Theoretical Foundations and Simulation of Diffusion Processes by Use of Finite Differences

Atharva Sinnarkar

14 February 2025

Task 1.1

Continuity Equation

The continuity equation expresses the conservation of mass:

$$\frac{\partial \rho(x,y)}{\partial t} + \nabla \cdot \mathbf{j}(x,y) = 0 \tag{1}$$

where:

- $\rho(x,y)$ is the concentration of the diffusing species.
- $\mathbf{j}(x,y)$ is the diffusion flux vector, defined as:

$$\mathbf{j}(x,y) = -\mathbf{D}(x,y)\nabla\rho(x,y) \tag{2}$$

- $\mathbf{D}(x,y)$ is the diffusion coefficient tensor.

Expanding the Flux Term

Substituting $\mathbf{j}(x,y)$ into the continuity equation, we get:

$$\frac{\partial \rho(x,y)}{\partial t} = \nabla \cdot (\mathbf{D}(x,y)\nabla\rho(x,y)) \tag{3}$$

Anisotropic Diffusion in 2D

In two dimensions, the diffusion coefficient tensor $\mathbf{D}(x,y)$ is a symmetric tensor:

$$\mathbf{D}(x,y) = \begin{bmatrix} D_{xx}(x,y) & D_{xy}(x,y) \\ D_{xy}(x,y) & D_{yy}(x,y) \end{bmatrix} \tag{4}$$

Expanding $\nabla \cdot (\mathbf{D}(x,y)\nabla\rho(x,y))$, we have:

$$\frac{\partial \rho(x,y)}{\partial t} = \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial \rho}{\partial x} + D_{xy}\frac{\partial \rho}{\partial y}\right) + \frac{\partial}{\partial y}\left(D_{xy}\frac{\partial \rho}{\partial x} + D_{yy}\frac{\partial \rho}{\partial y}\right) \tag{5}$$

Simplification Under Homogeneity Assumptions

Assuming that the diffusion properties are homogeneous and $\mathbf{D}(x, y)$ is constant, the equation simplifies to:

$$\frac{\partial \rho}{\partial t} = D_{xx}\frac{\partial^2 \rho}{\partial x^2} + 2D_{xy}\frac{\partial^2 \rho}{\partial x \partial y} + D_{yy}\frac{\partial^2 \rho}{\partial y^2} \tag{6}$$

This is Fick's second law for anisotropic diffusion in 2D.

Classification of the Partial Differential Equation

The general form of a second-order partial differential equation is:

$$A\frac{\partial^2 \rho}{\partial x^2} + B\frac{\partial^2 \rho}{\partial x \partial y} + C\frac{\partial^2 \rho}{\partial y^2} + \cdots = 0$$

The discriminant Δ determines the type of PDE:

$$\Delta = B^2 - AC$$

For anisotropic diffusion, the coefficients are defined as:

- $A = D_{xx}$
- $B = 2D_{xy}$
- $C = D_{yy}$

Substituting these values into the discriminant, we have:

$$\Delta = (2D_{xy})^2 - D_{xx}D_{yy}.$$

Justification of the Relation

This discriminant can be justified by considering a special orientation of the material in the Cartesian frame. In this orientation, the diffusion tensor D becomes diagonal ($D_{xy} = 0$), which simplifies the discriminant to:

$$\Delta = -D_{xx}D_{yy}.$$

Since the diffusion tensor D is positive-definite ($D_{xx} > 0$, $D_{yy} > 0$), the discriminant $\Delta < 0$, confirming that the PDE is elliptic for stationary diffusion.

Time-Dependent vs Stationary Diffusion

For time-dependent diffusion, t (time) and one spatial coordinate, say x, are considered as the two independent variables. In this case, the discriminant becomes zero ($\Delta = 0$), classifying the PDE as parabolic.

However, the equation solved in the tutorial corresponds to stationary diffusion, where only spatial variables are considered. For this case, the discriminant $\Delta < 0$, confirming the elliptic nature of the PDE.

Summary of Classifications

1. If $\Delta > 0$, the PDE is hyperbolic.
2. If $\Delta = 0$, the PDE is parabolic.
3. If $\Delta < 0$, the PDE is elliptic.

For stationary diffusion, the positive-definite diffusion tensor ensures that $\Delta < 0$, and the PDE is elliptic.

