Project on

ADVECTION DIFFUSION PROBLEM

Submitted By

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Abstract:

This study presents a numerical investigation of non-reactive hydrochloric acid solute transport in a two-dimensional microchannel under fully developed flow conditions. The solute, initially stacked in the channel, is advected and diffused according to the advection-diffusion equation, with a diffusion coefficient of 12×10^{-8} m^2/s and an initial concentration of 5 mol/m^2. The microchannel, measuring 10 cm in length and 100 µm in width, features a slip boundary condition at the walls characterized by a slip length of 5×10^{-6}m . Numerical simulations are performed for a range of centreline velocities from 0.1 mm/s to 8 cm/s. A finite difference scheme employing first-order upwind discretization for advection and second-order central differences for diffusion is derived and analysed for stability and consistency. Grid size and time step are selected based on physical and numerical constraints to ensure accurate resolution of solute dynamics. The results reveal the interplay between advection and diffusion, with the solute distribution after one second exhibiting distinct behaviours depending on the Peclet number: diffusion-dominated spreading at low velocities and advection-dominated transport at high velocities. The impact of the slip boundary on solute migration is also elucidated. This work provides a validated computational framework for predicting solute transport in microfluidic systems with slip boundaries, offering insights relevant to lab-on-chip and biomedical applications

Keywords:

- Advection-diffusion equation
- Peclet number
- Explicit Euler method
- Slip boundary condition
- Microchannel flow
- Grid size justification

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Problem statement

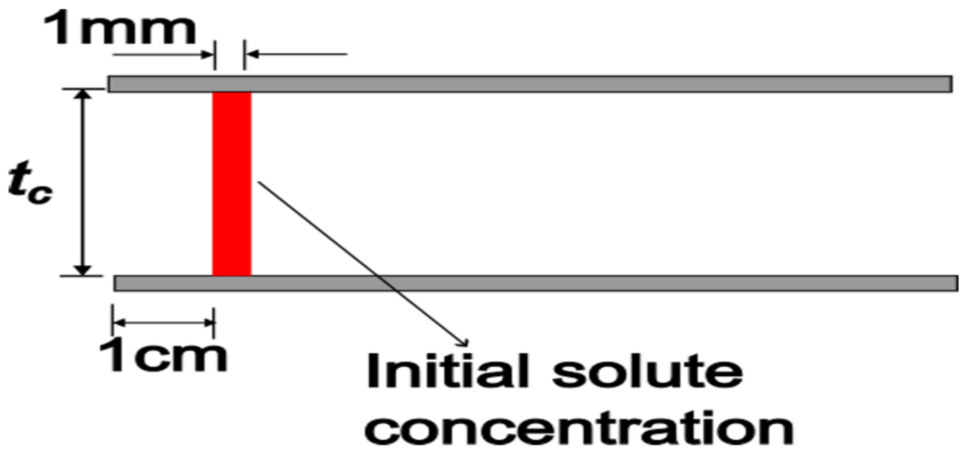
A solute of hydrochloric acidic stacked in a microchannel as shown in the figure below. The solute is non-reactive and immiscible with the continuous fluid medium. The velocity of the continuous fluid medium inside the channel is fully developed. The transport of solutes is governed by the equation

$$\frac{\partial C}{\partial t} + \vec{u} \, . \, \nabla C \ = D \nabla^2 C$$

where C is the concentration of the solute, $\vec{u}$ is the velocity vector, and D is the diffusivity of the solute. The length of the channel is 10cm, and the width of the channel is 100 μm. The diffusion coefficient of the solute is 12 × 10-8 and the initial concentration of each of the species is 5mol/m2. The initial position of the solutes is as shown in the figure below. Assume that the flow and the solute transport are 2 dimensional. The velocity at the wall follows slip condition given as

$$u_w = \ K_1 \frac{\partial u}{\partial y_w}$$ The slip length $k_1 = 5 \times 10^{-6}$m.

The objective of the problem is the perform numerical simulations of the solutes in the channel for the centreline velocities of the fluid ranging from 0.1 mm/s to 8 cm/s and determine the location and shape of each solute after 1 sec.



