POLLUTANT MIGRATION

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In Partial Fulfillment

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Academic Integrity Pledge:

On our honor, we did not give nor receive inappropriate aid in this Machine Problem.

ABSTRACT

One application of parabolic partial differential equations that would be of great interest in Civil Engineering is how we can describe the transport of various hazardous contaminants in a liner of a sanitary landfill. This Machine Problem aims to generate a model describing the migration of 6 contaminant species through the 3-meter liner of a single clay liner system sanitary landfill using the Forward-Time Center-Space and crank-Nicholson methods. Using the one-dimensional advection-dispersion-reaction equation and finite differential equations, the group were able to generate numerical models that could be used to program and find solutions to the problem. After graphing the concentration through the 3-m depth of the liner of all contaminants from 0 to 60 years, using the step sizes $\Delta t = 0.5\ yrs.$ and $\Delta z = 0.2\ m$, it was also found out that the contaminants from lowest to highest concentration were: Magnesium, Calcium, DCM, Sodium, Acetone, and Chloride. Chloride was also found to be the first contaminant specie to penetrate the 3-m liner. The two methods were then compared by tabulating their concentrations at 20 years, verifying that concentrations in the Crank-Nicholson method are slightly higher than that of the FTCS method. Finally, it was proved that Crank-Nicholson method is better and more accurate than Forward-Time Center-Space method because it is unconditionally stable and poses no restriction unlike the FTCS method.

I. Problem Statement

A. Physical Significance of the Problem

A problem of great importance in Civil Engineering, more commonly in its Environmental and Geotechnical Engineering branches is to understand how chemical or biological contaminants are transported through a system. In this machine problem, we consider the system to be a landfill liner, a low permeability barrier which is laid down under engineered landfill sites.

Until it deteriorates, a landfill liner retards the migration of leachate and its toxic constituents/contaminants into underlying aquifers or nearby rivers, causing spoliation of the local water.[4] In addition, landfills may also pose several hazards in public health through contamination of water resources, vegetation hazards, and hazardous air emissions. Which is why it is important that sanitary landfills must have adequate design, construction, and maintenance and that appropriate landfill liners with excellent characteristics must always be taken into consideration.

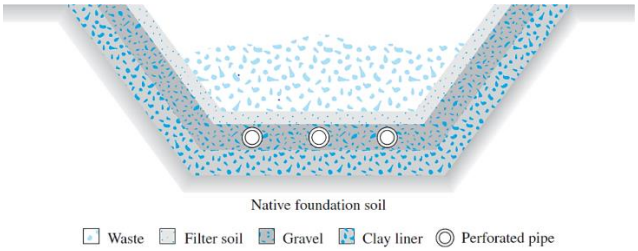


Figure 1. Cross section of a Single Clay Liner System

This Machine Problem aims to generate a model describing the migration of 6 contaminant species through the 3 m liner of a given single clay liner system sanitary landfill (Figure 1) using the Forward-Time-Center-Space (FTCS) and the Crank-Nicholson methods. The migration parameters of the 6 contaminant species - Acetone, DCM, Calcium, Chloride, Sodium, and Magnesium are shown in Table 1.

Table 1. Contaminant Species and their Migration Parameters

Parameter	Acetone	DCM	Calcium	Chloride	Sodium	Magnesium
Dispersion Coefficient, D	0.018	0.008	0.012	0.018	0.014	0.012
Retardation factor, R	1.770	1.240	6.000	1.000	1.450	13.500

An initial condition is shown in Equation 1 which signifies that the landfill was initially empty and has no sign of contamination anywhere. Equations 2 and 3 shows the boundary conditions for the problem. After a decade, the landfill then reached its full capacity. Equation 2.1 symbolizes the concentration of contaminant for the surface of the landfill until a decade. Then, after 8 years, the inflow of contaminants was constant, as portrayed in Equation 2.2. In the succeeding 2 years, the contents of the landfill were removed to use the land for residential use. As a result, the concentration of contaminant linearly decreased until there was no contamination left (Eq. 2.3). After 20 years, the landfill is now empty and no signs of any contamination were observed (Eq. 2.4). Equation 3 is a *Neumann boundary condition* wherein the value of the normal derivative of the function is defined to be zero. Since it is assumed that the soil layer below the clay liner is impermeable, there is no contamination beyond that area.

$$C(z,0) = 0 \tag{1}$$

$$c(0,t) = \begin{cases} 10{,}000 - 100(t-10)^2, & 0 \le t \le 10\ yrs & (2.1) \\ 10{,}000, & 10 < t \le 18\ yrs & (2.2) \\ -5000t + 100{,}000, & 18 < t \le 20\ yrs & (2.3) \\ 0, & t > 20\ yrs & (2.4) \end{cases} \quad \left(\frac{mg}{L}\right)$$

$$C_z(3,t) = 0 \tag{3}$$

B. The One-Dimensional Advection-Dispersion-Reaction Equation

In order for us to generate a model describing the migration of the six contaminants in the liner, we must first have a governing equation – the 1-D Advection-Dispersion-Reaction Equation. It is a parabolic partial differential equation that is derived from the conservation of mass, continuity equation, and mass balance. Using these concepts and processes will give us the final equation:

$$R\frac{\partial C}{\partial t} = v\frac{\partial C}{\partial z} + D\frac{\partial C^2}{\partial t^2} \tag{4}$$

Where *C(z,t)* is the concentration of the pollutant at a distance *z* from the surface at any time t, v is the given settling velocity 0.0063 m/year, D is the dispersion coefficient in m^2/yr, and R is the retardation factor.

Take note that in Equation 4, the term $v\frac{\partial C}{\partial z}$ represents the advective transport while $D\frac{\partial C^2}{\partial t^2}$ represents the dispersive transport.

II. Numerical Model

A. Forward-Time-Center-Space (Explicit) and Crank-Nicholson (Implicit) Methods.

In this machine problem, two numerical methods in solving parabolic partial differential equations (PDEs) namely, the Forward-Time-Center-Space (FTCS) and Crank-Nicholson Methods, were demonstrated. These two methods are considered part of the Finite Difference method wherein derivatives in a differential equation are replaced with differential formula or approximations. These differential formulas are purely composed of algebraic equations and therefore, can be solved algebraically to get approximate solutions. Both of these methods are based mainly on the forward (Equation 5) and central (Equations 6 and 7) finite difference formulas in getting the first and second derivatives of a function *f(x)*.

$$f'(x) = \frac{f(x+h)-f(x)}{h} \tag{5}$$

$$f'(x) = \frac{f(x+h)-f(x-h)}{2h} \tag{6}$$

$$f''(x) = \frac{f(x+h)-f(x)+f(x-h)}{h^2} \tag{7}$$

Where *f'(x)* and *f''(x)* are the first and second derivatives of the function *f(x)*, respectively, and *h* is the step size.

The first method to be used is the explicit finite difference Forward-Time-Center-Space (FTCS) method. This method is said to be explicit because the solution at a point at a time level *n+1* can be expressed explicitly in terms of a known solution at a previous time level *n*.[2] From the name itself, it uses forward finite difference in time using quantities from previous time steps and central difference in space using the values obtained previously. Having said that, we can use the forward and central finite difference equations (5), (6), and (7) to obtain equations for the first or second partial derivative of a time and space dependent function *u(x,t)* with respect to time or space. Equation 8 shows the second partial derivative of *u(x,t)* with respect to space.

