MA 203 Project: Numerical Modelling of Oil Spillage over Water Surface using Convection-Diffusion Equation

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1 Problem Statement

An oil spill is the release of a liquid petroleum hydrocarbon into the environment, especially the marine ecosystem, due to human activity, and is a form of pollution. The term is usually given to marine oil spills, where oil is released into the ocean or coastal waters, but spills may also occur on land. Oil spills may be due to releases of crude oil from tankers, offshore platforms, drilling rigs and wells, as well as spills of refined petroleum products (such as gasoline and diesel fuel) and their by-products, heavier fuels used by large ships such as bunker fuel, or the spill of any oily refuse or waste oil.

Spilled oil and seawater are considered in-compressible fluids, and it is assumed that there is no phase transition and slip at the oil–water interface[3].

The goal of this project is to stimulate diffusion of oil in water and the convection of oil movement of oil with respect to the velocity of water) during oil spillage. A theoretical and mathematical model of convection- diffusion of oil in water(2-D) will be developed and the resulting system of equations will be solved numerically on a computer. The specific objectives are presented below:

1. Develop a comprehensive mathematical model that represents the diffusion of oil in water and its convection, specifically during oil spillage.
2. Establish a set of reasonable assumptions that are essential for simplifying the problem while preserving its scientific relevance.
3. Derive the governing partial differential equation (PDE) from its preliminary form, taking into account the physical principles and relationships involved in the convection-diffusion of oil in water.
4. Formulate precise initial conditions that define the initial state of the oil concentration in the water domain. Additionally, establish boundary conditions that account for the interactions of oil with the environment, ensuring the model's realism.
5. Identify and select the correct values for relevant properties and parameters that describe the system.
6. Choose an appropriate numerical method to solve the derived PDE numerically.
7. Establish a stability analysis to confirm the discretized parameters chosen.
8. Solve the equation using Computer Program.
9. Investigate concentration profiles of oil under different velocity field scenarios, including zero velocity, constant velocity, and tilted velocity fields. Analyze how these different conditions impact the movement and dispersion of oil in water.

2 Physical Model

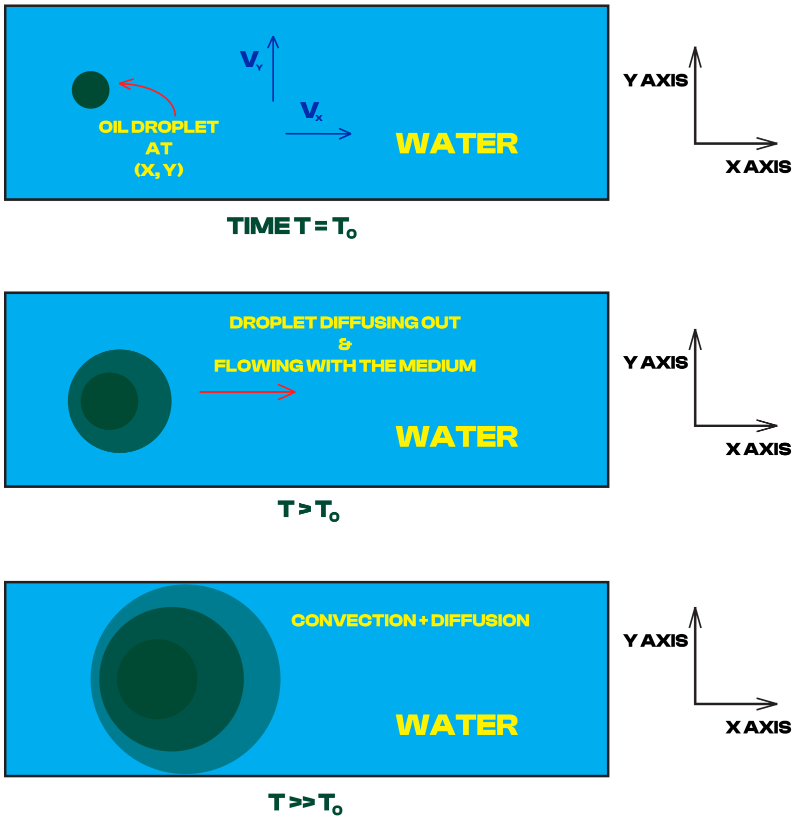

Figure 1: Diffusion of Oil Spill along with Convection with the medium

When oil particles (whose concentration is terms of particles/mm^3 is considered) are unintentionally introduced into water as highly concentrated blobs of oil, they experience both diffusion and convection. In the case of convection, the water is in motion with a certain velocity, and we use a reference frame attached to the moving water, which has velocities V_x and V_y. The diffusion process is governed by the Diffusion Coefficient D, while the convection part is dependent on the velocity field of the medium $\vec{\mathbf{V}}$. The whole problem is viewed in the 2D plane with entire medium being enclosed within a boundary L_x and L_y.