Task 1.2

Derivation of the Stationary Diffusion Equation

Starting from the anisotropic diffusion equation:

$$\frac{\partial \rho}{\partial t} = \nabla \cdot \left(D(x, y) \nabla \rho \right),$$

for stationary diffusion ($\frac{\partial \rho}{\partial t} = 0$), we have:

$$\nabla \cdot (D(x, y) \nabla \rho) = 0.$$

Assuming the coordinate system is aligned with the principal axes of the diffusion tensor, $D(x, y)$ becomes:

$$D(x, y) = \begin{bmatrix} D_{xx} & 0 \\ 0 & D_{yy} \end{bmatrix}.$$

Substituting this into the equation gives:

$$D_{xx} \frac{\partial^2 \rho}{\partial x^2} + D_{yy} \frac{\partial^2 \rho}{\partial y^2} = 0.$$

Defining P as the ratio of the diffusion coefficients:

$$P = \frac{D_{yy}}{D_{xx}},$$

the equation simplifies to:

$$\frac{\partial^2 \rho}{\partial x^2} + P \frac{\partial^2 \rho}{\partial y^2} = 0.$$

Interpretation of Parameters

- x, y: Represent the spatial directions in the 2D domain.
- P: A dimensionless number defined as $P = \frac{D_{yy}}{D_{xx}}$, which reflects the anisotropy in diffusion. If $P > 1$, diffusion is faster in the y-direction; if $P < 1$, diffusion is faster in the x-direction.

Simplification of the Diffusion Tensor

By aligning the coordinate system with the principal axes of the diffusion tensor, the off-diagonal terms (D_{xy}) vanish, and the tensor simplifies to:

$$D = \begin{bmatrix} D_{xx} & 0 \\ 0 & D_{yy} \end{bmatrix}.$$

This simplification reduces the anisotropic diffusion equation to its final form, where the directional dependence is captured by P.

Clarification of Assumptions

For stationary diffusion, the condition $\frac{\partial \rho}{\partial t} = 0$ implies that the system has reached a steady-state condition where the concentration no longer changes over time.

Task 1.3

We start with the stationary anisotropic diffusion equation:

$$\frac{\partial^2 \rho}{\partial x^2} + P \frac{\partial^2 \rho}{\partial y^2} = 0 \tag{7}$$

Step 1: Define the Transformation

To eliminate anisotropy, we introduce new coordinates:

$$x' = x, \quad y' = \frac{y}{\sqrt{P}} \tag{8}$$

Step 2: Compute the First-Order Derivatives

Using the chain rule:

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial x'} \tag{9}$$

$$\frac{\partial}{\partial y} = \frac{1}{\sqrt{P}} \frac{\partial}{\partial y'} \tag{10}$$

Step 3: Compute the Second-Order Derivatives

Now, we differentiate again to get the second-order derivatives:

$$\frac{\partial^2}{\partial x^2} = \frac{\partial^2}{\partial x'^2} \tag{11}$$

$$\frac{\partial^2}{\partial y^2} = \frac{\partial}{\partial y} \left(\frac{1}{\sqrt{P}} \frac{\partial}{\partial y'} \right) \tag{12}$$

Since $\frac{1}{\sqrt{P}}$ is a constant, we pull it out:

$$\frac{\partial^2}{\partial y^2} = \frac{1}{\sqrt{P}} \cdot \left(\frac{1}{\sqrt{P}} \frac{\partial^2}{\partial y'^2} \right) = \frac{1}{P} \frac{\partial^2}{\partial y'^2} \tag{13}$$

Step 4: Substitute into the Diffusion Equation

We now substitute these transformed derivatives into the original diffusion equation:

$$\frac{\partial^2 \rho}{\partial x^2} + P\frac{\partial^2 \rho}{\partial y^2} = 0 \tag{14}$$

Using the transformations:

$$\frac{\partial^2 \rho}{\partial x^2} = \frac{\partial^2 \rho}{\partial x'^2} \tag{15}$$

$$\frac{\partial^2 \rho}{\partial y^2} = \frac{1}{P}\frac{\partial^2 \rho}{\partial y'^2} \tag{16}$$

Substituting these into the equation:

$$\frac{\partial^2 \rho}{\partial x'^2} + P \cdot \left(\frac{1}{P}\frac{\partial^2 \rho}{\partial y'^2}\right) = 0 \tag{17}$$

Since P cancels out:

$$\frac{\partial^2 \rho}{\partial x'^2} + \frac{\partial^2 \rho}{\partial y'^2} = 0 \tag{18}$$

Step 5: Recognizing the Laplace Equation

This equation:

$$\frac{\partial^2 \rho}{\partial x'^2} + \frac{\partial^2 \rho}{\partial y'^2} = 0 \tag{19}$$

is exactly the **Laplace equation**, which describes isotropic diffusion.