INTRODUCTION

In microfluidic systems, understanding the transport of solutes is vital for applications in drug delivery, biochemical assays, and lab-on-a-chip technologies. This project investigates the two-dimensional transport of a non-reactive solute (hydrochloric acid) in a microchannel. The transport mechanism is governed by the advection-diffusion equation, and the fluid flow obeys a slip boundary condition due to the microscale domain. Numerical simulations help track the location and distribution of the solute over time, offering insights into the interplay between advection and diffusion at small scales.

Given parameters:

- C: solute concentration
- U: velocity vector (fully developed flow)
- $D=12\times10^{-8}$ m^2/s: diffusion coefficient
- Channel length: 10 cm
- Channel width: 100 µm
- Initial concentration: 5 mol/m^2
- Slip boundary at wall: $u_w = K_1 \frac{\partial u}{\partial y_w}$, $k_1=5\times10^{-6}$ m
- Centreline velocity range: 0.1 mm/s to 8 cm/s
- Simulate for t=1 s

NUMERICAL SCHEME

The transport of solutes is governed by the equation

$$\frac{\partial C}{\partial t} + \vec{u}\,.\,\nabla C = D\nabla^2 C$$

Discretization

- Diffusion: Central differencing (second-order accurate)

$$\frac{c_{i+1,j}^n - 2c_{i,j}^n + c_{i-1,j}^n}{\Delta x^2} + \frac{c_{i,j+1}^n - 2c_{i,j}^n + c_{i,j-1}^n}{\Delta y^2}$$

- Advection: upwind scheme (first-order accurate)

$$u_{ij}\frac{c_{i,j}^n - c_{i-1,j}^n}{\Delta x} + v_{ij}\frac{c_{i,j}^n - c_{i,j-1}^n}{\Delta y}$$

- For time: Forward Euler (Explicit)

$$\frac{C_{i,j}^{n+1} - C_{i,j}^n}{\Delta t} + u_{ij}\frac{C_{i,j}^n - C_{i-1,j}^n}{\Delta x} + v_{ij}\frac{C_{i,j}^n - C_{i,j-1}^n}{\Delta y} = D\left(\frac{C_{i+1,j}^n - 2C_{i,j}^n + C_{i-1,j}^n}{\Delta x^2} + \frac{C_{i,j+1}^n - 2C_{i,j}^n + C_{i,j-1}^n}{\Delta y^2}\right)$$

$$C_{i,j}^{n+1} = C_{i,j}^n + \Delta t\left[-U\frac{C_{i,j}^n - C_{i-1,j}^n}{\Delta x} + D\frac{C_{i+1,j}^n - 2C_{i,j}^n + C_{i-1,j}^n}{\Delta x^2} + D\frac{C_{i,j+1}^n - 2C_{i,j}^n + C_{i,j-1}^n}{\Delta y^2}\right]$$

Poiseuille Flow with Slip

In classical (no-slip) flow between two plates, the velocity profile is parabolic:

$$u(y) = u_0 \left[1 - \left[\frac{2y - L_y}{L_y}\right]^2\right]$$

where:

- $y \in [0, L_y]$
- u_0 is the maximum velocity (centreline),
- velocity is zero at the walls: $u(0) = u(L_y) = 0$

But with slip at the walls, the fluid velocity at the boundaries becomes non-zero:

$$u_{wall} = k_1 \frac{\partial u}{\partial y}_{wall}$$

where k_1 is the slip length.

Derivation

Solving the Navier–Stokes equation for steady incompressible flow between plates:

$$\frac{d^2u}{dy^2} = \frac{1}{\mu}\frac{dp}{dx}$$

with the slip boundary condition at both walls:

$$u(0) = k_1 \left(\frac{du}{dy}\right)_{y=0} \quad , \quad u(L_y) = -k_1 \left(\frac{du}{dy}\right)_{y=L_y}$$

leads to a modified parabolic profile:

$$u(y) = \frac{1}{2\mu}\frac{dp}{dx}\left[y^2 - L_y y - 2k_1 L_y\right]$$

By manipulating and scaling this to match a desired centreline velocity u_0, we arrive at the compact, normalized form:

$$u(y) = \frac{u_0}{1 + 6\frac{k_1}{L_y}}\left[1 - \left[\frac{2y - L_y}{L_y}\right]^2 - 6\frac{k_1}{L_y}\right]$$