3 Assumptions

1. The problem is considered to be two dimensional and the diffusion and convection of oil particles is considered planar.
2. The domain is infinite in all 3 directions, and as the problem is 2D, no variation in z-direction is considered.
3. Each spatial point is assumed to have constant velocity field and in steady state.
4. The neglect of the "R" term in the convection-diffusion equation during numerical analysis is typically based on the following factors:
   - Simplicity and Efficiency: Omitting the "R" term simplifies the mathematical model, making it computationally efficient.
   - Dominance of Convection and Diffusion: In cases where convection and diffusion dominate, source/sink effects may be small and can be safely ignored.

- Localized Effects: If source/sink effects are highly localized and don't significantly affect the overall system behavior, neglecting "R" is reasonable. However, in scenarios with significant source/sink processes, "R" should be included for accuracy.

5. In a common situation, the diffusion coefficient is constant, there are no sources or sinks, and the velocity field describes an in-compressible flow(i.e., it has zero divergence).

4 Governing Equations

4.1 Conservation of Mass Equation

The derivation of the one-dimensional convection-diffusion equation starts with the conservation of mass[2]:

$$\frac{d}{dt}\int_V C(x,t)\,dV + \int_A (u\cdot C)\cdot dA = 0$$

Where:

- $C(x,t)$ is the concentration of the substance at position x and time t.
- u is the velocity of the fluid flow in the positive x-direction.
- V represents the control volume.
- A represents the control surface.

Now, we introduce the diffusion term, representing the diffusion of the substance within the fluid:

$$\text{Diffusion} = -D\cdot\nabla^2 C$$

Where:

- D is the diffusion coefficient.
- $\nabla^2 C$ represents the Laplacian of concentration, indicating how concentration varies spatially.

$$\frac{d}{dt}\int_V C(x,t)\,dV + \int_A (u\cdot C)\cdot dA = -\int_V D\cdot\nabla^2 C\,dV$$

Using the divergence theorem to express the surface integral as a volume integral:

$$\frac{d}{dt}\int_V C(x,t)\,dV + \int_V \nabla\cdot(u\cdot C)\,dV = -\int_V D\cdot\nabla^2 C\,dV$$

Assuming in-compressible flow ($\nabla\cdot u = 0$), we obtain:

$$\frac{d}{dt}\int_V C(x,t)\,dV + \int_V u\cdot\nabla C\,dV = -\int_V D\cdot\nabla^2 C\,dV$$

Applying the Fundamental Theorem of Calculus for the time derivative:

$$\frac{d}{dt}\int_V C(x,t)\,dV = \int_V \frac{\partial C}{\partial t}\,dV$$

The complete one-dimensional convection-diffusion equation with the diffusion term included is:

$$\int_V \frac{\partial C}{\partial t}\,dV + \int_V u\cdot\nabla C\,dV = -\int_V D\cdot\nabla^2 C\,dV$$

In differential form:

$$\frac{\partial C}{\partial t} + u\cdot\nabla C = D\cdot\nabla^2 C$$

This equation describes the transport (convection) and diffusion of a substance $C(x,t)$ in a one-dimensional fluid flow with velocity u, accounting for both advection and diffusion.

4.2 Diffusion Equation

In the most simplest form, the diffusion equation as derived from the stochastic model of Einstein's Brownian Motion, resembles the heat equation. In its three-dimensional form it is written as:

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) \tag{1}$$

Where D represents the *Diffusion Coefficient* and the scalar quantity $C(x, y, z, t)$, a function of time and spatial coordinates, maybe anything of our interest. In the one-dimensional case, the diffusion takes the form of the classic *Heat Equation*:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \tag{2}$$

4.3 Convection-Diffusion Equation

$$\boxed{\frac{\partial C}{\partial t} = \boldsymbol{\nabla} \cdot (D\overrightarrow{\boldsymbol{\nabla} C}) - \boldsymbol{\nabla} \cdot (C\vec{\mathbf{V}}) + R} \tag{3}$$

Where $\vec{\mathbf{v}}$ represents the velocity vector of the medium in which the convection/diffusion takes place, the R term denotes the source or sinks in discussion. By expanding out the divergence and gradient parts and neglecting any source or sinks ($R = 0$), we obtain the following:

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) - \left(V_x\frac{\partial C}{\partial x} + V_y\frac{\partial C}{\partial y} + V_z\frac{\partial C}{\partial z}\right) \tag{4}$$