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{j,i+1}-2u_{j,i}+u_{j,i-1}}{(\Delta x)^2} \tag{8}$$

Where Δx is the step size corresponding in space. Since we are only dealing with a one-dimensional problem, Δx can be expressed as the length of consideration over the number of nodes.

In addition, we take note that i corresponds to a point in space (or a node) while j corresponds to a certain time.

$$\frac{\partial u}{\partial x} = \frac{u_{j,i+1} - u_{j,i-1}}{2\Delta x} \tag{9}$$

$$\frac{\partial u}{\partial t} = \frac{u_{j+1,i} - u_{j,i}}{\Delta t} \tag{10}$$

Equation 9 shows the first partial derivative of *u(x,t)* with respect to space while Equation 10 shows the first partial derivative of *u(x,t)* with respect to time. We can observe that Equations 8 and 9 are both based on the central finite difference equations 7 and 6, respectively to ensure a much more accurate partial derivative in space while Equation 10 is based on the forward difference formula (Eqn. 5).

The major advantage of explicit finite difference methods such as FTCS is that they are relatively simple and computationally fast. However, the main drawback is that stable solutions are obtained only when $0 < \frac{k\Delta t}{\Delta x^2} < 0.5$. That is, $u_{j,i}$ must have a positive coefficient or be absent in the equation.[1]

The second method is the implicit finite difference Crank-Nicholson Method. It is said to be implicit if the solution at a point in the solution time level *n+1* depends on the solution at neighboring points in the solution time level, which are unknown.[2] The output of the time step depends on itself, so a causal recursive computation is not specified. The main difference of the Crank-Nicholson method with FTCS method is that we get the average of the two first and second-order centered-space approximations. That is, you get the average of Equation 8 for the time steps j and j+1 as shown in Equation 11.

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{j+1,i+1} - 2u_{j+1,i} + u_{j+1,i-1}}{2(\Delta x)^2} + \frac{u_{j,i+1} - 2u_{j,i} + u_{j,i-1}}{2(\Delta x)^2} \tag{11}$$

In addition, Equation 9 must also be based on the central difference formula while Equation 10 also hold true for Crank Nicholson method. Also, this method is 2nd order accurate in both time and space approximations. One can prove that Crank-Nicholson's method is *unconditionally stable* which means that this method poses no restriction on the previously mentioned limitation of FTCS.

B. Formulation of the finite difference models

For the formulation of the Forward-Time Center-Space (FTCS) finite difference model of the problem, we start by using Equations 8, 9, and 10 and replacing the function *u(x,t)* with the pollutant concentration *C(z,t)* and x with the depth *z*. In addition, we take note that *j* still corresponds to a certain time but *i* now corresponds to a certain depth *z* within the 3-meter liner. Doing this will lead us to the equations:

$$\frac{\partial^2 C}{\partial z^2} = \frac{C_{j,i+1} - 2C_{j,i} + C_{j,i-1}}{(\Delta z)^2} \tag{12}$$

$$\frac{\partial C}{\partial z} = \frac{C_{j,i+1} - C_{j,i-1}}{2\Delta z} \tag{13}$$

$$\frac{\partial C}{\partial t} = \frac{C_{j+1,i} - C_{j,i}}{\Delta t} \tag{14}$$

Then, we plug in these three equations to the one-dimensional Advection-Dispersion-Reaction Equation (Eqn. 4). Taking note that R, *v*, and D are all constants, this will give us:

$$R\left(\frac{C_{j+1,i}-C_{j,i}}{\Delta t}\right) = v\left(\frac{C_{j,i+1}-C_{j,i-1}}{2\Delta z}\right) + D\left(\frac{C_{j,i+1}-2C_{j,i}+C_{j,i-1}}{(\Delta z)^2}\right) \quad (15)$$

Since we want to find the pollutant concentration for the next time step *j+1* at any given depth *I*, we must isolate the term $C_{j+1,i}$ which will lead us to:

$$C_{j+1,i} = C_{j,i}\left(1 - \frac{2D}{(\Delta z)^2}\cdot\frac{\Delta t}{R}\right) + C_{j,i+1}\left[\frac{\Delta t}{R}\left(\frac{v}{2\Delta z} + \frac{D}{(\Delta z)^2}\right)\right] + C_{j,i-1}\left[\frac{\Delta t}{R}\left(\frac{-v}{2\Delta z} + \frac{D}{(\Delta z)^2}\right)\right] \quad (16)$$

Letting $\alpha = 1 - \frac{2D}{(\Delta z)^2}\cdot\frac{\Delta t}{R}$, $\beta = \frac{\Delta t}{R}\left(\frac{v}{2\Delta z} + \frac{D}{(\Delta z)^2}\right)$, and $\gamma = \frac{\Delta t}{R}\left(\frac{-v}{2\Delta z} + \frac{D}{(\Delta z)^2}\right)$, simplifies the equation to:

$$C_{j+1,i} = \alpha C_{j,i} + \beta C_{j,i+1} + \gamma C_{j,i-1} \quad (17)$$

The next thing to do is to incorporate the boundary conditions given (Eqns. 2 and 3). For the topmost part of the 3-m liner (when depth z=0), we get the concentration from the piecewise Equation 2 and multiply the corresponding concentration to a multiplier. Using Equation 17, we set any number to the time index j (say, 0) and to the depth index i. Setting the boundary condition to be in the previous depth node i-1, we observe that the multiplier must be γ. For the Neumann Condition, we use the central finite difference formula (Eqn. 13). From Equation 3, $C_z(3,t) = 0$, and therefore,

$$\frac{\partial C}{\partial z} = \frac{C_{j,i+1}-C_{j,i-1}}{2\Delta z} = 0 \;\rightarrow\; C_{j,i+1} = C_{j,i-1} \quad (18)$$

Referring again to Equation 17 and the coefficient of the Neumann boundary is then the coefficient of the term $C_{j,i+1}$, which is β.

Transforming Equation 17 and the boundary conditions into its matrix form:

$$\begin{bmatrix} C_{j+1,1} \\ C_{j+1,2} \\ C_{j+1,3} \\ C_{j+1,4} \\ \vdots \end{bmatrix} = \begin{bmatrix} \alpha & \beta & 0 & 0 \cdots \\ \gamma & \alpha & \beta & 0 \cdots \\ 0 & \gamma & \alpha & \beta \cdots \\ 0 & 0 & \gamma+\beta & \alpha \cdots \\ \vdots & \vdots & \vdots & \vdots \ddots \end{bmatrix} \begin{bmatrix} C_{j,1} \\ C_{j,2} \\ C_{j,3} \\ C_{j,4} \\ \vdots \end{bmatrix} + \begin{bmatrix} \gamma \cdot C_{j,0} \\ 0 \\ 0 \\ 0 \\ \vdots \end{bmatrix} \quad (19)$$

Equation 19 will be the FTCS numerical model that will be used to code this part of the Machine Problem. Also take note that since the Neumann boundary condition has the same dependent variable with the main square matrix, we can just add its coefficient to the last row, second to the last column element of the main matrix. In addition, the size of the matrices in Equation 19 depends on the depth step size Δz and the number of nodes in the depth.