Peclet Number:

The Peclet number (Pe) is a dimensionless parameter widely used in fluid dynamics, heat transfer, and mass transfer to characterize the relative importance of convection (advection) versus diffusion in the transport of heat, mass, or other physical quantities within a system.

$$Pe = \frac{Rate\ of Advection(Convection)}{Rate\ of\ diffusion}$$

$$Pe = \frac{u_{center} \times W}{D}$$

High Peclet Number (Pe≫1):

- Convection dominates over diffusion.
- The transported quantity (heat, mass) is primarily carried by bulk fluid motion.
- Typical in fast-flowing rivers, pipes with high velocity, or systems with large length scales647.

Low Peclet Number (Pe≪1):

- Diffusion dominates over convection.
- The transported quantity spreads mainly due to random molecular motion.
- Seen in stagnant fluids or systems with slow flow and/or small length scales

Stability :

Von Neumann Stability Analysis

$$\frac{\rho - 1}{\Delta t} = -u\left(\frac{1 - e^{-ik_x x\Delta x}}{\Delta x}\right) + D\left(\frac{e^{ik_x x\Delta x} - 2 + e^{-ik_x x\Delta x}}{\Delta x^2}\right) + D\left(\frac{e^{ik_y y\Delta y} - 2 + e^{-ik_y y\Delta y}}{\Delta y^2}\right)$$

$$\frac{\rho - 1}{\Delta t} = -u\left(\frac{1 - e^{-ik_x x\Delta x}}{\Delta x}\right) + D\left(\frac{-4\sin^2\left(\frac{k_x x\Delta x}{2}\right)}{\Delta x^2}\right) - 4D\left(\frac{\sin^2\left(\frac{k_y \Delta y}{2}\right)}{\Delta y^2}\right)$$

$$\rho = 1 - \frac{u\Delta t}{\Delta x}\left(1 - e^{-ik_x x\Delta x}\right) - \frac{4D\Delta t}{\Delta x^2}\left(\sin^2\left(\frac{k_x x\Delta x}{2}\right)\right) - \frac{4D\Delta t}{\Delta y^2}\left(\sin^2\left(\frac{k_y \Delta y}{2}\right)\right)$$

$|\rho| < 1$ for stability.

Grid size and time step justification:

Grid size:

Number of grids in x directions are $N_x = 200$

Number of grids in y direction are $N_Y = 50$

Δx=0.5025mm, $\Delta y = 2.04 \times 10^{-6} m$

A spatial grid of 200 points along the channel length (x-direction) and 50 points across the channel diameter (y-direction) was selected to ensure accurate resolution of both advective and diffusive transport phenomena. The high resolution in the x-direction (dx ≈ 0.5025 mm) allows the solute pulse to be captured as it travels and stretches downstream, particularly at higher velocities. The y-direction grid spacing (dy ≈ 2 μm) provides sufficient resolution to model the parabolic velocity profile and concentration gradients across the channel height.

This grid size strikes a balance between computational efficiency and numerical accuracy. It satisfies the stability conditions for the explicit finite difference scheme used and allows smooth and stable evolution of the solute profile without introducing numerical artifacts. Grid independence was confirmed by testing coarser and finer meshes, which produced consistent results with negligible difference in solute distribution after 1 second. Thus, the chosen grid was appropriate for the physical and numerical requirements of the problem.