Task 2.1

The governing equation to discretize is:

$$\frac{\partial^2 \rho(x,y)}{\partial x^2} + P\frac{\partial^2 \rho(x,y)}{\partial y^2} = 0. \tag{20}$$

Using a second-order accurate central difference scheme:

$$\frac{\partial^2 \rho(x,y)}{\partial x^2} \approx \frac{\rho_{i+1,j} - 2\rho_{i,j} + \rho_{i-1,j}}{h_x^2},$$
$$\frac{\partial^2 \rho(x,y)}{\partial y^2} \approx \frac{\rho_{i,j+1} - 2\rho_{i,j} + \rho_{i,j-1}}{h_y^2}.$$

Substituting these into the governing equation gives:

$$\frac{\rho_{i+1,j} - 2\rho_{i,j} + \rho_{i-1,j}}{h_x^2} + P\frac{\rho_{i,j+1} - 2\rho_{i,j} + \rho_{i,j-1}}{h_y^2} = 0. \tag{21}$$

Multiplying through by $h_x^2 h_y^2$ results in:

$$\rho_{i+1,j}h_y^2 + P\rho_{i,j+1}h_x^2 - 2\rho_{i,j}(h_y^2 + Ph_x^2) + \rho_{i-1,j}h_y^2 + P\rho_{i,j-1}h_x^2 = 0. \tag{22}$$

For isotropic diffusion ($P = 1$, $h_x = h_y = h$), this simplifies to:

$$-4\rho_{i,j} + \rho_{i+1,j} + \rho_{i-1,j} + \rho_{i,j+1} + \rho_{i,j-1} = 0. \tag{23}$$

Task 2.2

(a) Node Numbering and Mapping

For a 5×5 grid, nodes are numbered row-wise from top-left to bottom-right. The mapping is shown below:

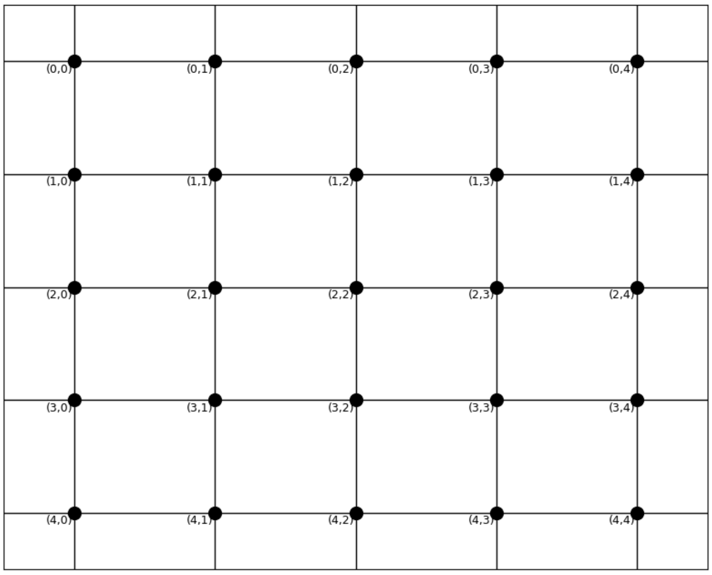

Figure 1: Sketch of the node numbering for a 5×5 grid.

To map the 2D indices (i, j) of a node in the grid to a linear index n, we use the formula:

$$n = (i - 1) \cdot N_y + j,$$

where:

- i: Row index (1 to N_x).
- j: Column index (1 to N_y).
- n: Linear index (1 to $N_x \cdot N_y$).

(b) Coefficient Matrix Construction

Finite Difference Discretization

For a 5×5 grid, the coefficient matrix A is constructed using the finite difference discretization from Task 2.1:

$$-4\rho_{i,j} + \rho_{i+1,j} + \rho_{i-1,j} + \rho_{i,j+1} + \rho_{i,j-1} = 0$$

Linear Index Mapping

To map a 2D index (i, j) to a linear index n:

$$n = (i - 1) \cdot Ny + j$$

Coefficient Matrix (25×25)

- The main diagonal contains -4, representing the central node.
- The subdiagonal and superdiagonal contain $+1$ for left and right neighbors.
- The off-diagonals spaced by 5 indices contain $+1$ for top and bottom neighbors.

