Homework 4

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BIOENG 104 Biological Transport Phenomena | Aaron Streets

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1 Problem 1

When examining diffusion out of (or into) a semi-infinite membrane, we applied the assumptions that there is no reaction in the membrane, we are not at steady-state, C_1 is constant in space and time, there and there is only diffusion in the x-direction, in order to reduce the general form of Fick's 2$^{\text{nd}}$ law to the following differential equation:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \tag{1.1}$$

Our goal is to solve for $c(x,t)$, but we cannot assume that $c(x,t)$ is separable, in other words $c(x,t) \neq f(x)g(t)$, because the boundary condition at $x = 0$ is not homogeneous, $c(0,t) = C_1$. Therefore, we performed a substitution to turn this second order partial differential equation into a dimensionless ordinary differential equation. The substitution for c, x, and t is defined below.

$$\theta = \frac{c - C_1}{C_0 - C_1}, \quad \eta = \frac{x}{\sqrt{4Dt}} \tag{1.2}$$

Show that when θ and η are substituted into the differential equation above, the resulting differential equation is:

$$-2\eta\frac{\mathrm{d}\theta}{\mathrm{d}\eta} = \frac{\mathrm{d}^2\theta}{\mathrm{d}\eta^2} \tag{1.3}$$

Show every step and provide a brief explanation when implementing a rule or identity.

This problem can be tackled by converting the first differential equation in terms of θ and η one side at a time. Doing the left-hand side first, we can use the chain rule so that we can express c in terms of θ in the differential equation.

$$\frac{\partial c}{\partial t} = \frac{\partial c}{\partial \theta}\frac{\partial \theta}{\partial t} \tag{1.4}$$

Solving for c in terms of θ from Equation (1.2),

$$\begin{aligned} c - C_1 &= \theta(C_0 - C_1) \\ c &= \theta(C_0 - C_1) + C_1 \end{aligned}$$

then differentiating in terms of θ,

$$\frac{\partial c}{\partial \theta} = C_0 - C_1 \tag{1.5}$$

We can substitute this result in Equation (1.4) to gain a new differential equation. Using the chain rule again, we aim to express the partial derivative in terms of η and t since η is a function of t also.

$$\begin{aligned}\frac{\partial c}{\partial \theta} &= (C_0 - C_1)\frac{\partial \theta}{\partial t} \\ &= (C_0 - C_1)\frac{\partial \theta}{\partial \eta}\frac{\partial \eta}{\partial t}\end{aligned} \tag{1.6}$$

Similarly, we differentiate η in terms of t and plug back in to Equation (1.6).

$$\begin{aligned}\frac{\partial \eta}{\partial t} &= \frac{\partial}{\partial t}\frac{x}{\sqrt{4Dt}} \\ &= x\big(-1/2\big)(4Dt)^{-3/2}(4D) \\ &= -x/2\ (4D)^{-1/2}t^{-3/2} \\ &= -x/2\ 1/t\ (4D)^{-1/2}t^{-1/2} \\ &= -\frac{1}{2t}\frac{x}{\sqrt{4Dt}} \\ &= -\frac{\eta}{2t} \\ \therefore \frac{\partial c}{\partial \theta} &= -(C_0 - C_1)\frac{\eta}{2t}\frac{\partial \theta}{\partial \eta}\end{aligned} \tag{1.7}$$

Doing the right-hand side of the original differential equation, we use the chain rule in anticipation of expressing everything in terms of θ and η. Equation (1.5) gives us a simple substitution for $\partial c/\partial \theta$.

$$\begin{aligned}\frac{\partial^2 c}{\partial x^2} &= \frac{\partial}{\partial x}\left(\frac{\partial c}{\partial x}\right) \\ &= \frac{\partial}{\partial x}\left(\frac{\partial c}{\partial \theta}\frac{\partial \theta}{\partial x}\right) \\ &= \frac{\partial}{\partial x}\left((C_0 - C_1)\frac{\partial \theta}{\partial x}\right) \\ &= (C_0 - C_1)\frac{\partial}{\partial x}\left(\frac{\partial \theta}{\partial x}\right)\end{aligned}$$

Similarly, the chain rule and the differentiation of η with respect to t allows us to develop $\partial\theta/\partial x$ further. We also know from $\eta = x/\sqrt{4Dt}$ that its partial derivative is simply the coefficient of x.