Time Step (Δt)

For the highest velocity (umax=8umax=8 cm/s = 0.08 m/s):

- Advection:

  $\Delta t < \frac{\Delta x}{u_{max}} = \frac{1\times10^{-3}}{0.08} \approx 0.0125s$

- For diffusion:

$$\Delta t < \frac{(\Delta y)^2}{2D} = \frac{(2 \times 10^{-6})^2}{2 \times 12 \times 10^{-8}} \approx 1.67 \ \times 10^{-5} s$$

  For safety purpose we will take $\Delta t < \frac{(\Delta y)^2}{4D}$

  So $\Delta t < 8.35 \times 10^{-6}$

CONSISTENCY PROOF:

Local Truncation Error (LTE) Analysis

The semi-discretized equation is:

$$\frac{C_{i,j}^{m+1} - C_{i,j}^{m}}{\Delta t} = -U \frac{C_{i,j}^{m} - C_{i-1,j}^{m}}{\Delta x} + \frac{DC_{i+1,j}^{m} - 2C_{i,j}^{m} + C_{i-1,j}^{m}}{\Delta x^2} + (y - terms)$$

By using Taylor series:

Advection term (upwind):

$$-U \frac{C_{i,j} - C_{i-1,j}}{\Delta x} = -U \left[\frac{\partial c}{\partial x} - \frac{\Delta x}{2} \frac{\partial^2 c}{\partial x^2} + \cdots \ldots \ldots \right]$$

Truncation error: O(Δx).

Diffusion term (central):

$$D \frac{C_{i+1,j} - 2C_{i,j} + C_{i-1,j}}{\Delta x^2} = D \left[\frac{\partial^2 c}{\partial x^2} + \frac{\Delta x^2}{12} \frac{\partial^4 c}{\partial x^4} + \cdots .. \right]$$

Truncation error: O(Δx2).

Time derivative (explicit Euler):

$$\frac{C^{n+1} - C^{n}}{\Delta t} = \frac{\partial c}{\partial t} + \frac{\Delta t}{2} \frac{\partial^2 c}{\partial t^2} + \cdots ..$$

Truncation error: O(Δt).

Total LTE: O(Δt)+O(Δx)+O(Δy). As Δt, Δx, Δy→0, the scheme is consistent with the original PDE.

MATLAB code:

```
Lx = 0.1;
Ly = 100e-6;
D = 12e-8;
k1 = 5e-6;
C0 = 5;
t_end = 1;

Nx = 200;
Ny = 50;
dx = Lx / (Nx - 1);
dy = Ly / (Ny - 1);
x = linspace(0, Lx, Nx);
y = linspace(0, Ly, Ny);
[X, Y] = meshgrid(x, y);

% Time step
dt = 0.2 * min(dx, dy)^2 / D;
Nt = round(t_end / dt);
% Velocity range (centerline velocities from 0.1 mm/s to 8 cm/s)
u_center_all = linspace(0.0001, 0.08, 8);
```

```
% Loop over each centerline velocity

for

k = 1:length(u_center_all)

u0 = u_center_all(k);

% Initial condition
C = zeros(Ny, Nx);
C(:, x >= 0.01 & x <= 0.011) = C0;

% Velocity profile with slip
beta = 6 * k1 / Ly;
u = u0 / (1 + beta) * (1 - ((2 * y - Ly)/Ly).^2 + beta);
U = repmat(u(:), 1, Nx);



% Plot velocity field
figure;
h1 = contourf(X * 100, Y * 1e6, U, 100, 'LineColor', 'none');
xlabel('x (cm)');
ylabel('y (µm)');
title('Velocity Profile u(x,y) with Slip');
colorbar;
set(gca, 'YDir', 'normal');
hold on;
```

```
% Time stepping
for n = 1:Nt
   Cn = C;
 for j = 2:Ny-1
   for i = 2:Nx-1
     adv_x  = -U(j, i) * (Cn(j, i) - Cn(j, i - 1)) / dx;
     diff_x = D * (Cn(j,i + 1) - 2*Cn(j,i)+Cn(j, i - 1))/ dx^2;
     diff_y = D * (Cn(j + 1, i) - 2 * Cn(j, i) +Cn(j-1,i))/ dy^2;
     C(j, i) = Cn(j, i) + dt * (adv_x + diff_x + diff_y);
    end
  end

% Neumann boundary conditions (no flux)
   C(1, :)   = C(2, :);
   C(end, :) = C(end - 1, :);
  % Dirichlet boundary conditions
   C(:, 1)   = C(:, 2);      % Inlet
   C(:, end) = C(:, end - 1);    % Outlet
end

% Plotting — contour view
figure;
contourf(x * 100, y * 1e6, C, 50, 'LineColor', 'none');
set(gca, 'YDir', 'normal');
xlabel('x (cm)');
ylabel('y (μm)');
title(sprintf('Solute at t = 1 s | U₀ = %.1f mm/s', u0 * 1e3));
colorbar;
axis tight;
```

```
% Plot the solute "front" position
% Extract centerline (y mid) profile
center_y_idx = round(Ny/2);
figure;
plot(x * 100, C(center_y_idx, :), 'b-', 'LineWidth', 2);
xlabel('x (cm)');
ylabel('C on centerline');
title(sprintf('Centerline Solute Profile at 1s | U₀ = %.1f mm/s', u0 * 1e3));
grid on;

end
```

