Homework 12

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BIOENG 104 Biological Transport Phenomena | Aaron Streets

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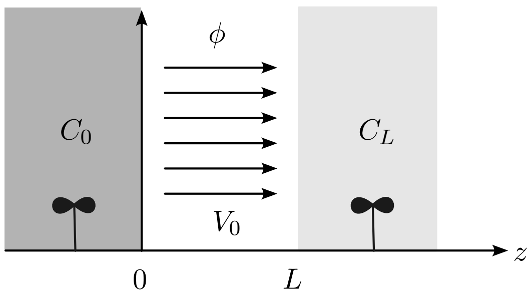
1 Problem 1

(*20 points*) Two large, well-mixed baths are separated by a membrane with thickness L and partition coefficient ϕ. The bath on the left is held at concentration C_0 and the bath on the right is held at concentration C_L. A pressure difference between the two baths is driving advection of the solute from the bath on the left to the bath on the right at constant uniform velocity of V_0.

(A) (*10 points*) Calculate the steady-state convective flux of solute through the membrane assuming no reaction.

Let $C(z)$ be the concentration of solute at position z. We assume the following.

- As given, we are at steady-state: $\partial c/\partial t = 0$.
- As given, no reaction is occurring: $R_i = 0$.
- C_0 and C_L are constant concentrations.
- As given, the baths are well-mixed.
- As given, bulk flow occurs at a constant uniform velocity in the z-direction.



Taking both diffusion and advection into account, we have the governing equations

$$\mathbf{N} = \mathbf{J} + \text{advection} = -D_M \boldsymbol{\nabla} C + \mathbf{v} C \tag{1.1}$$

$$\frac{\partial C}{\partial t} + \mathbf{v} \cdot \boldsymbol{\nabla} C = D_M \nabla^2 C + R_i \tag{1.2}$$

where $\mathbf{N}$ is the total flux, $\mathbf{J}$ is the flux only due to diffusion, and D_M is the diffusion coefficient of the solute in the membrane. From the steady-state and no-reaction assumption, we can simplify as follows:

$$\begin{aligned}\cancel{\frac{\partial C}{\partial t}} + \mathbf{v}\cdot\boldsymbol{\nabla} C &= D_M \nabla^2 C + \cancel{R_i} \\ \mathbf{v}\cdot\boldsymbol{\nabla} C &= D_M \nabla^2 C \\ V_0 \frac{\mathrm{d}C}{\mathrm{d}z} &= D_M \frac{\mathrm{d}^2 C}{\mathrm{d}z^2}\end{aligned}$$

This is an integrable second-order differential equation. Letting $U = \mathrm{d}C/\mathrm{d}z$,

$$\begin{aligned}V_0 U &= D_M \frac{\mathrm{d}U}{\mathrm{d}z} \\ \frac{1}{U}\frac{\mathrm{d}U}{\mathrm{d}z} &= \frac{V_0}{D_M} \\ U &= A_0 \mathrm{e}^{V_0 z/D_M}\end{aligned}$$

Substituting back in U and integrating again to solve for C,

$$C = \underbrace{\frac{A_0 D_M}{V_0}}_{A} \mathrm{e}^{V_0 z/D_M} + B = A\mathrm{e}^{V_0 z/D_M} + B$$

We have the following boundary conditions.

Boundary conditions:
- $C(z=0) = \phi C_0$ (BC1)
- $C(z=L) = \phi C_L$ (BC2)

From the boundary conditions, we have

$$\begin{aligned}\phi C_0 &= A + B \\ \phi C_L &= A\mathrm{e}^{V_0 L/D_M} + B\end{aligned}$$

Then, eliminate B to solve for A.

$$\begin{aligned}A(1 - \mathrm{e}^{V_0 L/D_M}) &= \phi(C_0 - C_L) \\ A &= \frac{\phi(C_0 - C_L)}{1 - \mathrm{e}^{V_0 L/D_M}}\end{aligned}$$