$$\frac{\partial \eta}{\partial x} = \frac{1}{\sqrt{4Dt}} \implies \frac{\partial \theta}{\partial x} = \frac{\partial \theta}{\partial \eta}\frac{\partial \eta}{\partial x} = \frac{\partial \theta}{\partial \eta}\frac{1}{\sqrt{4Dt}} \tag{1.8}$$

When differentiating $\partial\theta/\partial x$ when it's in terms of t requires an additional application of the chain rule.

$$\begin{aligned}
\frac{\partial}{\partial x}\left(\frac{\partial\theta}{\partial x}\right) &= \frac{\partial}{\partial x}\left(\frac{\partial\theta}{\partial\eta}\frac{1}{\sqrt{4Dt}}\right) \\
&= \frac{\partial\eta}{\partial x}\frac{\partial}{\partial\eta}\left(\frac{\partial\theta}{\partial\eta}\frac{1}{\sqrt{4Dt}}\right) \\
&= \frac{1}{\sqrt{4Dt}}\frac{\partial}{\partial\eta}\left(\frac{\partial\theta}{\partial\eta}\frac{1}{\sqrt{4Dt}}\right) \\
&= \frac{1}{4Dt}\frac{\partial^2\theta}{\partial\eta^2} \\
\therefore \frac{\partial^2 c}{\partial x^2} &= (C_0 - C_1)\frac{1}{4Dt}\frac{\partial^2\theta}{\partial\eta^2} \qquad (1.9)
\end{aligned}$$

The replacement of $\partial\eta/\partial x$ by $1/\sqrt{4Dt}$ comes from Equation (1.8). Bringing in Equation (1.7) and Equation (1.9) together, we have the new differential equation in terms of θ and η.

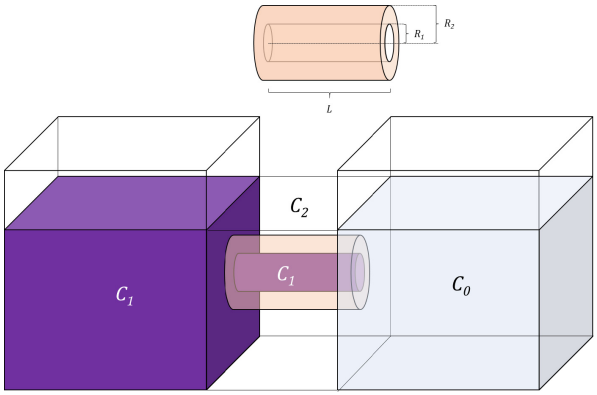
$$\begin{aligned}
-(C_0 - C_1)\frac{\eta}{2t}\frac{\partial\theta}{\partial\eta} &= D(C_0 - C_1)\frac{1}{4Dt}\frac{\partial^2\theta}{\partial\eta^2} \\
-\frac{\eta}{2t}\frac{\partial\theta}{\partial\eta} &= \frac{1}{4t}\frac{\partial^2\theta}{\partial\eta^2}
\end{aligned}$$

and multiplying the equation by $4t$, assuming $t \neq 0$, we get the final result.

$$-2t\frac{\partial\theta}{\partial\eta} = \frac{\partial^2\theta}{\partial\eta^2}$$

2 Problem 2

Imagine a cylindrical membrane with a hollow core, depicted in orange below, of length L, inner radius R_1 and outer radius R_2. This membrane connects two large, well-mixed tanks of solution that are held at constant concentrations C_1 and C_0 respectively. The inner core of the membrane is held at C_1 and the membrane is submerged in a third tank that is also well-mixed and held at a concentration C_2. All of the surfaces of the membrane (inner, outer, and the left and right faces) are exposed to the solution in the respective tanks and solute can diffuse into or out of the membrane at all of these interfaces. The diffusivity of the solute in the membrane is D_m and the partition coefficient of the membrane is Φ_m. Define a coordinate system and use the general vector form of Fick's second law to derive a differential equation that defines concentration c throughout the membrane at steady-state. Then define all the boundary conditions that are necessary to solve this differential equation. Show all your work and clearly state your assumptions. In this problem, you do not have to solve the differential equation, only set it up.