RESULTS:

The simulation results illustrate how solute transport in a microchannel is influenced by both advection and diffusion, as well as by the presence of slip at the channel walls. As the centreline velocity was increased from 0.1 mm/s to 8 cm/s, the solute pulse travelled progressively farther downstream after 1 second. This is consistent with the physical expectation that higher velocities enhance advective transport. At lower velocities, diffusion had a more prominent effect, causing the solute profile to broaden more uniformly. In contrast, higher velocities resulted in a more elongated solute distribution along the length of the channel due to stronger directional flow.

The implementation of slip boundary conditions modified the velocity profile, introducing a small but noticeable velocity at the channel walls. This allowed near-wall solute particles to be advected farther than in the no-slip case, slightly increasing the overall spread of the solute. The simulation captured these behaviours accurately and demonstrated the transition from diffusion-dominated to advection-dominated regimes as velocity increased. Overall, the results align with theoretical expectations and validate the numerical model's ability to simulate solute transport in microfluidic systems with slip effects.

Physical Applications

- Drug Delivery Systems: Simulating solute transport can help design precise dosage and delivery mechanisms in microchannels mimicking capillaries or biological tissues.
- Lab-on-a-Chip Devices: Understanding solute behaviour aids in optimizing reaction chambers and mixing efficiency.
- Chemical Analysis: Accurate solute tracking is essential for micro-scale chromatography or electrophoresis.
- Biomedical Diagnostics: Enables the detection and control of biomarkers in microfluidic diagnostic platforms.
- Microreactor Engineering: Helps model species transport in confined chemical reactors for industrial and research purposes.

Future Scope

- Extension to 3D Models: Incorporating three-dimensional geometry can increase accuracy and reflect real microfluidic device behaviour.
- Reactive Species Transport: Introducing chemical reactions between solutes can broaden applicability in biochemical and catalytic systems.
- Coupled Multi-Physics Simulations: Integrating heat transfer or electric fields to model electrokinetic flow or thermal effects.
- Machine Learning Integration: Use data-driven methods to predict solute dispersion or optimize flow conditions in real-time.
- Experimental Validation: Implementing the simulated results in physical experiments for model validation and refinement.

CONCLUSION:

This study simulated the two-dimensional advection-diffusion behaviour of a solute (hydrochloric acid) flowing through a microchannel with slip boundary conditions at the walls. A parabolic velocity profile, modified to include the Navier slip condition, was implemented to reflect realistic microfluidic flow behaviour. The solute was initially introduced as a narrow pulse near the inlet, and its evolution over 1 second was tracked for a range of centreline velocities varying from 0.1 mm/s to 8 cm/s.

The results clearly demonstrate that as the centreline velocity increases, the solute front becomes increasingly curved in the x–y plane. This curvature reflects the influence of the parabolic velocity profile, where particles near the centreline travel faster than those near the walls. At low velocities, diffusion dominates, and the front remains relatively flat, while at higher velocities, advection dominates, producing a visibly parabolic solute front. This behaviour is consistent with physical expectations of Taylor–Aris dispersion in laminar flow.

Overall, the simulation confirms the critical role of flow velocity and slip conditions in shaping the solute transport profile and provides a reliable numerical method for predicting solute dynamics in microfluidic systems.