Homework 3

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BIOENG 104 Biological Transport Phenomena | Aaron Streets

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1 Problem 1

For diffusion in Cartesian coordinates through a flat membrane between two well stirred baths, with no reaction, we found that the flux of a solute was constant in the x-direction ($\mathrm{d}J/\mathrm{d}x = 0$). For diffusion through a cylindrical membrane we used cylindrical coordinates and found that the flux in the r-direction was a function of r ($\mathrm{d}J/\mathrm{d}r = 0$). Show that for radial diffusion through a cylindrical membrane of length L, the product of flux and area is a constant in the r-direction. In other words, show that

$$\frac{\mathrm{d}}{\mathrm{d}r}[J(r) \times A(r)] = 0$$

1.1 Solution 1

Assuming the fluid is incompressible, the flow rate of mass of solute passing through an area at radial position r is also equal at position $r + \Delta r$, where Δr is some distance. This results from mass balance.

$$\dot{m}|_r = \dot{m}|_{r+\Delta r}$$

The definition of flux is the mass flow rate per area per unit time. In other words,

$$\dot{m}|_r = J(r)A(r)\Delta t \qquad \text{and} \qquad \dot{m}|_{r+\Delta r} = J(r+\Delta r)A(r+\Delta r)\Delta t$$

The result can be quickly obtained using the definition of derivative.

$$\begin{aligned} J(r)A(r)\Delta t &= J(r+\Delta r)A(r+\Delta r)\Delta t \\ 0 &= J(r+\Delta r)A(r+\Delta r) - J(r)A(r) \\ \therefore \frac{\mathrm{d}}{\mathrm{d}r}J(r)A(r) &= \lim_{\Delta r \to 0} \frac{J(r+\Delta r)A(r+\Delta r) - J(r)A(r)}{\Delta r} = \lim_{\Delta r \to 0} \frac{0}{\Delta r} = 0 \end{aligned}$$

1.2 Solution 2

Assume that in and out of the cylindrical membrane are two well-mixed baths, each with constant concentrations, and that there is no reaction occurring. Suppose that the bath within the cylindrical membrane has concentration c_0 and that on the outside has concentration c_L. Suppose also that the membrane has inner radius R_0 and outer radius R_1. By Fick's second law, we have that

$$\begin{aligned}\frac{\partial c}{\partial t} &= -\frac{D}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right) + R \\ 0 &= -\frac{D}{r}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}c}{\mathrm{d}r}\right)\end{aligned}$$

where D is the diffusivity of the solute in the membrane. Since the domain we are concerned with is $R_0 \le r \le R_1$, then it is valid to multiply both sides of the above equation by r.

$$\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}c}{\mathrm{d}r}\right) = 0$$

Integrating the above differential equation,

$$\begin{aligned}\int \frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}c}{\mathrm{d}r}\right)\mathrm{d}r &= \int 0\,\mathrm{d}r \\ \frac{\mathrm{d}c}{\mathrm{d}r} &= \frac{A}{r}\end{aligned}$$

where $A \in \mathbb{R}$ is a constant of integration. Integrating again,

$$\begin{aligned}\int \frac{\mathrm{d}c}{\mathrm{d}r}\,\mathrm{d}r &= \int \frac{A}{r}\,\mathrm{d}r \\ c(r) &= A\ln|r| + B \\ &= A\ln r + B\end{aligned}$$

since r is always positive. Again, $B \in \mathbb{R}$ serves as another constant of integration. Since we have two unknowns A and B to solve for, this requires two boundary conditions. These boundary conditions can be easily found by accounting for the concentration profile at $r = R_1$ and $r = R_2$.