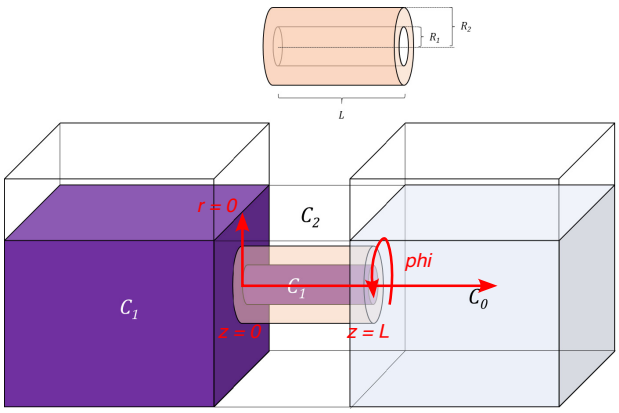


First, we assign an appropriate coordinate system. Since we're dealing with a cylindrical membrane, it's most natural to assign a cylindrical coordinate system with the z-axis parallel to the tube, directed such that $z = 0$ is located at the left end of the tube where it meets the surface of the left tank, and $z = L$ is located at the right end of the tube, where it meets the surfaces of the right tank (Figure (2)).

The general form of Fick's second law is

$$\frac{\partial c}{\partial t} = D_m \nabla^2 c + R_i \tag{2.10}$$

Since we can safely assume there is no reaction between the solute and the membrane, we can set $R_i = 0$ so that the differential equation can be solvable. Additionally, we are



given that the system is in steady state, so the left side $\frac{\partial c}{\partial t}$ is zero also.

$$\begin{aligned} \frac{\partial c}{\partial t}^{0} &= D_m \nabla^2 c + R_i^{0} \\ 0 &= D_m \nabla^2 c \\ 0 &= \nabla^2 c \end{aligned}$$

Expanding the Laplacian of c out in terms of cylindrical coordinates, we get

$$\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial c}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 c}{\partial \phi^2} + \frac{\partial^2 c}{\partial z^2} = 0$$

and since there is no gradient in the angular (ϕ) direction, then $\partial^2 c / \partial \phi^2 = 0$.

$$\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial c}{\partial r}\right) + \frac{\partial^2 c}{\partial z^2} = 0 \tag{2.11}$$

Then, we find the appropriate initial conditions. When we look at the left side of the tube ($z = 0$) within the membrane ($R_1 \leq r \leq R_2$), we have that

$$c(R_1 \leq r \leq R_2; z = 0) = \Phi_m C_1$$

where Φ_m is the partition coefficient. When we look at the right side of the tube within the membrane, we also have

$$c(R_1 \leq r \leq R_2; z = L) = \Phi_m C_0$$

When we look at the membrane between the left and right sides of the tube, we have along the inner face of the membrane,

$$c(r = R_1; 0 < z < L) = \Phi_m C_1$$

and along the outer face of the membrane,

$$c(r = R_2; 0 < z < L) = \Phi_m C_0$$

Bringing the differential equation to solve and the boundary conditions, we have

$$\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial c}{\partial r}\right) + \frac{\partial^2 c}{\partial z^2} = 0 \qquad \begin{cases} c(R_1 \leq r \leq R_2; z = 0) = \Phi_m C_1 \\ c(R_1 \leq r \leq R_2; z = L) = \Phi_m C_0 \\ c(r = R_1; 0 \leq z \leq L) = \Phi_m C_1 \\ c(r = R_2; 0 \leq z \leq L) = \Phi_m C_2 \end{cases}$$

3 Lab Questions

3.1 Problem 3

> The default rate of glucose consumption is given in Lab 04 as $0.0077\,\mathrm{mol\,m^{-3}\,s^{-1}}$. At some point we might want to put various types of cells in these devices. Assuming there are 800 cells in the trap, and you never want the glucose concentration to fall below $2.0\,\mathrm{mol\,m^{-3}}$, what is the maximum rate of glucose consumption in mol/cell/s for a given cell type in this device?

To solve for the maximum rate of glucose consumption, we perform several parametric sweeps for the value R in COMSOL such that the glucose concentration is no lower than $2.0\,\mathrm{mol\,m^{-3}}$.