Notice that the second term on the RHS represents the convection part of the equation. In an even more simplied form for a one-dimensional case, the equation maybe further reduced to:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - V_x\frac{\partial C}{\partial x} \tag{5}$$

And again, $C(x, t)$, D is the diffusion coefficient, and V is the velocity in the said direction of the medium of the convection.
In 2-Dimensional scenario where $C(x, y, t)$ is involved, we have:

$$\boxed{\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right) - V_x\frac{\partial C}{\partial x} - V_y\frac{\partial C}{\partial y}} \tag{6}$$

4.4 Velocity Field

A two-dimensional velocity field in fluid dynamics describes the speed and direction of fluid motion within a two-dimensional plane. It is represented as a vector field where each point in the plane corresponds to a velocity vector.

$$\text{2D Velocity Field:} \quad \boxed{\vec{\mathbf{V}}(x, y, t) = (u(x, y, t), v(x, y, t))} \tag{7}$$

For example for a rotatory swirl velocity field we may describe the relation as:

$$u = \omega \cdot (Y - y_c) \tag{8a}$$

$$v = -\omega \cdot (X - x_c) \tag{8b}$$

where,

$$r = \sqrt{(X - x_c)^2 + (Y - y_c)^2} \tag{8c}$$

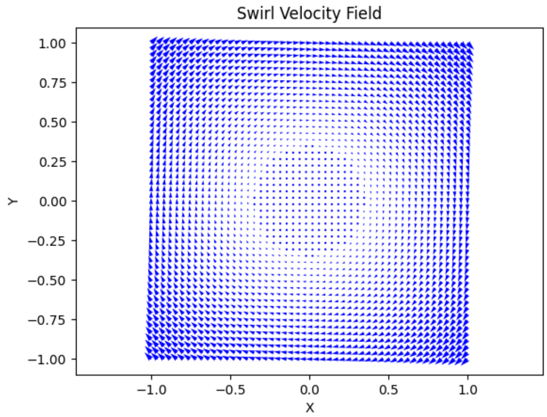

Figure 2: Swirl Velocity Field with ω = 2.0rad/s and center at($x_c = 0, y_c = 0$)

For our case we considered three velocity profiles:

1. Zero Velocity Field
2. Constant Velocity Field
3. Tilted Velocity Field

5 Boundary Conditions

For our scenario of oil spillage, we have considered the **Dirichlet Boundary Condition** only.

5.1 Dirichlet Boundary Condition

The Dirichlet boundary condition for concentration at the edges of the computational domain is given by:

$$C(x, y, t) = 0 \quad \text{for } (x, y) \in \partial\Omega$$

where:

- $C(x, y, t)$ is the concentration of oil at position (x, y) and time t.
- $\partial\Omega$ represents the boundary of the computational domain Ω.

This condition implies that the concentration of oil is fixed at 0 at the domain boundaries, indicating impermeable boundaries, no inflow or outflow of oil, and containment of the spill within the modeled domain. The oil spillage is, therefore, contained within the modeled area, and no inflow or outflow of oil occurs through the boundaries. It is a suitable choice for certain modeling scenarios but may not capture the full dynamics of real-world oil spill situations.

5.2 Neumann Boundary Condition

The Neumann boundary condition for concentration at the edges of the computational domain is given by:

$$\frac{\partial C}{\partial n} = 0 \quad \text{for } (x, y) \in \partial\Omega$$

where:

- $C(x, y, t)$ is the concentration of oil at position (x, y) and time t.
- $\frac{\partial C}{\partial n}$ represents the normal derivative of concentration, indicating that there is no flux of oil normal to the boundary.

- $\partial\Omega$ represents the boundary of the computational domain Ω.

This condition implies that there is no net flow of oil across the domain boundaries. In practical terms, it suggests that the concentration gradient at the boundary is zero, which can be interpreted as a condition of no oil entering or leaving the domain through the boundaries.

5.3 Parameters Involved

Parameter	Value
L_x (horizontal limit on water boundary)	$1.00m$
L_y (vertical limit on water boundary)	$1.00m$
D (Diffusion Coefficient)	$10^{-5}m^2/s$
N_x (Spatial x grid points)	50
N_Y (Spatial y grid points)	50
τ_s (Total Simulation Time)	$100.00s$
Δx (X-Grid Size)	$0.02m$
Δy (Y-Grid Size)	$0.02m$
Δt (Time Step)	$0.1s$