The matrix structure is as follows:

$$A = \begin{bmatrix} -4 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & \dots \\ 1 & -4 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & \dots \\ 0 & 1 & -4 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & 1 & -4 & 1 & 0 & 0 & 0 & 1 & 0 & \dots \\ 0 & 0 & 0 & 1 & -4 & 0 & 0 & 0 & 0 & 1 & \dots \\ 1 & 0 & 0 & 0 & 0 & -4 & 1 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & \dots \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & -4 & 1 & 0 & \dots \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & -4 & 1 & \dots \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & -4 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

Difficulties in the Boundary Regions

- **Dirichlet boundary conditions** impose fixed values at the edges, reducing the number of unknowns and modifying the coefficient matrix.
- **Neumann boundary conditions** introduce ghost nodes, requiring additional equations to approximate derivatives at the boundaries.
- The **sparse nature of the matrix** is affected as boundary rows need special treatment to incorporate fixed values or flux conditions.
- Boundary nodes **do not have five neighbors**, requiring modifications in the finite difference formulation at the edges.

Task 3.1

Discrete Equation for Node 3

Using the central difference scheme, the governing equation at node 3 is given by:

$$-4\rho_3 + \rho_C + \rho_2 + \rho_4 + \rho_8 = 0.$$

Task 3.2

The Neumann boundary condition specifies the normal derivative at a boundary to be either zero or a constant. This is different from Dirichlet boundary conditions, which directly specify the concentration at the boundary.

From Fick's law, the Neumann boundary condition is given by:

$$\frac{\partial \rho}{\partial x} = -\frac{j}{D}$$

Using the finite difference approximation for the first derivative at node 10:

$$\frac{\rho_G - \rho_9}{2h} = -\frac{j}{D}$$

Rearranging for the ghost node ρ_G:

$$\rho_G = \rho_9 - 2h\frac{j}{D}$$

where:

- ρ_G is the ghost node outside the right boundary.
- ρ_9 is the concentration at the adjacent interior node.
- j is the prescribed flux at the boundary.
- D is the diffusion coefficient.
- h is the step size in the x-direction.

The diffusion equation in two dimensions is given by:

$$\rho_{i+1,j} + \rho_{i-1,j} + \rho_{i,j+1} + \rho_{i,j-1} - 4\rho_{i,j} = 0$$

For node 10, its neighboring nodes are:

- **Left**: ρ_9
- **Above**: ρ_5
- **Below**: ρ_{15}
- **Right**: Ghost node ρ_G

Substituting these into the finite difference equation:

$$\rho_G + \rho_9 + \rho_5 + \rho_{15} - 4\rho_{10} = 0$$

Replacing ρ_G with $\rho_9 - 2h\frac{j}{D}$:

$$(\rho_9 - 2h\frac{j}{D}) + \rho_9 + \rho_5 + \rho_{15} - 4\rho_{10} = 0$$

Simplifying:

$$-4\rho_{10} + 2\rho_9 + \rho_5 + \rho_{15} = 2h\frac{j}{D}$$

Grid Sketch for Reference

The grid structure is shown in Fig. 2, which illustrates the node layout and boundary positions.

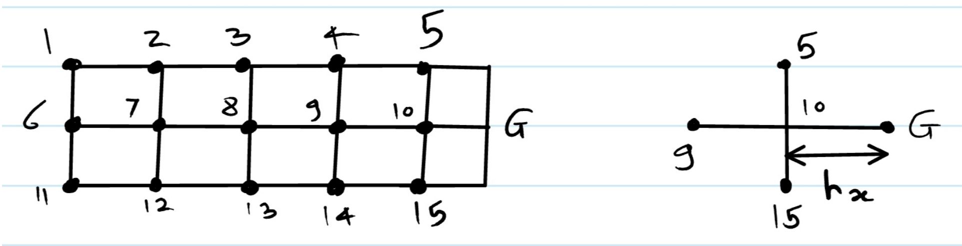

Figure 2: Sketch of the grid layout for Task 3.2.