On the other hand, we formulate the Crank-Nicholson finite difference model of the problem by using Equations 9, 10, and 11 and also replacing the function *u(x,t)* with the pollutant concentration *C(z,t)* and x with the depth *z*. Modifying Equation 11:

$$\frac{\partial^2 C}{\partial z^2} = \frac{C_{j+1,i+1}-2C_{j+1,i}+C_{j+1,i-1}}{2(\Delta z)^2} + \frac{C_{j,i+1}-2C_{j,i}+C_{j,i-1}}{2(\Delta z)^2} \quad (20)$$

$$\frac{\partial C}{\partial z} = \frac{C_{j,i+1}-C_{j,i-1}+C_{j+1,i+1}-C_{j+1,i-1}}{4\Delta z} \quad (21)$$

Also, we can use Equation 14 for the first partial derivative with respect to time. Plugging in equations 14, 20, and 21 to the one-dimensional Advection-Dispersion-Reaction Equation (Eqn. 4) and also taking note that R, *v*, and D are all constants will give us:

$$R\left(\frac{C_{j+1,i}-C_{j,i}}{\Delta t}\right)=v\left(\frac{C_{j,i+1}-C_{j,i-1}+C_{j+1,i+1}-C_{j+1,i-1}}{4\Delta z}\right)+D\left(\frac{C_{j+1,i+1}-2C_{j+1,i}+C_{j+1,i-1}}{2(\Delta z)^2}+\frac{C_{j,i+1}-2C_{j,i}+C_{j,i-1}}{2(\Delta z)^2}\right) \quad (22)$$

$$\frac{R}{\Delta t}(C_{j+1,i}-C_{j,i})=\frac{v}{4\Delta z}(C_{j,i+1}-C_{j,i-1}+C_{j+1,i+1}-C_{j+1,i-1})+\frac{D}{2(\Delta z)^2}(C_{j+1,i+1}-2C_{j+1,i}+C_{j+1,i-1}+C_{j,i+1}-2C_{j,i}+C_{j,i-1}) \quad (23)$$

Letting $\alpha=\frac{R}{\Delta t}$, $\beta=\frac{v}{4\Delta z}$, & $\gamma=\frac{D}{2(\Delta z)^2}$ and isolating all *C(z,t)* containing the next time step *j+1* regardless of any position step *i*, simplifies the equation to:

$$(-\gamma+\beta)C_{j+1,i+1}+(\alpha+2\gamma)C_{j+1,i}+(-\gamma+\beta)C_{j+1,i-1}=(\beta+\gamma)C_{j,i+1}+(\alpha-2\gamma)C_{j,i}+(-\beta+\gamma)C_{j,i-1} \quad (24)$$

The next thing to do is to incorporate the boundary conditions. The process is also similar to what we did in FTCS, but the difference is that we incorporate two boundary conditions matrices on both sides of the equation (at time j and j+1). The boundary condition in z=0 is still multiplied to a multiplier which, in this case, is the upper part of corresponding to the tri-diagonal square matrix (when time is j+1). These multipliers are shown in the matrices of Equation 25. The process in incorporating the Neumann boundary condition is also the same as that in FTCS (Eqn. 18). Equation 25 shows the equivalent matrix of Equation 24.

$$\begin{bmatrix}\alpha+2\gamma & -\gamma-\beta & 0 & 0 & \cdots\\ -\gamma+\beta & \alpha+2\gamma & -\gamma-\beta & 0 & \cdots\\ 0 & -\gamma+\beta & \alpha+2\gamma & -\gamma-\beta & \cdots\\ 0 & 0 & -2\gamma & \alpha+2\gamma & \cdots\\ \vdots & \vdots & \vdots & \vdots & \ddots\end{bmatrix}\begin{bmatrix}C_{j+1,1}\\ C_{j+1,2}\\ C_{j+1,3}\\ C_{j+1,4}\\ \vdots\end{bmatrix}+\begin{bmatrix}(-\gamma+\beta)\cdot C_{j+1,0}\\ 0\\ 0\\ 0\\ \vdots\end{bmatrix}=\begin{bmatrix}\alpha-2\gamma & \gamma+\beta & 0 & 0 & \cdots\\ \gamma-\beta & \alpha-2\gamma & \gamma+\beta & 0 & \cdots\\ 0 & \gamma-\beta & \alpha-2\gamma & \gamma+\beta & \cdots\\ 0 & 0 & 2\gamma & \alpha-2\gamma & \cdots\\ \vdots & \vdots & \vdots & \vdots & \ddots\end{bmatrix}\begin{bmatrix}C_{j,1}\\ C_{j,2}\\ C_{j,3}\\ C_{j,4}\\ \vdots\end{bmatrix}+\begin{bmatrix}(\gamma-\beta)\cdot C_{j,0}\\ 0\\ 0\\ 0\\ \vdots\end{bmatrix} \quad (25)$$

Equation 25 will be the Crank-Nicholson numerical model that will be used to code this other part of the Machine Problem. Also take note that since the Neumann boundary condition has the same dependent variable with the main square matrix, we can just add its coefficient to the last row, second to the last column element of the corresponding main matrices of the left and right sides of the equation. In addition, the size of the matrices in Equation 25 depends on the depth step size Δz and the number of nodes in the depth.

III. Implementation of Numerical Model

A. Usage of the finite difference models

To use Equation 19 for the FTCS method, we must know matrix addition, multiplication, and the inverse of a matrix. But before anything else, we must first set-up the coefficients and boundary matrices. The boundary array is shown in lines 74 to 88 for FTCS and lines 239 to 253 for Crank-Nicholson method. Then the initial condition was also set in the concentrations array. The constants array was then created, as seen in lines 97 to 113. Now that we have set all the arrays/matrices needed to use Equation 19, we can now perform matrix operations. We first multiply the constants matrix with the previous concentrations matrix. The boundary conditions matrix was then added using an if statement and is seen in lines 124 to 128. The code for this part is shown in a snippet below:

```
115         for(j=0;j<st;j++)
116         {
117  //Matrix Multiplication
118             for (i = 1; i < sz; i++)
119             {
120                 for (k = 1; k < sz; k++)
121                 {
122                   sum = sum + A[i-1][k-1]*C[k][j];
123                 }
124  //BC matrix
125             if(i==1)
126                 C[i][j+1] = sum + C[0][j];
127             else
128                 C[i][j+1] = sum;
129
130             sum = 0;
131             }
132         }
```

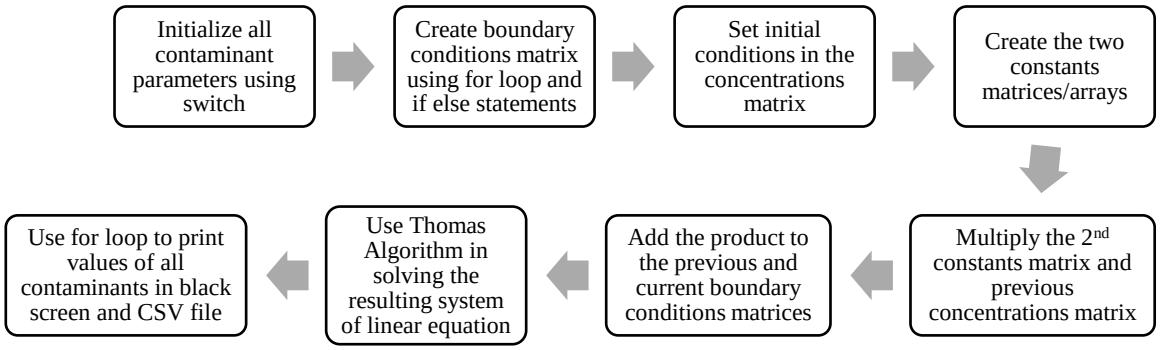
The FTCS method is that fast and simple. After the matrix operations, we can now print the computations in the black screen and in the CSV file as seen in lines 137 to 200. In addition, for loop and case structures were used to iterate all of the previously mentioned codes for all six contaminants.