Table 1: List of Parameters involved

6 Numerical Solution & Results

6.1 Discretizing the Spatial Domain

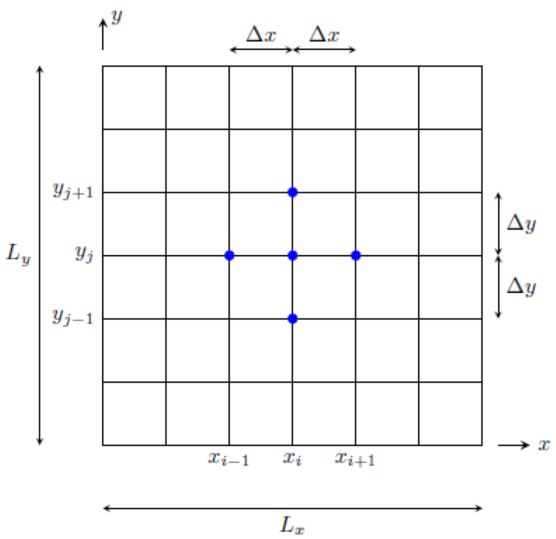

Figure 3: Discretizing the spatial domain (x, y)

Discretizing the spatial coordinates (x, y) and the time axis t using the relations:

$$\frac{\partial^2 C}{\partial x^2} \approx \frac{C_{i+1} - 2C_i + C_{i-1}}{(\Delta x)^2} \tag{9}$$

$$\frac{\partial^2 C}{\partial y^2} \approx \frac{C_{j+1} - 2C_j + C_{j-1}}{(\Delta y)^2} \tag{10}$$

$$\frac{\partial C}{\partial t} \approx \frac{C^{N+1} - C^N}{\Delta t} \tag{11}$$

Using all these, we eventually get the finite Volume/Difference Analysis as: For 1-Dimensional Case:

$$\frac{C_i^{N+1} - C_i^N}{\Delta t} = D\left(\frac{C_{i+1}^N - 2C_i^N + C_{i-1}^N}{(\Delta x)^2}\right) - V_x\left(\frac{C_{i+1}^N - C_i^N}{\Delta x}\right) \tag{12}$$

For 2-Dimensional Case:

$$\frac{C_{i,j}^{N+1} - C_{i,j}^N}{\Delta t} = D\left(\frac{C_{i+1,j}^N - 2C_{i,j}^N + C_{i-1,j}^N}{(\Delta x)^2} + \frac{C_{i,j+1}^N - 2C_{i,j}^N + C_{i,j-1}^N}{(\Delta y)^2}\right) - V_x\left(\frac{C_{i+1,j}^N - C_{i,j}^N}{\Delta x}\right) - V_y\left(\frac{C_{i,j+1}^N - C_{i,j}^N}{\Delta y}\right) \tag{13}$$

where $C_{i,j}^N$ represents the $x = i^{th}, y = j^{th}$ grid point in the N^{th} time step. Notice that for each time-step, we are evaluating an entire 2D array of spatial grid points! And each $C_{i,j}^{N+1}$ cell in the grid is dependent on five values from the previous time-step which enclose around the grid point $C_{i,j}^N$. Hence we can determine $C_{i,j}^{N+1}$ for all points except the BOUNDARY POINTS!

6.2 Initial and Boundary Conditions

Using the Dirichlet Boundary Criteria, we set the concentration $C(x, y, t)$ at boundary points equal to zero at all times.
For the initial condition, we set three points on the spatial grid to be having a high concentration of oil. The concentration and the corresponding points are:

1. $C(\frac{L_x}{4\Delta x}, \frac{L_y}{4\Delta y}, t = 0) = 100.00$ particles$/mm^3$
2. $C(\frac{3L_x}{4\Delta x}, \frac{3L_y}{4\Delta y}, t = 0) = 75.00$ particles$/mm^3$
3. $C(\frac{2L_x}{3\Delta x}, \frac{L_y}{3\Delta y}, t = 0) = 100.00$ particles$/mm^3$

These three points are shown in the top view of the 2D spatial grid in Figure 4.

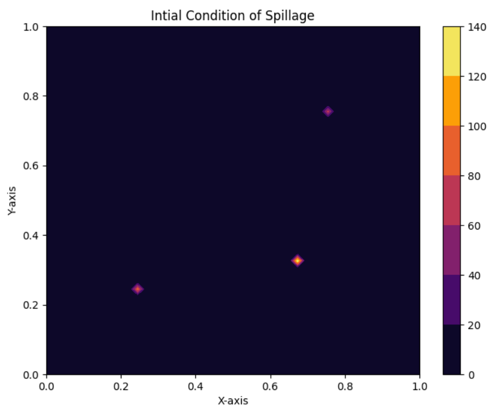

Figure 4: Initial location oil spills

6.3 Diffusion in Zero Velocity Field

In a zero velocity field medium, the oil spills do not move with the convection of water as the medium is a stationary frame. Hence in the absence of the convection term ($u = 0, v = 0$), the equation changes to a simple diffusion equation in 2D. The green trail in Figure 6. represents the concentration descent of the spatial point with the highest concentration. The linearity of the path confirms that only due to diffusion no lateral movement has happened in the 2D space.