Since $B = \phi C_0 - A$, then

$$\begin{aligned}C &= A\mathrm{e}^{V_0 z/D_M} + (\phi C_0 - A) \\ &= \phi C_0 - A(1 - \mathrm{e}^{V_0 z/D_M}) \\ &= \phi C_0 - \phi(C_0 - C_L)\frac{1 - \mathrm{e}^{V_0 z/D_M}}{1 - \mathrm{e}^{V_0 L/D_M}}\end{aligned}$$

Letting $Pe = V_0 L/D_M$ be the Péclet number, we have the concentration profile

$$C = \phi C_0 - \phi(C_0 - C_L)\frac{1 - \mathrm{e}^{Pe(z/L)}}{1 - \mathrm{e}^{Pe}}$$

From Equation (1.1), the flux is

$$\begin{aligned}
N_z &= -D_M \frac{\partial C}{\partial z} + V_0 C \\
&= -\underbrace{D_M \frac{Pe}{L}}_{V_0} \phi(C_0 - C_L)\frac{\mathrm{e}^{Pe(z/L)}}{1 - \mathrm{e}^{Pe}} + V_0\phi C_0 - V_0\phi(C_0 - C_L)\frac{1 - \mathrm{e}^{Pe(z/L)}}{1 - \mathrm{e}^{Pe}} \\
&= V_0\phi\left[C_0 - (C_0 - C_L)\left(\frac{\mathrm{e}^{Pe(z/L)}}{1 - \mathrm{e}^{Pe}} - \frac{1 - \mathrm{e}^{Pe(z/L)}}{1 - \mathrm{e}^{Pe}}\right)\right] \\
&= \boxed{V_0\phi\left(C_0 - \frac{C_0 - C_L}{1 - \mathrm{e}^{Pe}}\right) = D_M \frac{Pe}{L}\phi\left(C_0 - \frac{C_0 - C_L}{1 - \mathrm{e}^{Pe}}\right)}
\end{aligned}$$

(B) (*5 points*) What does this convective flux reduce to for very large Péclet number ($Pe \gg 1$)? And for very small Péclet number ($Pe \ll 1$)?

For $Pe \gg 1$, the quantity $1 - \mathrm{e}^{Pe}$ gets closer to infinity, so

$$N_z = \phi V_0\left(C_0 - \frac{C_0 - C_L}{1 - \mathrm{e}^{Pe}}\right) \approx \boxed{\phi C_0 V_0}$$

For $Pe \ll 1$, the quantity e^{Pe} is approximately $1 + Pe$, so

$$\begin{aligned}
N_z &\approx \phi V_0\left(C_0 - \frac{C_0 - C_L}{1 - (1 + Pe)}\right) = \phi V_0\left(C_0 + \frac{C_0 - C_L}{Pe}\right) \\
&= \phi V_0 C_0 + \frac{\phi V_0(C_0 - C_L)}{Pe} = \cancel{\phi Pe \frac{D_M}{L} C_0} + D_M \frac{\phi(C_0 - C_L)}{L} \\
&\approx \boxed{D_M \frac{\phi(C_0 - C_L)}{L}}
\end{aligned}$$

The approximation $\mathrm{e}^{Pe} \approx 1 + Pe$ for very small Pe comes from the Taylor series expansion

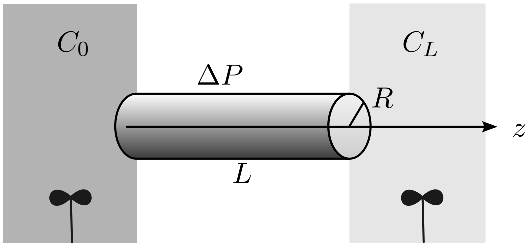
$$\mathrm{e}^{Pe} = \sum_{n=0}^{\infty} \frac{Pe^n}{n!} = \frac{Pe^0}{0!} + \frac{Pe^1}{1!} + \underbrace{\frac{Pe^2}{2!} + \frac{Pe^2}{3!} + \cdots}_{\approx 0} \approx 1 + Pe$$

since powers of Pe higher than one are negligible.