For Crank-Nicholson method we refer to Equation 25 to find the solutions to the problem. Just like what we did in FTCS method, matrix addition and multiplication were also used, but we now add the concept of matrix algorithm in solving the corresponding systems of linear equations per iteration. The boundary conditions array has a similar process to FTCS, except that the multiplier now changed, as shown in Equation 25. This is seen in lines 239 to 253. Another difference of Crank-Nicholson method is that it requires two constants matrices, one on the left-hand side and one on the right-hand side of the Equation 25. The initialization of these two constant matrices are shown in lines 262 to 297. After setting up these arrays/matrices, we now multiply the second constants matrix (right-hand side of eqn. 25) with the previous concentrations matrix. Then, we add the boundary conditions matrices for both previous and current time steps. Finally, we can now use *Thomas Algorithm* to solve the resulting system of linear equation for that specific time step, wherein its code is in a separate function. After this, we can now print the values obtained. A snippet of the code for finding the solutions using Crank-Nicholson method is shown below:

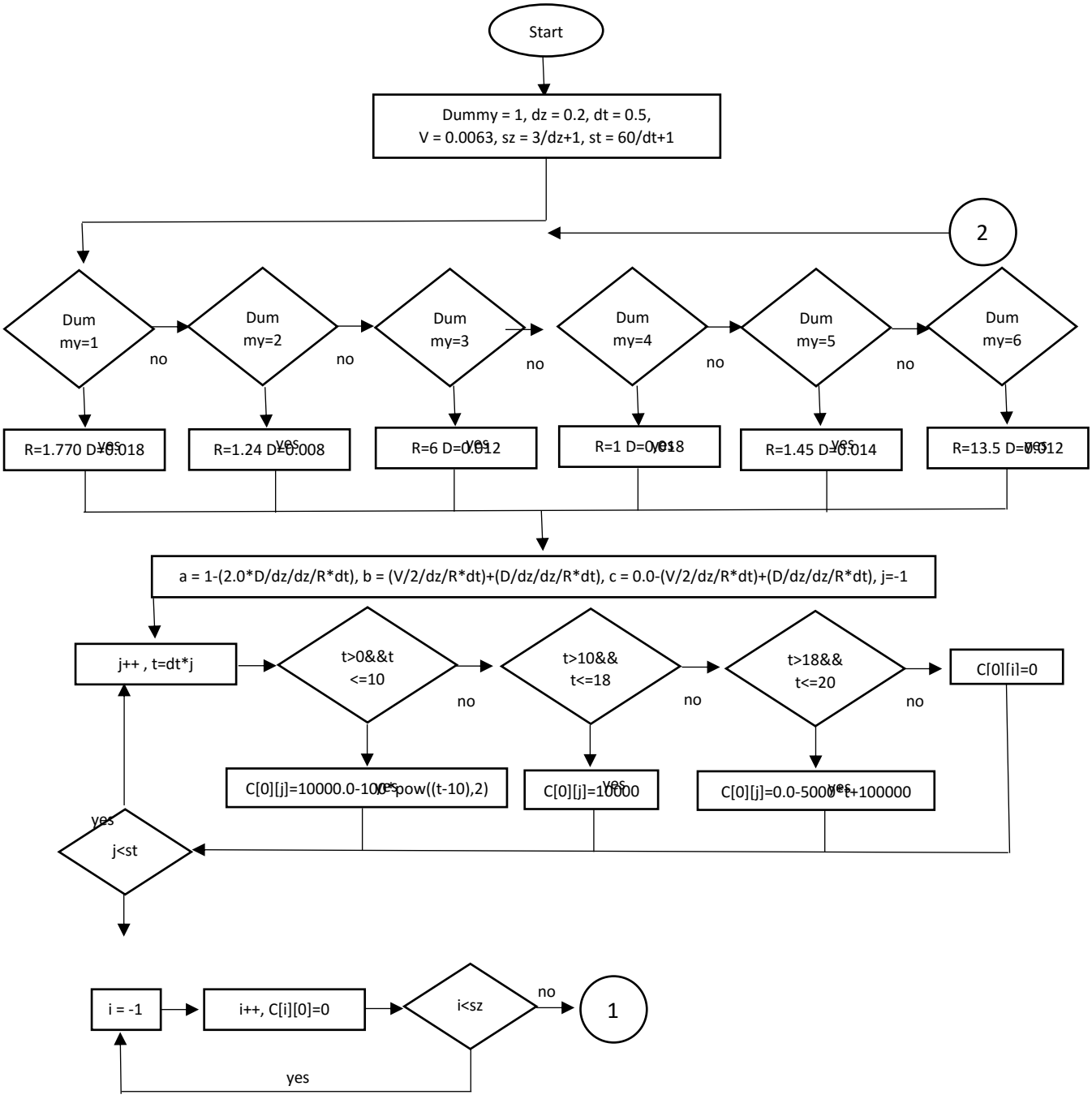
```
300 //Multiplication
301             for (i = 1; i < sz; i++)
302             {
303                 for (k = 1; k < sz; k++)
304                 {
305                   sum = sum + A2[i-1][k-1]*C2[k][j];
306                 }
307 //BC matrix
308             if(i==1)
309                 {C2[i][j+1] = sum + C2[0][j+1]+C2[0][j];} //added current and prev bound matrix only
310             else{
311                 C2[i][j+1] = sum ;
312             }
313             sum = 0;
314             }
315             for(i=0; i<sz;i++){
316                 dum2[i][j]=C2[i+1][j+1];
317             }
318
319     //THOMAS ALGORITHM
320
321             thomas(A1, dum2, sz-1, i, j, C2);
```