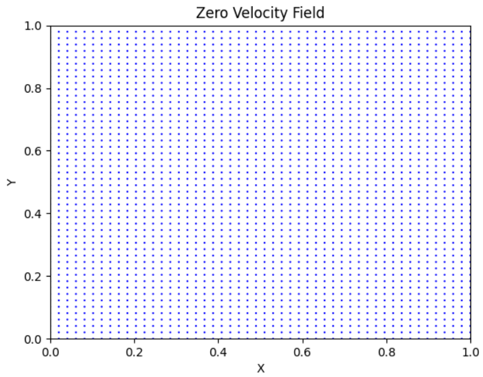

Figure 5: Zero Velocity Field

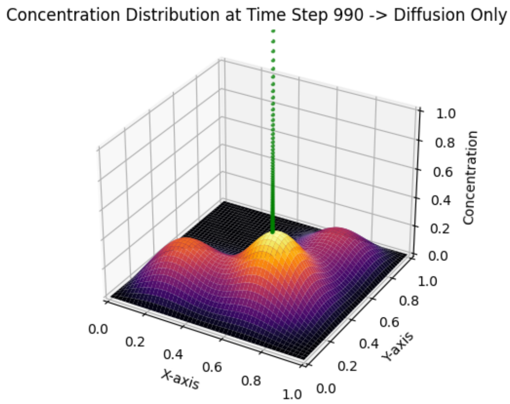

Figure 6: Final Contour of Oil Concentration with the green line showing the trail of the highest concentration point

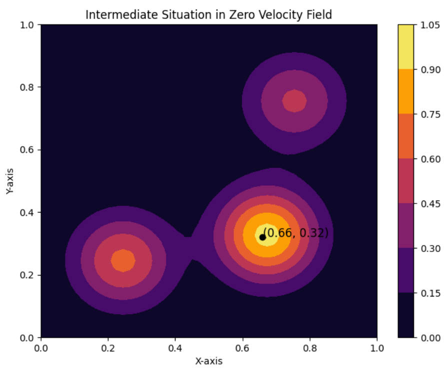

Figure 7: 2D view of concentration of oil at an intermediate time step (notice the coordinates of the highest concentration point)

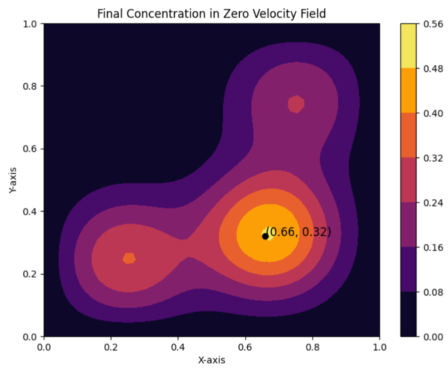

Figure 8: 2D view of the concentration of oil after the final time step

This can be clearly seen from Figure 7. and Figure 8. that the highest point has landed in the same $(x, y) = (0.66, 0.32)$ coordinates as it started with.

6.4 Convection-Diffusion in a Constant Velocity Field

In a constant velocity field with $(u = 0.01m/s, v = 0.01m/s)$, in addition to the diffusion term, the oil particles now advect with velocity field of the medium water too. This is observable in the green trail as shown in Figure 10. where the highest concentration point traverses laterally in addition to diffusion as time progresses.

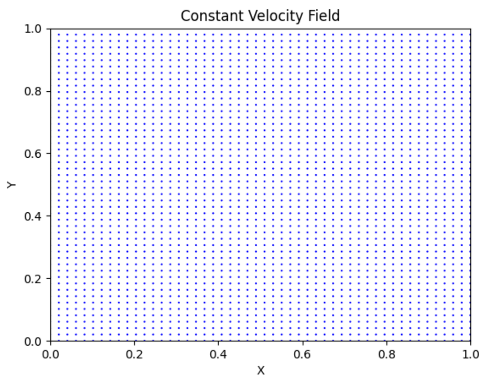

Figure 9: Constant Velocity Field with u = v = $0.01 m/s$

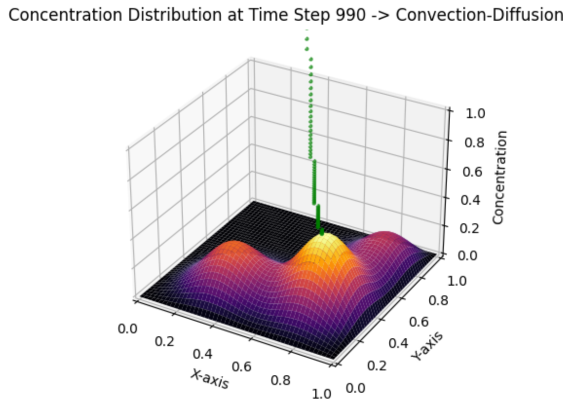

Figure 10: Final Contour of Oil Concentration with the green line showing the trail of the highest concentration point