Suppose that the membrane has partition coefficient Φ. Then, the proper boundary conditions would be that the concentration at $r = R_0$ would be Φc_0 and the concentration at $r = R_1$ would be Φc_L:

$$c(R_0) = \Phi c_0 \qquad \text{and} \qquad c(R_1) = \Phi c_L$$

Then, plugging these boundary conditions in, we have

$$c(R_1) = A\ln R_0 + B = \Phi c_0 \tag{1.1}$$
$$c(R_2) = A\ln R_1 + B = \Phi c_L \tag{1.2}$$

Subtracting Equation (1.2) from Equation (1.1) yields

$$\begin{aligned}A(\ln R_0 - \ln R_1) &= \Phi(c_0 - c_L) \\ \Phi c_0 - \frac{\Phi(c_0 - c_L)}{\ln\bigl(R_0/R_1\bigr)}\ln R_0 &= B\end{aligned}$$

Plugging these values into the concentration profile $c(r) = A \ln r + B$, we obtain

$$\begin{aligned} c(r) &= \Phi c_0 + \frac{\Phi(c_0 - c_L)}{\ln\bigl(R_0/R_1\bigr)} \ln r - \frac{\Phi(c_0 - c_L)}{\ln\bigl(R_0/R_1\bigr)} \ln R_0 \\ &= \Phi c_0 - \frac{\Phi(c_0 - c_L)}{\ln\bigl(R_0/R_1\bigr)} \ln\left(\frac{R_0}{r}\right) \end{aligned} \tag{1.3}$$

From Equation (1.3), we can determine the flux by Fick's first law.

$$J_r(r) = -D\frac{\partial c}{\partial r} = -D\Phi \frac{c_0 - c_L}{\ln\bigl(R_0/R_1\bigr)} \frac{1}{r} \tag{1.4}$$

The area of the membrane at radial position r is

$$A(r) = 2\pi r h \tag{1.5}$$

where h is the height of the membrane. Typing Equations (1.4) and (1.5) together,

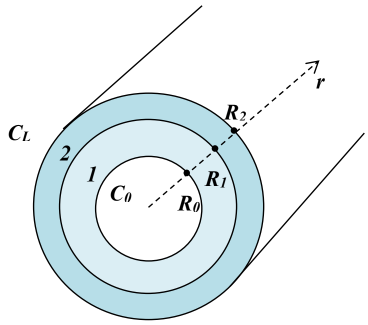
$$\begin{aligned} J(r)A(r) &= -D\Phi \frac{c_0 - c_L}{\ln\bigl(R_0/R_1\bigr)} \frac{1}{r} \cdot 2\pi r h \\ &= -2\pi D h \Phi \frac{(c_0 - c_L)}{\ln\bigl(R_0/R_1\bigr)} \end{aligned}$$

Since all variables shown on the right hand side are constant with respect to r, then

$$\frac{\mathrm{d}}{\mathrm{d}r}[J(r)A(r)] = 0$$

2 Problem 2

Here we consider mass transfer (without reaction) through the walls of a cylinder that consists of two membranes (as shown). For simplicity's sake, assume that the partition coefficients for each membrane are ~ 1.0.



Membrane 1 has a diffusivity D_1 from $r = R_0$ to R_1 and membrane 2 has a diffusivity D_2 from $r = R_1$ to R_2. Given that the concentration profile through a single membrane is $C(r) = A\ln(r) + B$, solve for the flux through the membranes *in terms of a sum of resistors in series*. Your final equation should be in a form that makes it easy to recognize the individual membrane resistances.

Assume that the system is steady-state, that the concentrations inside and outside the dual membrane are constant, and that the baths at the same locations are well-stirred. As given, the concentration through each membrane do not vary with respect to time (from the steady-state assumption) and can be modeled by the following equations:

$$C_1(r) = A_1 \ln r + B_1$$
$$C_2(r) = A_2 \ln r + B_2$$

where A_1, B_1, A_2, and B_2 are unknown quantities. Because we have four unknowns, we need four boundary conditions to fully solve the concentration equations.