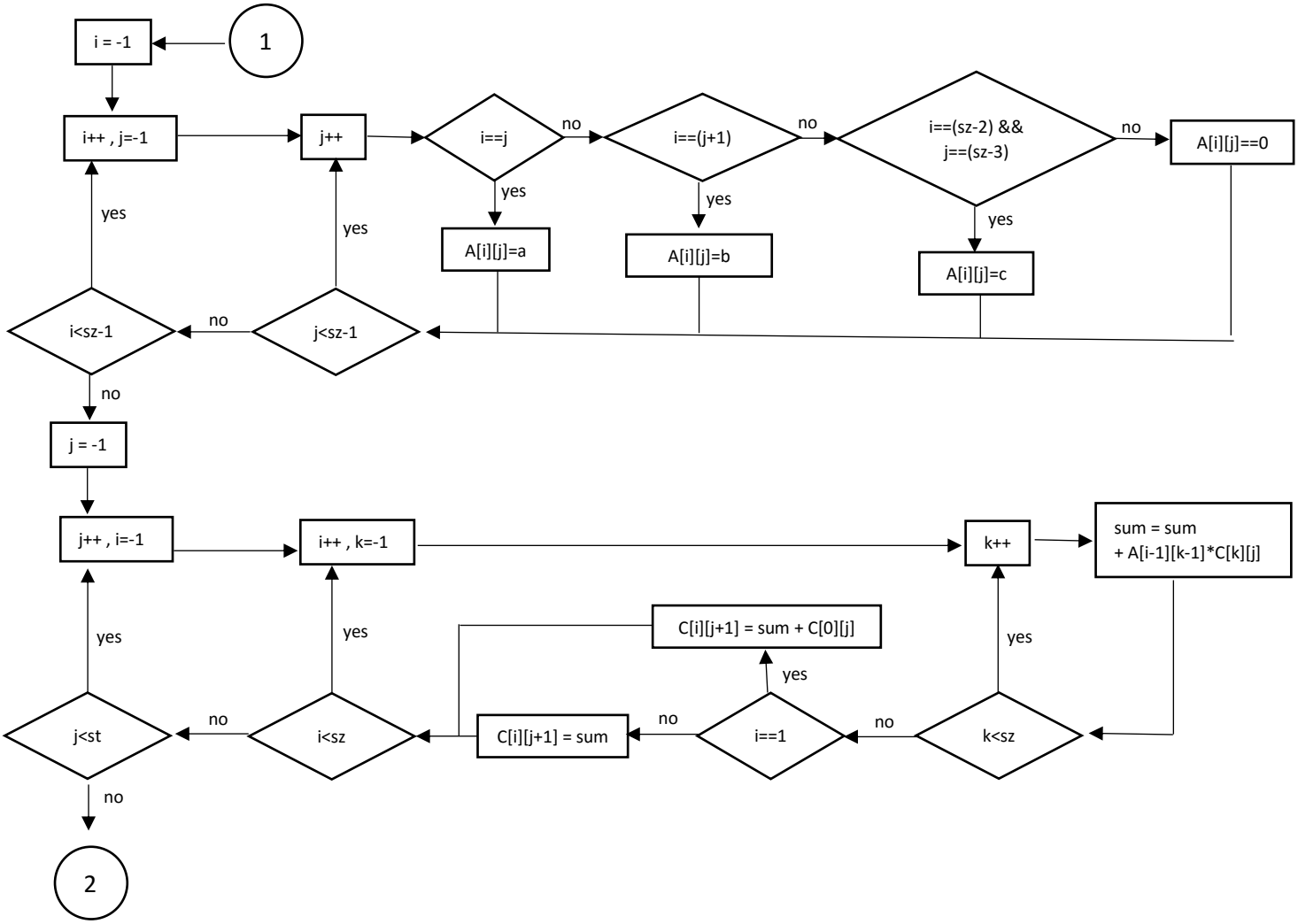
B. Flowcharts/Pseudocodes

1. Crank-Nicholson Method



2. Forward-Time Center-Space Method




1
i = -1
i++ , j=-1
j++
i==j
no
i==(j+1)
no
i==(sz-2) &&
j==(sz-3)
no
A[i][j]==0
yes
yes
yes
A[i][j]=a
A[i][j]=b
A[i][j]=c
yes
yes
i<sz-1
no
j<sz-1
no
j = -1
j++ , i=-1
i++ , k=-1
k++
sum = sum
+ A[i-1][k-1]*C[k][j]
C[i][j+1] = sum + C[0][j]
yes
yes
yes
j<st
no
i<sz
no
C[i][j+1] = sum
no
i==1
no
k<sz
yes
no
2

IV. Results and Discussion

Before creating the main code for the problem, the group first brainstormed on how will the program be user-friendly, organized and more efficient. The first thought that they had in mind is that an introductory text showing the title of the problem, some notes, and the pre-defined step sizes $\Delta z = 0.2\ m$ and $\Delta t = 0.5\ years$ to be used would give a good impression to the user. A sample output is shown in Figure 2.

```
=================================== MP 1: ONE-DIMENSIONAL POLLUTANT MIGRATION ===================================

Given:
> Delta z = 0.2 m
> Delta t = 0.5 years
[NOTE]: Please open the file 'output.csv' to check the summary of calculated data for ALL methods.
=================================================================================================================

Please input anything to continue:
```

Figure 2. Introductory text at the start of the program

Right after the user continues by inputting any key, the program then runs and prints all methods (FTCS and Crank-Nicholson) for all six contaminants in the black screen. The program also prints all data computed in the CSV file "output.csv" for both methods and all contaminants. A sample ouput for both methods and a contaminant Acetone is shown in Figure 2. Note that the first row corresponds to years (up to 60 yrs) while the first column corresponds to the depth for every 0.2 m.

FTCS METHOD

ACETONE:

	0.00	0.50	1.00	1.50	2.00	2.50	3.00	3.50	4.00	4.50	5.00	5.50	6.00	6.50	7.00	7.50	8.00	8.50	9.00	9.50	10.00
0.00	0.00	119.60	233.07	340.41	441.61	536.68	625.61	708.42	785.08	855.62	920.02	978.29	1030.42	1076.42	1116.29	1150.03	1177.63	1199.09	1214.43	1223.63	1226.69
0.20	0.00	0.00	119.60	322.27	582.67	882.79	1209.42	1552.66	1904.91	2260.17	2613.66	2961.46	3300.32	3627.50	3940.68	4237.84	4517.25	4777.36	5016.83	5234.43	5429.07
0.40	0.00	0.00	0.00	14.67	50.47	109.35	190.83	293.18	414.08	550.97	701.28	862.53	1032.33	1208.49	1388.95	1571.80	1755.30	1937.80	2117.81	2293.93	2464.87
0.60	0.00	0.00	0.00	0.00	1.80	7.53	19.06	37.77	64.55	99.85	143.79	196.19	256.67	324.69	399.61	480.73	567.28	658.47	753.50	851.58	951.90
0.80	0.00	0.00	0.00	0.00	0.00	0.22	1.09	3.15	7.01	13.21	22.26	34.58	50.47	70.14	93.73	121.27	152.72	187.99	226.90	269.26	314.82
1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.03	0.15	0.50	1.24	2.55	4.66	7.78	12.11	17.86	25.18	34.22	45.09	57.88	72.64	89.40
1.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.08	0.21	0.47	0.93	1.66	2.75	4.28	6.36	9.07	12.49	16.72	21.81
1.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.03	0.08	0.18	0.34	0.59	0.98	1.52	2.28	3.28	4.57
1.60	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.03	0.07	0.12	0.21	0.35	0.55	0.82
1.80	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.02	0.04	0.08	0.13
2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.02
2.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2.60	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2.80	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

CRANK NICHOLSON METHOD

ACETONE:

	0.00	0.50	1.00	1.50	2.00	2.50	3.00	3.50	4.00	4.50	5.00	5.50	6.00	6.50	7.00	7.50	8.00	8.50	9.00	9.50	10.00
0.00	0.00	216.30	421.51	615.63	798.66	970.59	1131.43	1281.18	1419.84	1547.40	1663.87	1769.25	1863.54	1946.73	2018.83	2079.84	2129.76	2168.58	2196.31	2212.95	2218.50
0.20	0.00	54.38	203.10	420.93	688.89	992.52	1320.59	1664.27	2016.54	2371.70	2725.08	3072.81	3411.62	3738.76	4051.85	4348.84	4627.92	4887.53	5126.25	5342.83	5536.16
0.40	0.00	3.03	16.75	48.00	99.82	172.88	266.42	378.86	508.18	652.15	808.47	974.88	1149.19	1329.32	1513.31	1699.32	1885.61	2070.59	2252.75	2430.69	2603.12
0.60	0.00	0.17	1.24	4.58	11.86	24.59	44.00	70.95	106.00	149.36	201.00	260.71	328.06	402.55	483.53	570.33	662.20	758.38	858.09	960.52	1064.89
0.80	0.00	0.01	0.09	0.39	1.23	3.00	6.20	11.33	18.87	29.27	42.89	60.04	80.93	105.70	134.41	167.05	203.55	243.78	287.56	334.67	384.86
1.00	0.00	0.00	0.01	0.03	0.11	0.33	0.77	1.59	2.94	5.02	8.02	12.14	17.56	24.46	33.00	43.31	55.50	69.65	85.82	104.05	124.33
1.20	0.00	0.00	0.00	0.00	0.01	0.03	0.09	0.20	0.41	0.77	1.34	2.19	3.40	5.06	7.25	10.06	13.58	17.88	23.06	29.16	36.25
1.40	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.02	0.05	0.11	0.20	0.36	0.60	0.95	1.44	2.12	3.01	4.17	5.63	7.43	9.63
1.60	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.03	0.05	0.10	0.16	0.26	0.41	0.61	0.89	1.26	1.74	2.35
1.80	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.03	0.04	0.07	0.11	0.18	0.26	0.38	0.53
2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.02	0.03	0.05	0.08	0.11
2.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.02
2.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2.60	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2.80	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Figure 3. Sample output for FTCS and Crank-Nicholson Methods

All data printed in the CSV file will now be used to create the merged plot of the concentration of the six contaminants versus the depth of the 3m liner at times t=5, 10, 15, 20, 40, and 60 years for both FTCS and Crank-Nicholson methods.

Figure 2 shows the concentration vs. depth graph of all contaminants using the Forward-Time Center-Space (FTCS) method. Take note again that $\Delta z = 0.2\ m$ and $\Delta t = 0.5\ yrs$. We can observe from these graphs that the contaminants from lowest to highest concentration are: Magnesium, Calcium, DCM, Sodium, Acetone, and Chloride. This order of the contaminants is constant throughout the time span of 60 years. We can also observe that the graph is parabolic, signifying that the governing equation is indeed, a parabolic PDE.

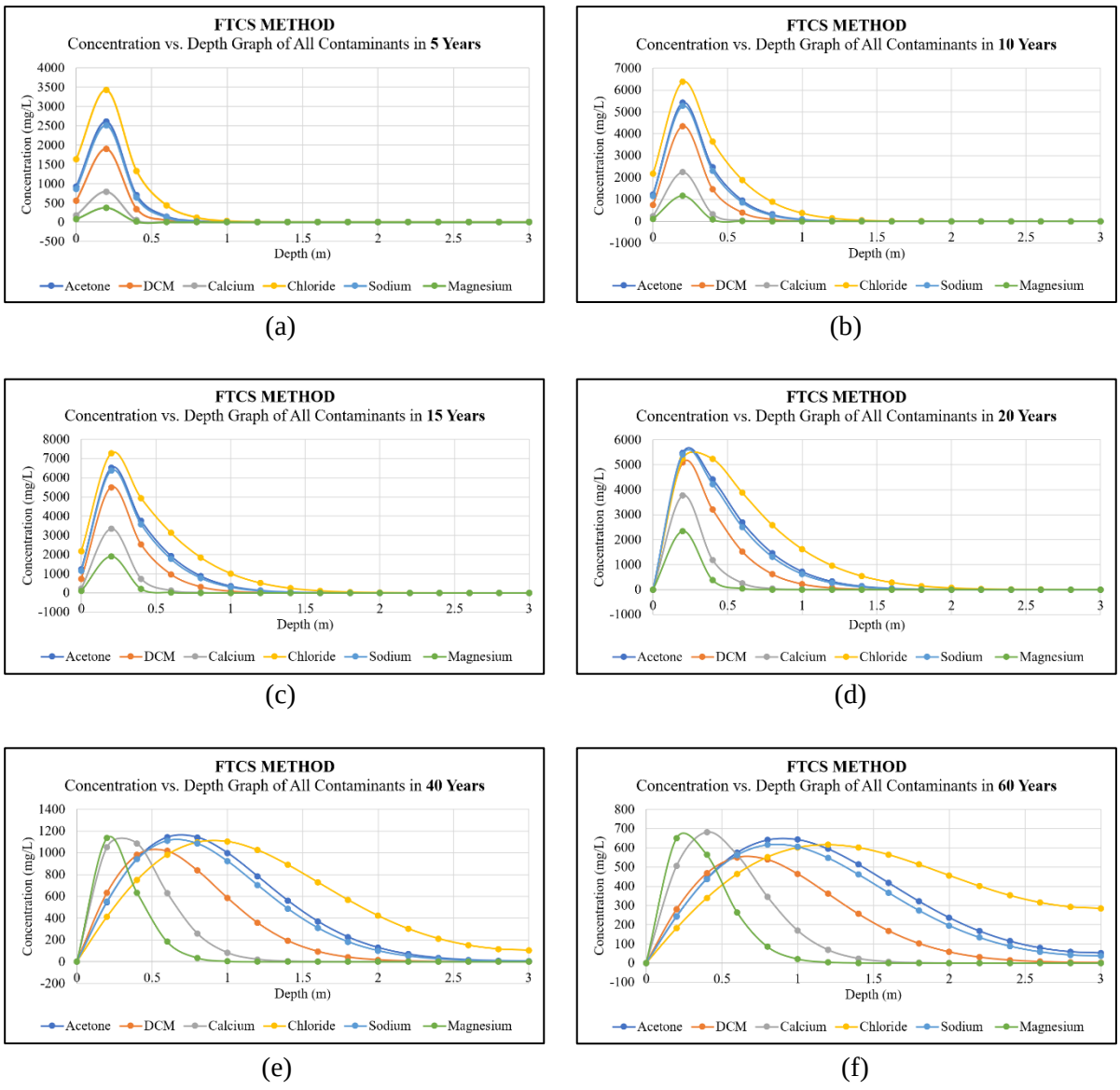


Figure 4. Concentration vs. Depth Graph of the Six Contaminants using the Forward-Time Center-Space (FTCS) Method in (a) 5 years, (b) 10 years, (c) 15 years, (d) 20 years, (e) 40 years, and (f) 60 years.

After 5 years, the concentrations of the contaminants range in between 0 to 3500 mg/L while after 10 years, the concentrations increased, ranging from 0 to 6500mg/L. These concentrations are evident only from 0 to 1.5 m depth in this time span. Then, after 15 years, the contaminants start to spread beyond the 1.5 m depth as the concentration in that area start to rise. The spreading out then continues after 20 years, reaching up the depth of 2 m. Moreover, the concentration in between 0 to 1 m depth decreased. After 40 years, the contaminants have spread throughout the 3-m thickness of the liner but their concentrations decreased further from 0 to 0.75 m depth ranging in between 0 to 1200 mg/L only. Higher concentrations are now more evident in the middle of the liner (0.5-1.5 m). Finally, after 60 years, the concentrations in between the depths 1.2 to 3.0 m increased, but concentrations in lower depths (0 – 1.2 m) decreased further.