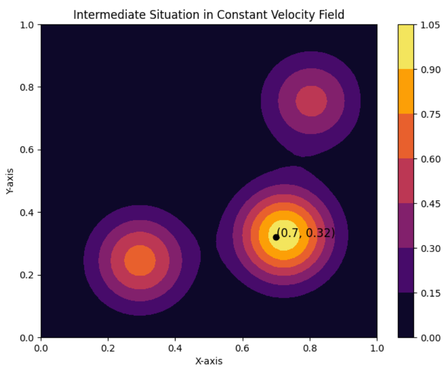

Figure 11: 2D view of concentration of oil at an intermediate time step (notice the coordinates of the highest concentration point)

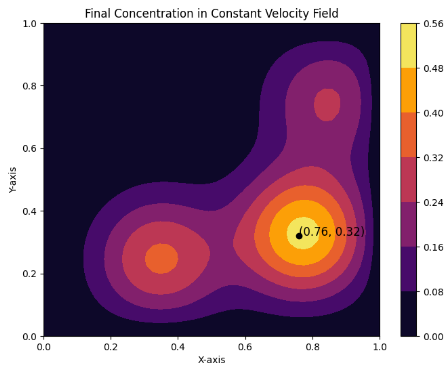

Figure 12: 2D view of concentration of oil after the final time step

This is evident from the Figure 11. and Figure 12. where the highest concentration point starts off at $(x, y) = (0.66, 0.32)$, moves on to the point $(x, y) = (0.70, 0.32)$ at an intermediate stage and thereby eventually ending up at the point $(x, y) = (0.76, 0.32)$.

6.5 Convection-Diffusion in a Tilted Velocity Field

In a constant velocity field with $(u = 0.01cos(\frac{\pi}{4})m/s, v = 0.01sin(\frac{\pi}{4}m/s)$, the motion though similar to that in the constant velocity field, has the particles sway in a slightly different direction.

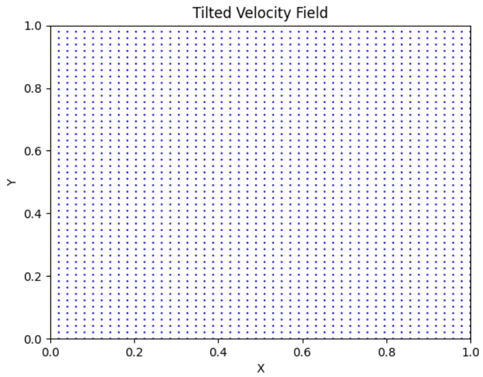

Figure 13: Tilted Constant Velocity Field

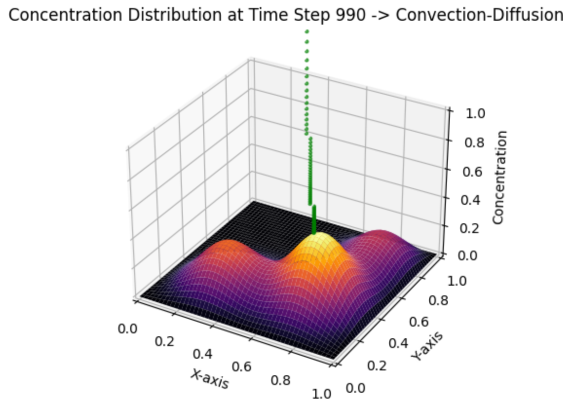

Figure 14: Final Contour of Oil Concentration with the green line showing the trail of the highest concentration point

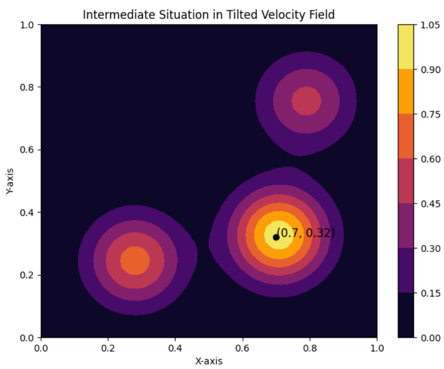

Figure 15: 2D view of concentration of oil at an intermediate time step (notice the coordinates of the highest concentration point)