In particular, I ran a parametric sweep first at R at start value $-0.5\,\mathrm{mol\,m^{-3}\,s^{-1}}$ and end value $-1\,\mathrm{mol\,m^{-3}\,s^{-1}}$ with number of values 7. Narrowing it down, I reran the parametric sweep between the values of R that yielded the closest volume average concentration to $2.0\,\mathrm{mol\,m^{-3}}$, with number of values 5. I repeated this step until I obtained a final value of $R = -0.6156\,\mathrm{mol\,m^{-3}\,s^{-1}}$, which gave a concentration of $2.0000\,\mathrm{mol\,m^{-3}}$.

R	Concentration (mol/m^3)
-0.50000	7.6162
-0.58333	4.7182
-0.66667	1.8225
-0.75000	-1.0729
-0.83333	-3.9698
-0.91667	-6.8661
-1.0000	-9.7627

R	Concentration (mol/m^3)
-0.67000	1.7066
-0.66438	1.9022
-0.65875	2.0977
-0.65313	2.2933
-0.64750	2.4888

R	Concentration (mol/m^3)
-0.66438	1.9020
-0.66297	1.9509
-0.66157	1.9999
-0.66016	2.0488
-0.65875	2.0977

R	Concentration (mol/m^3)
-0.66157	1.9997
-0.66122	2.0119
-0.66087	2.0242
-0.66051	2.0364
-0.66016	2.0487

R	Concentration (mol/m^3)
-0.66157	1.9997
-0.66148	2.0027
-0.66140	2.0058
-0.66131	2.0088
-0.66122	2.0119

R	Concentration (mol/m^3)
-0.66157	1.9997
-0.66155	2.0005
-0.66152	2.0012
-0.66150	2.0020
-0.66148	2.0028

R	Concentration (mol/m^3)
-0.66157	1.9997
-0.66157	1.9999
-0.66156	2.0000
-0.66156	2.0002
-0.66155	2.0004

Since there are 800 cells in the cell plate, and the cell plate has an area of

$$(80\,\mu\mathrm{m})(200\,\mu\mathrm{m})(10\,\mu\mathrm{m}) \times \left(\frac{1\,\mathrm{m}}{10^6\,\mu\mathrm{m}}\right)^3 = 1.6 \times 10^{-13}\,\mathrm{m^3}$$

then, using basic stoichiometry, we can obtain the maximum rate of glucose consumption in mol/cell/s.

$$0.6156\,\mathrm{mol\,m^{-3}\,s^{-1}} \times \frac{1.6 \times 10^{-13}\,\mathrm{m^3}}{800\,\mathrm{cells}} = \boxed{1.23 \times 10^{-16}\,\mathrm{mol/cell/s}}$$

3.2 Problem 4

> Enable the flow through the "thin channel" and solve the problem again. Plot the concentration distribution on a slice and compare it with the case that you solved in the labs. What differences do you see in the concentration distribution, and in the flow streamlines?

When enabling the laminar flow through the thin channel, the solution does have the velocity field pointing inwards, as well as the flux passing through the thin channel and cell plate. This makes sense since we allowed the glucose to flow through a new component of the microfluidic chip.

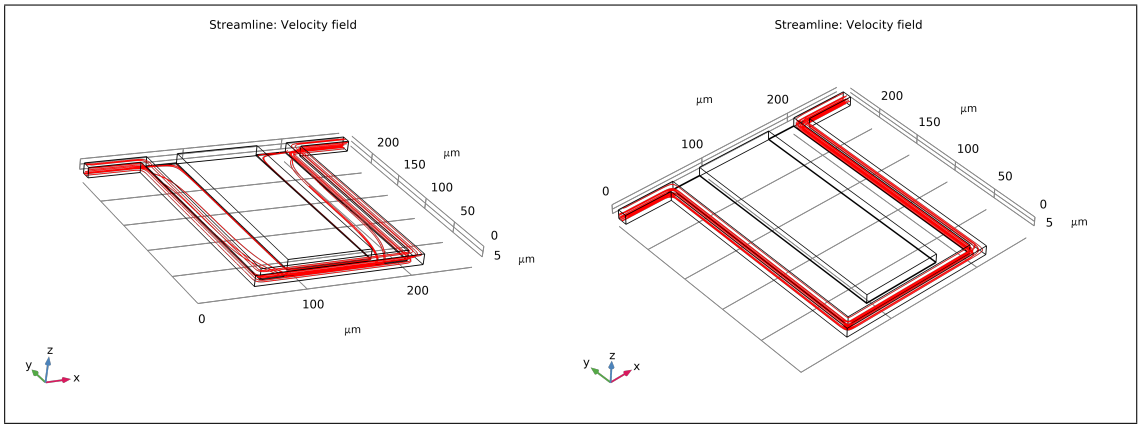


Figure 1: Velocity field with laminar flow enabled in the thin plate (left) and with it disabled (right).