Task 4.1

Linear system of equations

$$
\begin{bmatrix}
-4 & 2 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & -4 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & -4 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & -4 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & -4 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & -4 & 2 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & -4 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -4 & 2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & -4 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & -4 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & -4 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & -4
\end{bmatrix}
\begin{bmatrix}
\rho_1 \\ \rho_2 \\ \rho_3 \\ \rho_4 \\ \rho_5 \\ \rho_6 \\ \rho_7 \\ \rho_8 \\ \rho_9 \\ \rho_{10} \\ \rho_{11} \\ \rho_{12} \\ \rho_{13} \\ \rho_{14} \\ \rho_{15}
\end{bmatrix}
=
\begin{bmatrix}
\frac{2h}{D} J_{\text{left}} \\ 0 \\ 0 \\ 0 \\ \frac{2h}{D}(-J_{\text{right}}) \\ \frac{2h}{D} J_{\text{left}} \\ 0 \\ 0 \\ 0 \\ \frac{2h}{D}(J_{\text{right}}) \\ \frac{2h}{D} J_{\text{left}} \\ 0 \\ 0 \\ 0 \\ \frac{2h}{D}(-J_{\text{right}})
\end{bmatrix}
-
\begin{bmatrix}
\rho_A \\ \rho_B \\ \rho_C \\ \rho_D \\ \rho_E \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \rho_F \\ \rho_G \\ \rho_H \\ \rho_J
\end{bmatrix}
$$

Grid and Discretization

The system is defined on a 3×5 grid, as per Figure 2 from the instruction manual. The nodes are labeled as follows:

- **Dirichlet boundary nodes**: $\rho_A, \rho_B, ..., \rho_E$ (top) and $\rho_F, \rho_G, ..., \rho_J$ (bottom) are known values.
- **Interior nodes**: These are the 15 unknowns that form the vector ρ.

Task 4.2

The coefficient matrix A for the linear system of equations has the following numerical properties:

- **5-band matrix**: A is a sparse matrix with five non-zero diagonals:
  - The main diagonal contains -4, representing the central node in the finite difference discretization.
  - Two adjacent diagonals contain $+1$, representing the connections to neighboring nodes in the same row.
  - Two additional diagonals spaced by the grid width (N_y) contain $+1$, representing connections to nodes in adjacent rows.
- **Quadratic**: The matrix A is square ($n \times n$), where n is the number of interior nodes in the grid.
- **Not symmetric**: Due to the Neumann boundary conditions on the left and right boundaries, the matrix is not symmetric. Contributions from ghost nodes modify the sparsity pattern asymmetrically.
- **Sparsity**: The matrix A is highly sparse, with non-zero elements only on the five bands described above. Most of the matrix elements are zero, which allows for efficient numerical solvers.

Key Observations

1. The matrix is quadratic ($n \times n$), where n is the number of interior nodes. 2. It is a sparse 5-band matrix, with non-zero diagonals for connections in the grid. 3. The matrix is not symmetric due to contributions from Neumann boundary conditions, which break symmetry in the sparsity pattern. 4. The sparsity of A allows for efficient numerical solutions using specialized solvers such as ‘scipy.sparse.linalg‘ in Python.

Task 5.1

The python implementation is provided with this report.

Task 5.2

5.2(1)

The concentration is constant everywhere.

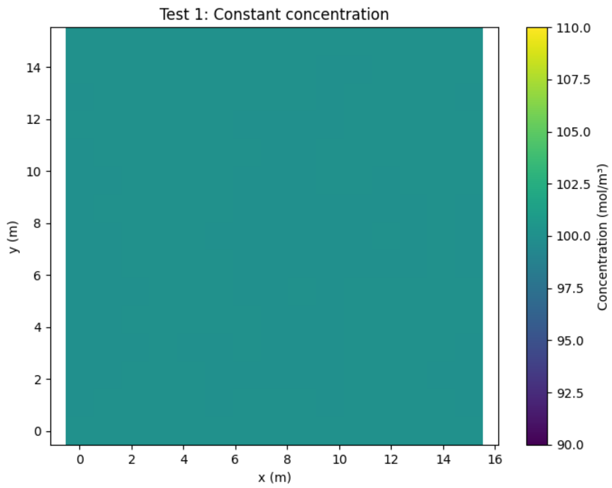

Figure 3: Contant Concentration Profile.

5.2(2)

The plot is linear.