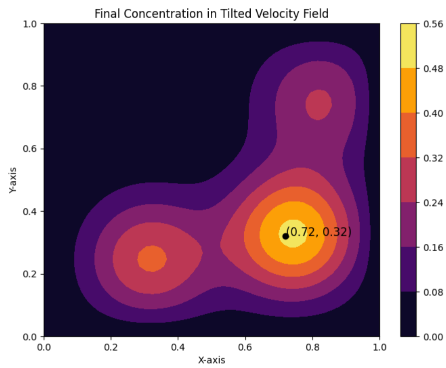

Figure 16: 2D view of concentration of oil after the final time step

This is evident from the Figure 15. and Figure 16. where the highest concentration point starts off at $(x, y) = (0.66, 0.32)$, moves on to the point $(x, y) = (0.70, 0.32)$ at an intermediate stage and thereby eventually ending up at the point $(x, y) = (0.72, 0.32)$. Which is different from that in the case of constant velocity field case $(x, y) = (0.76, 0.32)$.

7 Algorithms Used

7.1 Finite-Volume Method using Explicit Scheme

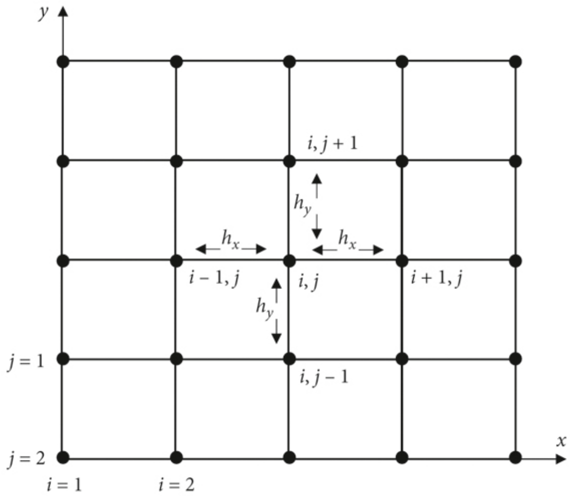

Figure 17: Finite Volume Method

At each step of discretizing the first-order or the second-order derivatives, we have used the forward difference method:

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} \tag{14}$$

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} \tag{15}$$

Both these have been employed for the spatial derivatives and the time derivatives to obtain an iterative solution to find the i^{th} and j^{th} spatial coordinate at time $t = N + 1$ from the volume surrounded by the cells at the previous time step $t = N$.

```python
import numpy as np
import matplotlib.pyplot as plt

# Define parameters
Lx = 1.0
Ly = 1.0
Nx = 50
Ny = 50
D = 10e-5

# # Zero Velocity Field
# u, v = 0, 0

# # Constant Velocity Field
# u, v = 0.001, 0.001

# Constant Tilted Velocity Field
u = 0.001 * np.cos(np.pi/4)    # Horizontal airflow velocity (m/s)
v = 0.001 * np.sin(np.pi/4)  # Vertical airflow velocity (m/s)


x = np.linspace(0, Lx, Nx)
y = np.linspace(0, Ly, Ny)
X, Y = np.meshgrid(x, y)
```

```python

delta_x = Lx / Nx
delta_y = Ly / Ny
delta_t = 0.1
t_simulation = 100.0
num_time_steps = int(t_simulation / delta_t)

C = np.zeros((Nx, Ny))

# Initial condition (a point source at the center)
C[Nx//4, Ny//4] = 100.0
C[3*Nx//4, 3*Ny//4] = 75.0
C[2*Nx//3, Ny//3] = 150.0


fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')

Concentration_snapshots = []

for step in range(num_time_steps):
    C_new = C.copy()
    # Finite difference calculations for interior grid points
    for i in range(1, Nx - 1):
        for j in range(1, Ny - 1):
            C_new[i, j] = C[i, j] + D * delta_t * (
                (C[i+1, j] - 2 * C[i, j] + C[i-1, j]) / delta_x**2 +
                (C[i, j+1] - 2 * C[i, j] + C[i, j-1]) / delta_y**2) -
                u * delta_t * (C[i + 1, j] - C[i, j])/delta_x
            - v * delta_t * (C[i, j + 1] - C[i, j])/delta_y
    C = C_new
    Concentration_snapshots.append(C.copy())

```

8 Error Analysis

8.1 Courant–Friedrichs–Lewy (CFL) condition

The Courant–Friedrichs–Lewy (CFL) condition ensures that the time step used in a numerical simulation is small enough to accurately capture the propagation of information within the system. This ensures that the Δt is small enough to not miss any information between the time-steps[1].