$$C_1(R_0) = \Phi_0 C_0 = C_0 \tag{2.6}$$
$$C_2(R_2) = \Phi_1 C_L = C_L \tag{2.7}$$
$$C_1(R_1) = C_2(R_1) \tag{2.8}$$
$$J_{r(1)}(R_1) = J_{r(2)}(R_1) \tag{2.9}$$

where $\Phi_i \cong 1$ is the partition coefficient of membrane i, and J_r is the flux through the radial position. We obtain the boundary condition (2.8) from the fact that, although the concentration may be discontinuous through $x = R_1$, there must be some concentration X such that at $x = R_1$,

$$C_1(R_1) = \Phi_0 X \qquad \text{and} \qquad C_2(R_1) = \Phi_1 X$$

so, the value of concentration X itself is

$$X = \frac{C_1(R_1)}{\Phi_0} = \frac{C_2(R_1)}{\Phi_1}$$

A system of four unknowns can be obtained from the boundary conditions (Equations (2.6) to (2.9)). The fourth boundary condition, Equation (2.13), is obtained from Fick's first law ($J_{r(i)} = -D_i \, \mathrm{d}c_i/\mathrm{d}r = -D_i A_i/r$), which immediately gives the equation $-D_1 A_1/R_1 = -D_2 A_2/R_1$.

$$C_1(R_0) = A_1 \ln R_0 + B_1 = C_0 \tag{2.10}$$

$$C_2(R_2) = A_2 \ln(R_2) + B_2 = C_L \tag{2.11}$$

$$A_1 \ln R_1 + B_1 = A_2 \ln R_1 + B_2 \tag{2.12}$$

$$D_1 A_1 = D_2 A_2 \tag{2.13}$$

One approach to solving these boundary conditions is to solve for other unknown variables in terms of one unknown, e.g. A_1, and substituting them in Equation (2.12).

$$\begin{aligned}
&A_2 = D_1 A_1/D_2 \\
&B_1 = C_0 - A_1 \ln R_0 \\
&B_2 = C_L - A_2 \ln R_2 = C_L - D_1 A_1/D_2 \, \ln R_2
\end{aligned}$$

Then, we solve for A_1.

$$\begin{aligned}
A_1 \ln R_1 + C_0 - A_1 \ln R_0 &= \frac{D_1 A_1}{D_2} \ln R_1 + C_L - \frac{D_1 A_1}{D_2} \ln R_2 \\
A_1 \ln\left(\frac{R_1}{R_0}\right) &= \frac{D_1 A_1}{D_2} \ln\left(\frac{R_1}{R_2}\right) - (C_0 - C_L) \\
-(C_0 - C_L) &= A_1 \left[\ln\left(\frac{R_1}{R_0}\right) + \frac{D_1}{D_2} \ln\left(\frac{R_2}{R_1}\right)\right] \\
A_1 &= -(C_0 - C_L) \left[\ln\left(\frac{R_1}{R_0}\right) + \frac{D_1}{D_2} \ln\left(\frac{R_2}{R_1}\right)\right]^{-1}
\end{aligned}$$

Solving for the other unknowns,

$$\begin{aligned}
A_2 &= -\frac{D_1}{D_2}(C_0 - C_L) \left[\ln\left(\frac{R_1}{R_0}\right) + \frac{D_1}{D_2} \ln\left(\frac{R_2}{R_1}\right)\right]^{-1} \\
&= (C_0 - C_L) \left[\ln\left(\frac{R_1}{R_2}\right) - \frac{D_2}{D_1} \ln\left(\frac{R_1}{R_0}\right)\right]^{-1} \\
B_1 &= C_0 + (C_0 - C_L) \ln R_0 \left[\ln\left(\frac{R_1}{R_0}\right) + \frac{D_1}{D_2} \ln\left(\frac{R_2}{R_1}\right)\right]^{-1} \\
B_2 &= C_L - (C_0 - C_L) \ln R_2 \left[\ln\left(\frac{R_1}{R_2}\right) - \frac{D_2}{D_1} \ln\left(\frac{R_1}{R_0}\right)\right]^{-1}
\end{aligned}$$