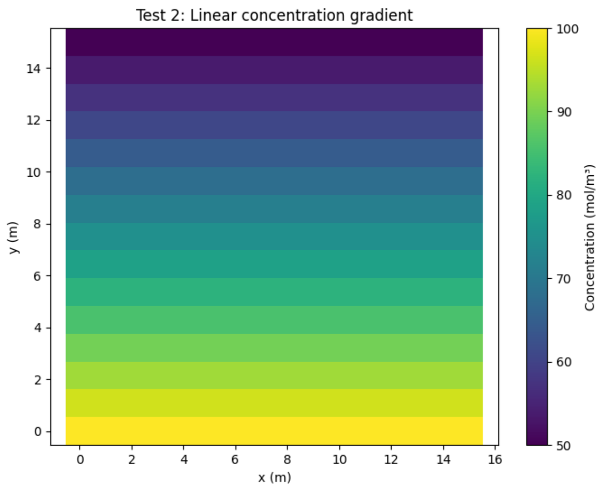

Figure 4: Linear Profile.

5.2(3)

Even after changing the boundary conditions, the plots are linear.

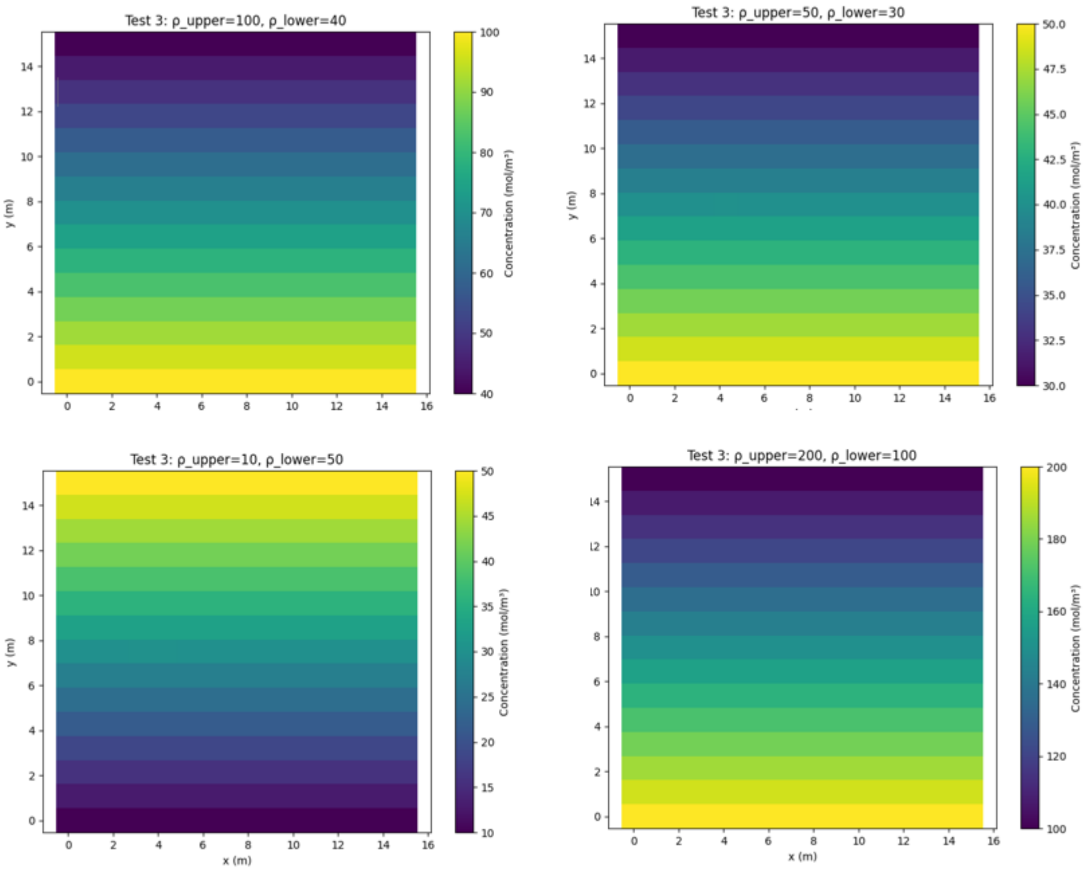

Figure 5: Plots after changing the boundary conditions.

5.2(4)

To obtain an analytical solution, we need to increase the number of nodes as much as possible. By making comparisons, it becomes clear that the number of nodes significantly impacts the discrepancy in a coarse grid.