For our Convection-Diffusion Equation:

$$\boxed{\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right) - V_x\frac{\partial C}{\partial x} - V_y\frac{\partial C}{\partial y}} \tag{16}$$

The CFL criteria for the Convection part of the equation:

$$C_{\text{convection}} = \frac{V_x \Delta t}{\Delta x} + \frac{V_y \Delta t}{\Delta y} \leq CFL_{\max} \tag{17}$$

For the Diffusion part of the equation the CFL condition is now:

$$C_{\text{diff}} = \frac{D\Delta t}{(\Delta x^2 + \Delta y^2)} \leq CFL_{max} \tag{18}$$

Combining these two we have:

$$C_{\text{convection}} + C_{\text{diff}} \leq C_{\max} \tag{19}$$

On further simplifying we get:

$$\boxed{\Delta t \leq \min\left(\frac{\Delta x^2}{2(|V_x| + |V_y|) + 2D}, \frac{\Delta y^2}{2(|V_x| + |V_y|) + 2D}\right)} \tag{20}$$

9 Visualizations

Open the PDF in Acrobat and click on the graphics to play the GIF.

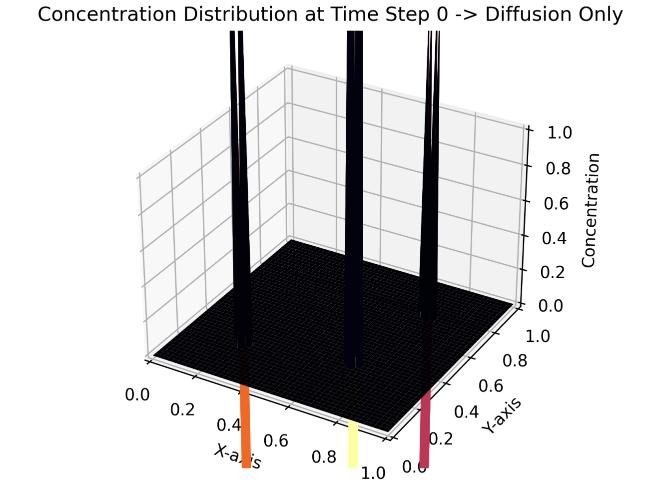

Figure 18: Zero Velocity Field Animation

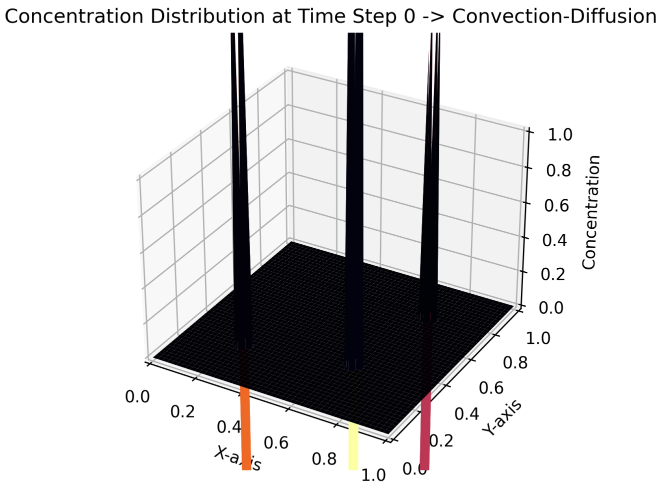

Figure 19: Constant Velocity Field Animation

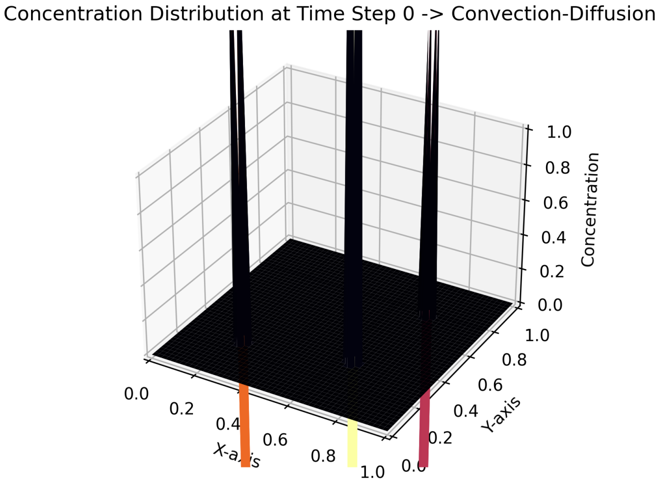

Figure 20: Tilted Velocity Field Animation

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