So, the concentration profiles of the two membranes are

$$C_1(r) = \left[-(C_0 - C_L)\ln r + C_0 + (C_0 - C_L)\ln R_0\right]\left[\ln\left(\frac{R_1}{R_0}\right) + \frac{D_1}{D_2}\ln\left(\frac{R_2}{R_1}\right)\right]^{-1}$$

$$= \left[C_0 - (C_0 - C_L)\ln\left(\frac{r}{R_0}\right)\right]\left[\ln\left(\frac{R_1}{R_0}\right) + \frac{D_1}{D_2}\ln\left(\frac{R_2}{R_1}\right)\right]^{-1} \tag{2.14}$$

$$C_2(r) = \left[(C_0 - C_L)\ln r + C_L - (C_0 - C_L)\ln R_2\right]\left[\ln\left(\frac{R_1}{R_2}\right) - \frac{D_2}{D_1}\ln\left(\frac{R_1}{R_0}\right)\right]^{-1}$$

$$= \left[C_L + (C_0 - C_L)\ln\left(\frac{r}{R_2}\right)\right]\left[\ln\left(\frac{R_1}{R_2}\right) - \frac{D_2}{D_1}\ln\left(\frac{R_1}{R_0}\right)\right]^{-1} \tag{2.15}$$

By Fick's first law, the flux at radial position r is, according to Equation (2.14) and Equation (2.15),

$$J_{r(i)}(r) = -D_i\frac{\mathrm{d}C_i}{\mathrm{d}r} \tag{2.16}$$

$$J_{r(1)}(r) = D_1\frac{C_0 - C_L}{r}\left[\ln\left(\frac{R_1}{R_0}\right) + \frac{D_1}{D_2}\ln\left(\frac{R_2}{R_1}\right)\right]^{-1} \tag{2.17}$$

$$J_{r(2)}(r) = -D_2\frac{C_0 - C_L}{r}\left[\ln\left(\frac{R_1}{R_2}\right) - \frac{D_2}{D_1}\ln\left(\frac{R_1}{R_0}\right)\right]^{-1} \tag{2.18}$$

We can additionally prove that $J_{x(1)} = J_{x(2)}$ from Equations (2.17) and (2.18), making sure that everything makes sense physically.

$$\begin{aligned}
D_1\frac{C_0 - C_L}{r}\left[\ln\left(\frac{R_1}{R_0}\right) + \frac{D_1}{D_2}\ln\left(\frac{R_2}{R_1}\right)\right]^{-1} &= -D_1\frac{C_0 - C_L}{r}\left[-\ln\left(\frac{R_1}{R_0}\right) - \frac{D_1}{D_2}\ln\left(\frac{R_2}{R_1}\right)\right]^{-1} \\
&= -D_1\frac{C_0 - C_L}{r}\left[\frac{D_1}{D_2}\ln\left(\frac{R_1}{R_2}\right) - \ln\left(\frac{R_1}{R_0}\right)\right]^{-1} \\
&= -D_2\frac{C_0 - C_L}{r}\left[\ln\left(\frac{R_1}{R_2}\right) - \frac{D_2}{D_1}\ln\left(\frac{R_1}{R_0}\right)\right]^{-1}
\end{aligned}$$

Finally, we divide both sides of Equation (2.17) by $(1/D_1)/(1/D_1)$ to express the flux in terms of mass transfer resistances.

$$\begin{aligned}
J_r &= D_1\left(\frac{1}{D_1}\right)\frac{C_0 - C_L}{r}\left[\ln\left(\frac{R_1}{R_0}\right) + \frac{D_1}{D_2}\ln\left(\frac{R_2}{R_1}\right)\right]^{-1}\left[\frac{1}{D_1}\right]^{-1} \\
&= \boxed{\frac{C_0 - C_L}{r}\left[\frac{1}{D_1}\ln\left(\frac{R_1}{R_0}\right) + \frac{1}{D_2}\ln\left(\frac{R_2}{R_1}\right)\right]^{-1}}
\end{aligned}$$

3 Problem 3

NASA is working on a bioreactor designed to produce oxygen from carbon dioxide via photosynthesis and you have been commissioned as a consultant in the project. The device will consist of a well-stirred bath of cyanobacteria with a concentration of $0.02\,\mathrm{g\,L^{-1}}$ CO_2 (held constant by the photosynthetic cyanobacteria) separated by three flat membranes from a bath of water with 0.75 g/L CO_2 (also constant). Both baths are well mixed. One of the membranes is designed to keep the bacteria sterile; the middle membrane is required to protect the first membrane from the light source providing energy to the system, and the third membrane provides structural integrity.