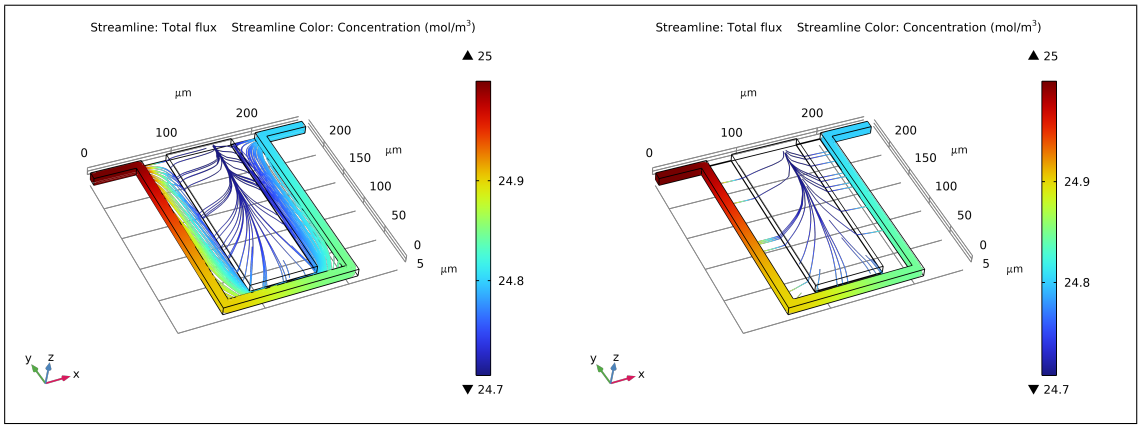


Figure 2: Total flux streamline with laminar flow enabled in the thin plate (left) and with it disabled (right).

There is no noticeable difference between the concentrations. When calculating the (volume average) concentration over the thin plate, there is a slight increase from $24.712\,\mathrm{mol\,m^{-3}}$ to $24.726\,\mathrm{mol\,m^{-3}}$. This makes sense since we expect the concentration to slightly increase as more glucose solution flows into the cell plate.

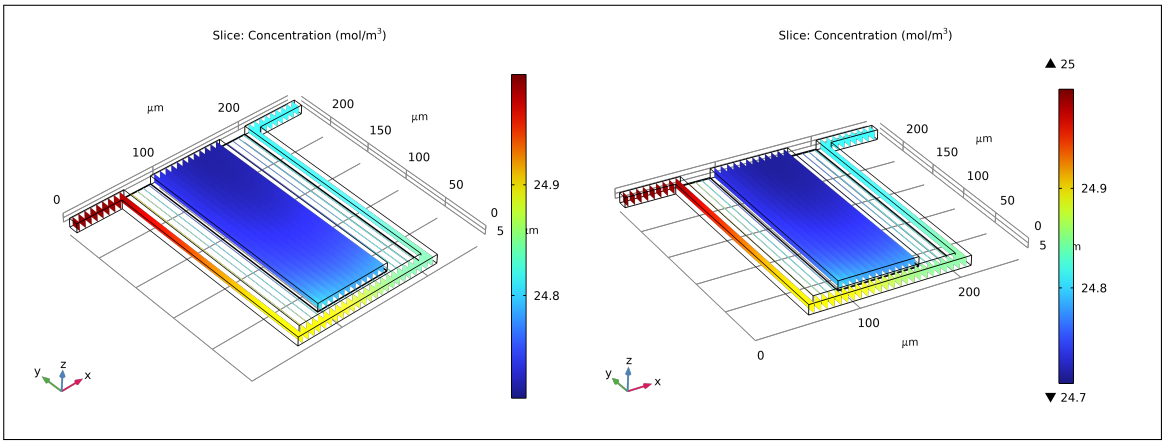


Figure 3: A slice plot for the concentration of glucose throughout the system, with laminar flow disabled (left) and with it enabled (right).