For the Crank Nicholson Method, Figure 5 illustrates the merged concentration vs. depth plot of all contaminants in the six-time frames.

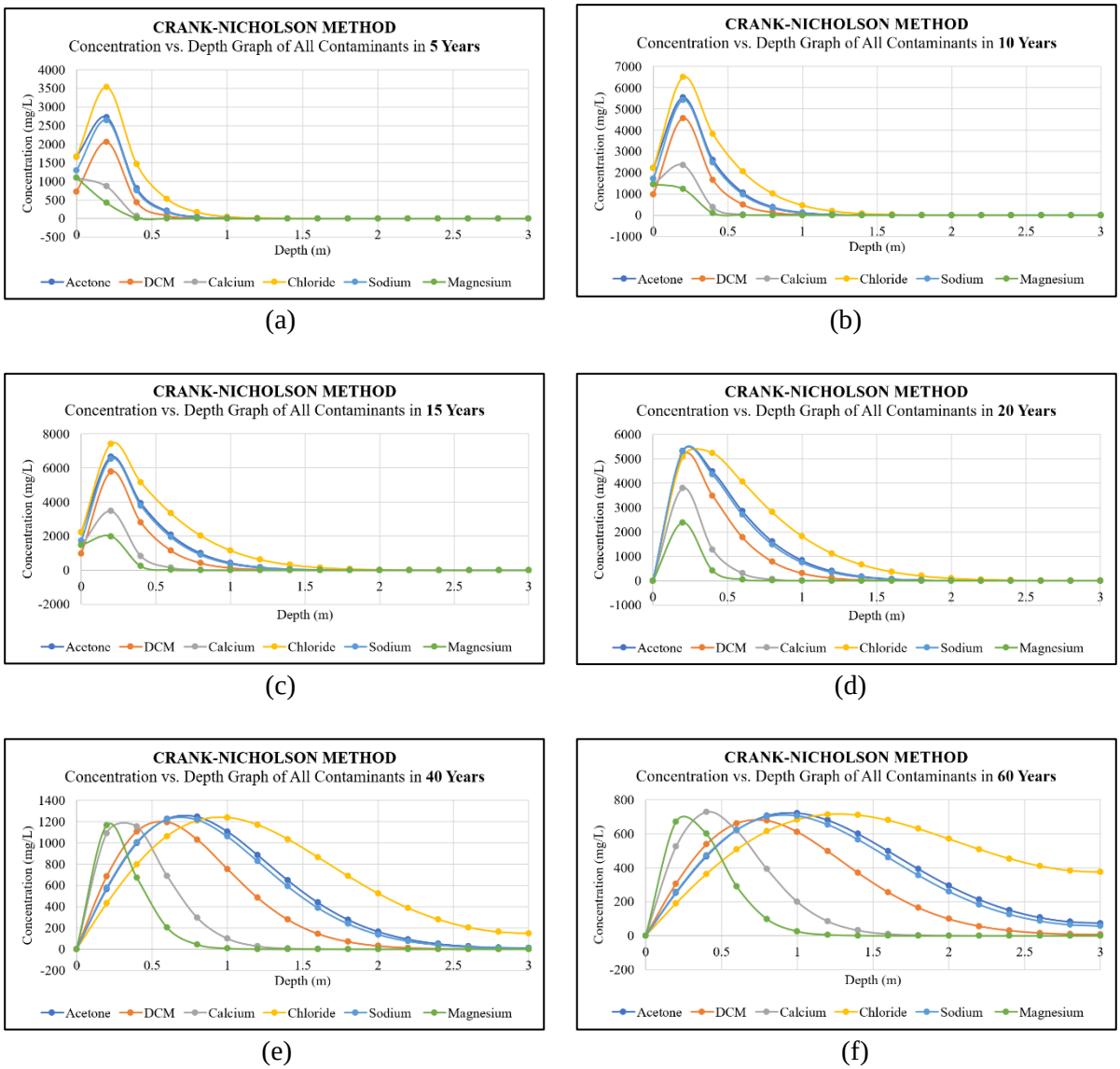


Figure 5. Concentration vs. Depth Graph of the Six Contaminants using the Crank-Nicholson Method in (a) 5 years, (b) 10 years, (c) 15 years, (d) 20 years, (e) 40 years, and (f) 60 years.

One difference of Crank-Nicholson with the FTCS method is that in the next time step, t=0.5 yrs. and beyond the depth z=0.2 m, no values can be seen in FTCS while in Crank-Nicholson, there are values already. This is because Crank-Nicholson method adds the boundary matrices first before it is multiplied to the inverse constants matrix of the left hand side of Equation 25. Another thing that the group immediately observed after creating the graphs in Figure 5 is that the curve for Magnesium in Figures 5a., 5b, and 5c is different than its curve in the FTCS method. In FTCS, the concentration of Magnesium in the 0 m depth started in less than 100mg/L, but in Crank-Nicholson method, its concentration was more than 1100mg/L. Hence, the curve is sloping down instead of a "hill-like" curve as portrayed using FTCS. The trend along the 3-m depth throughout the span of 0 to 6 years is the same as that in the FTCS as said in the previous paragraph.

To further see the differences between the two methods, the concentration for every 0.2 m depth at 20 years was tabulated in all the contaminants for each method. These are shown in Tables 2 and 3.

Table 2. Concentration of All Contaminants along the 3-m Liner in **20 years** using the FTCS method

Forward-Time Center-Space Method						
Depth (m)	Concentration (mg/L)					
	Acetone	DCM	Calcium	Chloride	Sodium	Magnesium
0	0	0	0	0	0	0
0.2	5475.603	5091.324	3770.035	5244.100	5415.569	2347.831
0.4	4415.537	3207.576	1191.836	5240.157	4230.177	378.281
0.6	2690.964	1523.677	261.737	3880.566	2499.304	40.293
0.8	1461.361	625.311	45.092	2586.926	1312.410	3.253
1	724.163	225.785	6.336	1625.706	626.444	0.209
1.2	328.223	72.172	0.745	968.380	272.493	0.011
1.4	136.233	20.535	0.074	546.349	108.186	5.02E-04
1.6	51.855	5.227	0.006	291.806	39.271	1.94E-05
1.8	18.125	1.195	4.91E-04	147.487	13.055	6.5E-07
2	5.824	0.246	3.28E-05	70.520	3.980	2E-08
2.2	1.722	0.045	1.95E-06	31.892	1.114	0
2.4	0.469	0.007	1.00E-07	13.656	0.286	0
2.6	0.117	0.001	0	5.600	0.067	0
2.8	0.028	1.7E-04	0	2.391	0.015	0
3	0.012	4.62E-05	0	1.573	0.006	0

Table 3. Concentration of All Contaminants along the 3-m Liner in **20 years** using the Crank-Nicholson method