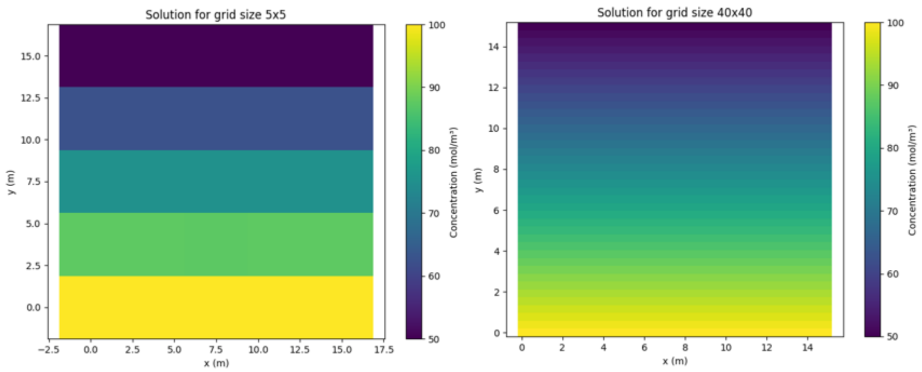

Figure 6: Numerical solution of coarse grid vs Analytical solution.

5.2(5)

Increasing the number of nodes improves the spatial resolution. Additionally, when the number of nodes (N) is smaller, the computational cost is reduced.

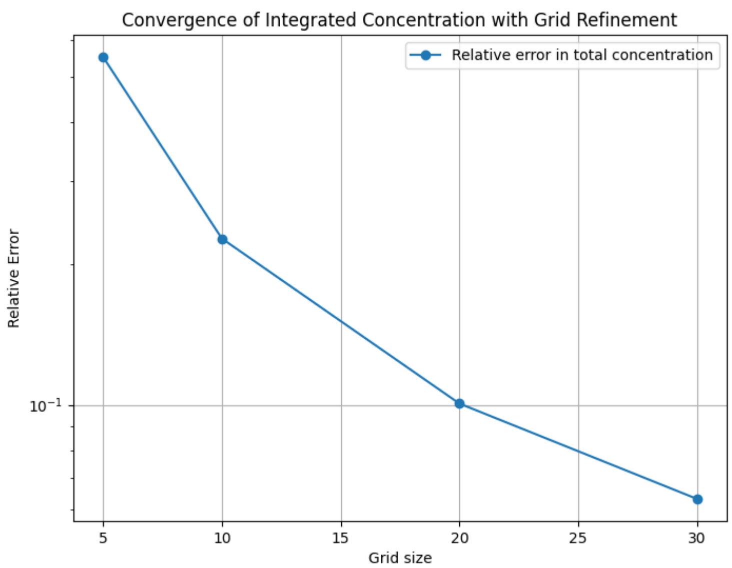

Figure 7: Convergence Plot.

5.2(6)

As observed, there will be no change in concentration in the X-direction when we set Jleft = Jright = 0.

5.2(7)

As we can observe, since J_{left} and J_{right} are equal, and the upper and lower boundary conditions are the same, the flux distribution is uniform on both sides of the boundary.

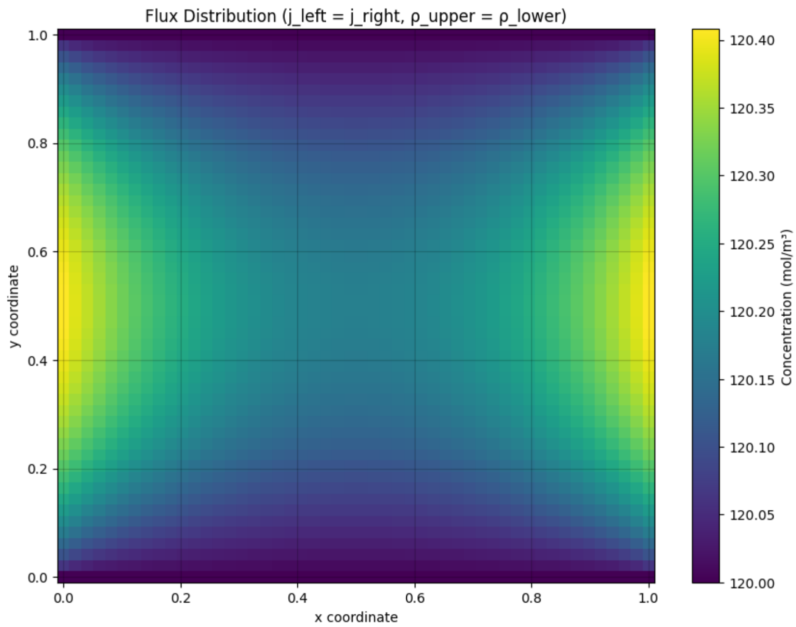

Figure 8: Plot with different boundary conditions.