(C) (*5 points*) Now imagine that a cylindrical membrane is separating the two baths and that the pressure in bath 1 is P_1 and the pressure in bath 2 is P_2. Instead of a constant advective velocity vector field, the velocity profile is given by the equation

$$v_z(r) = \frac{R^2 \Delta P}{4\mu L}\left[1 - \left(\frac{r}{R}\right)^2\right]$$

where R is the radius of the membrane, L is the length of the membrane, ΔP is $P_2 - P_1$, and μ is the effective viscosity of the fluid in the membrane. Using the convection form of Fick's second law, write the simplified differential equation that can be used to solve for $c(r, z)$ in the membrane at steady state.



The convection–diffusion equation states that for C the solute concentration, D the diffusivity of the membrane, $\mathbf{v}$ the velocity field induced by convection, and R the reaction rate of solute in the membrane,

$$\frac{\partial C}{\partial t} + \mathbf{v} \cdot \boldsymbol{\nabla} C = D\nabla^2 C + R \tag{1.3}$$

Under steady state, $\partial C/\partial t = 0$, and there is no reaction occurring $R = 0$, so we can reduce this to

$$\mathbf{v} \cdot \boldsymbol{\nabla} C = D\nabla^2 C \tag{1.4}$$

In cylindrical coordinates, we can expand the advection and Laplacian operators out to

$$v_r \frac{\partial C}{\partial r} + \frac{v_\theta}{r}\frac{\partial C}{\partial \theta} + v_z \frac{\partial C}{\partial z} = D\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 C}{\partial \theta^2} + \frac{\partial^2 C}{\partial z^2}\right] \tag{1.5}$$

Here, we will assume that the advective velocity field is nonzero only in the z direction. This means that $v_r = v_\theta = 0$. We will also assume that $\partial C/\partial \theta = 0$, so that our concentration profile will only vary in terms of r and z.

$$v_z \frac{\partial C}{\partial z} = D\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right) + \frac{\partial^2 C}{\partial z^2}\right]$$

Plugging in the velocity profile v_z as shown above,

$$\boxed{\frac{R^2 \Delta P}{4\mu L}\left[1 - \left(\frac{r}{R}\right)^2\right]\frac{\partial C}{\partial z} = D\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right) + \frac{\partial^2 C}{\partial z^2}\right]}$$

2 Problem 2

(*10 points*) A cylindrical membrane has an inner radius R_0, outer radius R_1, diffusivity D_M, and a partition coefficient of ~ 1.0. Assume that the concentrations at the inner and outer walls are held constant at C_0 and C_1, respectively. Assume that there is no flow in the z- or θ-directions.
The velocity in the radial direction v_r is equal to:

$$v_r = \frac{Q_L}{2\pi r}$$

where Q_L is the constant volumetric flow rate per length of the membrane ($\mathrm{m^3\,s^{-1}\,m^{-1}}$). Show that the steady-state concentration profile through the pipe is given by the equation:

$$c_i(r) = \frac{r^{Pe} - R_0^{Pe}}{R_0^{Pe} - R_1^{Pe}}(c_0 - c_1) + c_0$$

where the P'eclet number Pe is defined as $Q_L/2\pi D_{ij}$.

The convection–diffusion equation states that, for solute concentration c_i and velocity field $\mathbf{v}$,

$$\frac{\partial c_i}{\partial t} + \mathbf{v} \cdot \boldsymbol{\nabla} c_i = D_M \nabla^2 c_i + R$$