Crank-Nicholson Method						
Depth (m)	Concentration (mg/L)					
	Acetone	DCM	Calcium	Chloride	Sodium	Magnesium
0	0	0	0	0	0	0
0.2	5319.024	5127.981	3792.176	5083.036	5299.499	2386.811
0.4	4478.386	3486.996	1282.106	5241.008	4353.181	415.182
0.6	2850.094	1779.888	303.561	4054.25	2702.739	48.479
0.8	1606.354	785.582	57.57	2809.322	1482.977	4.401
1	828.6044	308.705	9.146	1823.763	742.579	0.328
1.2	394.8502	109.31	1.251	1123.043	342.544	0.021
1.4	174.6765	35.183	0.15	658.493	146.329	0.001
1.6	72.0318	10.371	0.016	368.314	58.144	5.67E-05
1.8	27.793	2.818	0.002	196.798	21.578	2.51E-06
2	10.0698	0.71	1.39E-04	100.598	7.507	1.01E-07
2.2	3.437	0.166	1.12E-05	49.288	2.457	3.72E-09
2.4	1.109	0.036	8.52E-07	23.247	0.759	1.27E-10
2.6	0.3407	0.007	6.00E-08	10.751	0.223	4.05E-12
2.8	0.106	0.002	3.97E-09	5.333	0.066	1.21E-13
3	0.055	5.67E-04	5.03E-10	3.849	0.033	7.00E-15

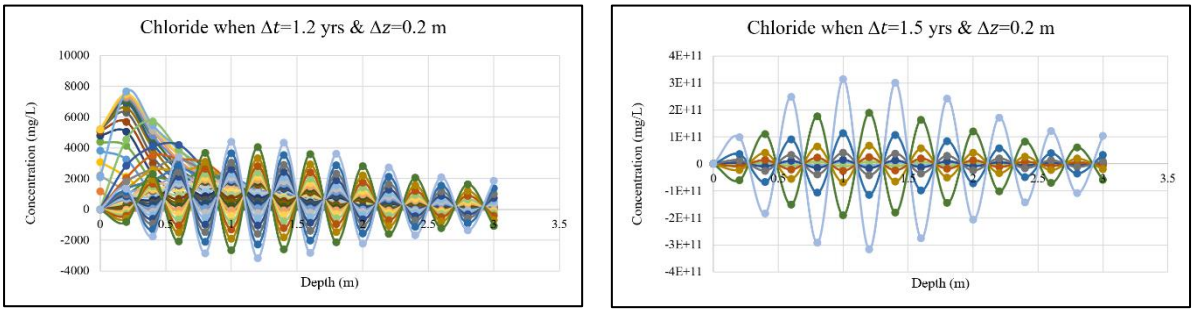
Excluding the boundary (depth = 0 m) having 0 concentrations for all contaminants, it is evident that the corresponding concentrations in each contaminant along the 3-m depth isn't the same as it has a few differences in each other. For an instance, the concentrations of every contaminant in and beyond the 0.2 m depth are a bit higher in the Crank-Nicholson method than that of the FTCS method. However, even though concentrations in Crank-Nicholson method are higher, it can still be observed that the concentration vs. depth graphs of both methods have a very similar trend/shape with each other. Another difference that can also be observed with the two tables is that in FTCS method, some parts, more commonly in depths closer to the very bottom 3-m depth, still have zero values in them while in Crank-Nicholson method, there are already values even though very small.

One of the goals of this Machine Problem is to also identify what contaminant specie will first break through the 3-m liner. This would be very important because we would know what contaminant is easily penetrating ideally impermeable boundaries, more hazardous, and is most likely to contaminate the soil or aquifers beneath the liner. From the data computed, it is found that ***Chloride*** is the first contaminant to penetrate the 3-m single clay liner. Its details are shown below.

Table 4. Concentration of Chloride in the 3-m Depth on the Year it First Penetrated and in 20 Years

	FTCS Method	Crank-Nicholson Method
	Concentration at z =3.0 m (mg/L)	Concentration at z =3.0m (mg/L)
Year it first penetrated	2.3×10^{-7} after 8 years	5.1×10^{-13} after 0.5 years
In 20 years	1.573	3.849

We tackled previously that the major advantage of FTCS is that it is relatively simple and computationally fast. However, the main drawback is that if the condition $0 < \frac{k\Delta t}{\Delta x^2} < 0.5$ is not satisfied, unstable solutions will be obtained. Through trial and error and by inputting various Δt and Δz, it is found out that the solution of the first contaminant specie to penetrate the 3-m liner (Chloride) will start to be unstable for the values $\Delta t = 1.2\ years$ and $\Delta z = 0.2\ m$ (Fig. 6a). To clearly see the instability of the solution, we can also set $\Delta z = 1.5\ years$ and $\Delta t = 0.2\ m$ for a more sinusoidal-like graph (Fig.6b).



(a) (b)

Figure 6. Verification of the Instability of the Solutions for Chloride with (a) $\Delta t = 1.2\ years$ and (b) $\Delta t = 1.5\ years$ using the FTCS Method

V. Conclusions and Recommendations

In this Machine Problem, a numerical model describing the migration of the 6 contaminant species through the given 3-m single clay liner system of a sanitary landfill was successfully generated using the Forward-Time-Center-Space (FTCS) and the Crank-Nicholson methods. In addition, the one-dimensional advection-dispersion-reaction equation was also used as the governing equation and the central and forward finite difference formulas were also used to generate the model for both methods. For the usage and implementation of the numerical model, matrix addition and multiplication were used in the FTCS method while the concept of Thomas algorithm was also used to find the solution in the Crank-Nicholson Method.

Based from the results, it is shown that with $\Delta z = 0.2\ m$ and $\Delta t = 0.5\ yrs.$, we can observe that the plotted concentrations vs. depth graph is parabolic and that the contaminants from lowest to highest concentration are: Magnesium, Calcium, DCM, Sodium, Acetone, and Chloride. The concentrations spread out throughout the 3-m liner and also decrease through the years. Interestingly, the contaminant with the lowest concentration is Magnesium, which means that it is the least likely to easily penetrate the 3-m clay liner. On the other hand, Chloride has the highest concentration out of all contaminants and was also found to be the first contaminant to penetrate the 3-m liner. This information is very important because chloride is most likely to be more hazardous to the environment & people and to contaminate the soil or aquifers beneath the liner. Therefore, the group recommends that Engineers or researchers must innovate a more impenetrable, robust, and efficient clay liner to be used in the construction of future sanitary landfills to prevent these hazardous instances.

Although both FTCS and Crank-Nicholson methods have similar trend/shape of the graphs, there are still a few differences. It can be observed that the concentrations computed for a certain depth and time in Crank-Nicholson method are slightly higher than that of the FTCS. Unlike the FTCS method, it can be observed that there are already concentrations computed in some parts of the depth even at an earlier time step (say, 0.5 years) when the Crank-Nicholson method is used, which may be due to their difference in the usage of numerical model (e.g. Thomas algorithm was used in Crank-Nicholson method). Finally, Crank-Nicholson was found to be a better and more accurate method than Forward-Time Center-Space since it is 2nd degree accurate in both time and space approximations. It is also proved to be unconditionally stable as it poses no restriction on the previously mentioned limitation of the FTCS method.

VI. Source Code

The files included in this Machine Problem are:

- MP1_LITANA_YAP.c
- output.csv

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[4] Hughes, Kerry L. "Ohio State University Fact Sheet." Landfill Types and Liner Systems, CDFS-138-05 (2005). Retrieved from the website: http://ohioline.osu.edu/cd-fact/0138.htm