Flux Values and Boundary Conditions

The flux values and boundary conditions used in the simulations are as follows:

- $j_{\text{left}} = 1.0$, $j_{\text{right}} = -1.0$, $\rho_{\text{upper}} = 120.0$, $\rho_{\text{lower}} = 80.0$.
- $j_{\text{left}} = -1.0$, $j_{\text{right}} = 1.0$, $\rho_{\text{upper}} = 150.0$, $\rho_{\text{lower}} = 50.0$.
- $j_{\text{left}} = 0.5$, $j_{\text{right}} = -0.5$, $\rho_{\text{upper}} = 100.0$, $\rho_{\text{lower}} = 100.0$.
- $j_{\text{left}} = 2.0$, $j_{\text{right}} = -2.0$, $\rho_{\text{upper}} = 200.0$, $\rho_{\text{lower}} = 50.0$.

Combined Flux Study Results

The results for all flux studies are shown in the figure below, illustrating the concentration distributions for the selected flux and boundary condition values:

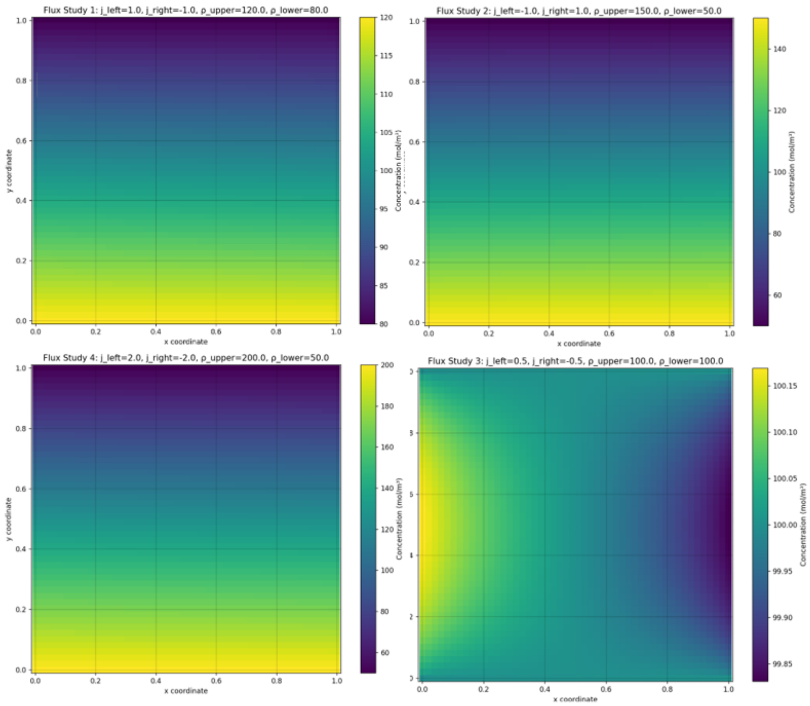

Figure 9: Combined results for the extended flux study, showing the steady-state concentration distributions for varying j_{left}, j_{right}, ρ_{upper}, and ρ_{lower}.

Matching Influx and Outflux

In each case, the simulations demonstrate that the flux values (j_{left} and j_{right}) are consistent with the boundary conditions:

- Positive and negative fluxes produce symmetrical or balanced distributions when inflow equals outflow.
- Unequal fluxes result in gradients aligned with the prescribed flux direction and boundary conditions.

Additional Observations

The steady-state concentration distributions reflect the effect of flux and boundary conditions on diffusion. Notable trends include:

- Larger flux magnitudes ($j_{\text{left}}, j_{\text{right}}$) result in steeper gradients.
- Symmetrical fluxes with equal upper and lower boundary concentrations lead to uniform distributions.
- Concentration gradients align with the flux direction and are influenced by boundary concentrations ($\rho_{\text{upper}}, \rho_{\text{lower}}$).