Assuming steady-state and no reaction occurring, meaning $\partial c_i/\partial t = R = 0$,

$$\mathbf{v} \cdot \boldsymbol{\nabla} c_i = D_M \nabla^2 c_i$$

Expanding this equation out in cylindrical coordinates along the r-direction,

$$v_r \frac{\partial c_i}{\partial r} + \frac{v_\theta}{r}\frac{\partial c_i}{\partial \theta} - \frac{v_\theta^2}{r} + v_z \frac{\partial c_i}{\partial z} = D_M \left[\frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial c_i}{\partial r} \right) + \frac{1}{r^2}\frac{\partial^2 c_i}{\partial \theta^2} + \frac{\partial^2 c_i}{\partial z^2} \right]$$

We can apply the assumption that there is no flow in the z- or θ-directions. This means any term in the equation above that contains either v_z or v_θ can be eliminated.

$$v_r \frac{\partial c_i}{\partial r} = D_M \left[\frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial c_i}{\partial r} \right) + \frac{1}{r^2}\frac{\partial^2 c_i}{\partial \theta^2} + \frac{\partial^2 c_i}{\partial z^2} \right]$$

Additionally, the concentration profile has no gradient along the z- or θ-directions, so $\partial c_i/\partial \theta = \partial c_i/\partial z = 0$.

$$v_r \frac{\partial c_i}{\partial r} = \frac{D_M}{r}\frac{\partial}{\partial r}\left(r \frac{\partial c_i}{\partial r} \right)$$

Plugging v_r as given above,

$$
\begin{aligned}
\frac{Q_L}{2\pi r}\frac{\partial c_i}{\partial r} &= \frac{D_M}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c_i}{\partial r}\right) \\
\frac{Q_L}{2\pi D_M}\frac{\partial c_i}{\partial r} &= \frac{\partial}{\partial r}\left(r\frac{\partial c_i}{\partial r}\right) \\
Pe \cdot u &= \frac{\mathrm{d}c_i}{\mathrm{d}r} + r\frac{\mathrm{d}^2 c_i}{\mathrm{d}r^2}
\end{aligned} \tag{2.6}
$$

since the Péclet number is $Pe = Q_L/2\pi D_M$. To solve Equation (2.6), we can perform a substitution $u = \partial c_i/\partial r$, which yields

$$
\begin{aligned}
Pe \cdot u &= u + r\frac{\mathrm{d}u}{\mathrm{d}r} \\
\frac{1}{u}\frac{\mathrm{d}u}{\mathrm{d}r} &= \frac{Pe-1}{r} \\
\ln u &= (Pe-1)\ln r + \ln A \\
u &= Ar^{Pe-1}
\end{aligned}
$$

Substituting u back in and integrating again,

$$
c_i = \underbrace{\frac{A}{Pe}}_{A_0} r^{Pe} + B = \boxed{A_0 r^{Pe} + B} \tag{2.7}
$$

To solve for the particular concentration profile, we use two boundary conditions.

$$
\begin{aligned}
c_i(r = R_0) &= \Phi_M c_0 \approx c_0 \\
c_i(r = R_1) &= \Phi_M c_1 \approx c_1
\end{aligned}
$$

where $\Phi_M \approx 1$ is the partition coefficient. We therefore have

$$
\begin{aligned}
c_0 &= A_0 R_0^{Pe} + B \\
c_1 &= A_0 R_1^{Pe} + B
\end{aligned}
$$

Subtracting one of the two equations from the other yields

$$
\begin{aligned}
c_0 - c_1 &= A_0(R_0^{Pe} - R_1^{Pe}) \\
A_0 &= \frac{c_0 - c_1}{R_0^{Pe} - R_1^{Pe}}
\end{aligned}
$$

And since the first boundary condition implies $B = c_0 - A_0 R_0^{Pe}$, we can solve for the complete concentration profile as follows:

$$
\begin{aligned}
c_i &= A_0 r^{Pe} + c_0 - A_0 R_0^{Pe} \\
&= A_0(r^{Pe} - R_0^{Pe}) + c_0
\end{aligned}
$$

$$
\boxed{c_i = \frac{r^{Pe} - R_0^{Pe}}{R_0^{Pe} - R_1^{Pe}}(c_0 - c_1) + c_0}
$$