- The first membrane has a diffusivity for CO_2 of $2.7 \times 10^{-6}\,\mathrm{cm^2\,s^{-1}}$ and a Φ for CO_2 of 0.75.
- The second membrane has a diffusivity for CO_2 of $2.3 \times 10^{-7}\,\mathrm{cm^2\,s^{-1}}$ and a Φ for CO_2 of 0.75.
- The third membrane has a diffusivity for CO_2 of $9.2 \times 10^{-10}\,\mathrm{cm^2\,s^{-1}}$ and a Φ for CO_2 of 0.15.

The total cross-sectional area of the membranes is $1.7\,\mathrm{m^2}$. You're in charge of optimizing these membranes for maximum CO_2 flux. What should the thickness of each membrane be in order to maximize CO_2 flux through these membranes in series? You have the following design constraints: The total combined thicknesses must be 5 mm. Each membrane must be at least 1 mm thick.

Hint: *Which membrane will have the largest resistance to diffusive flux? You should probably make that membrane as small as possible.*

Assume the system is at steady state (meaning $\partial c/\partial t = 0$). We are given that

$$D_1 = 2.7 \times 10^{-6}\,\mathrm{cm^2\,s^{-1}};\, \Phi_1 = 0.75$$
$$D_2 = 2.3 \times 10^{-7}\,\mathrm{cm^2\,s^{-1}};\, \Phi_2 = 0.75$$
$$D_3 = 9.2 \times 10^{-10}\,\mathrm{cm^2\,s^{-1}};\, \Phi_3 = 0.15$$
$$C_0 = 0.02\,\mathrm{g\,L^{-1}CO_2};\, C_L = 0.75\,\mathrm{g\,L^{-1}}$$

We use the equation describing diffusion across N membranes assuming no reaction and steady-state.

$$J(x) = \frac{1}{R_{\text{tot}}}(C_0 - C_L) \tag{3.19}$$

where R_{tot} is the sum of the mass transfer resistances of all membranes concerned.

$$R_{\text{tot}} = \sum_i R_i = \sum_i \frac{L_i}{D_i \Phi_i} \tag{3.20}$$

Since C_0 and C_L are constant, all we need to do to maximize $J(x)$ is to minimize R_{tot}.

The first step is to determine which membrane has the greatest resistance.

$$R_1 = \frac{L_1}{D_1\Phi_1} = \frac{L_1}{(2.7\times10^{-6}\,\mathrm{cm^2\,s^{-1}})(0.75)} = (4.9\times10^{5}\,\mathrm{s\,cm^{-2}})L_1 \tag{3.21}$$

$$R_2 = \frac{L_2}{D_2\Phi_2} = \frac{L_2}{(2.3\times10^{-7}\,\mathrm{cm^2\,s^{-1}})(0.75)} = (5.8\times10^{6}\,\mathrm{s\,cm^{-2}})L_2 \tag{3.22}$$

$$R_3 = \frac{L_3}{D_3\Phi_3} = \frac{L_3}{(9.2\times10^{-10}\,\mathrm{cm^2\,s^{-1}})(0.15)} = (7.2\times10^{9}\,\mathrm{s\,cm^{-2}})L_3 \tag{3.23}$$

meaning membrane 3 has the greatest resistance. To minimize resistance R_{tot}, we make the length L_3 as small as possible. Due to our given constraints, the smallest length L_3 can be is 1 mm.

Since $L_3 = 1\,\mathrm{mm}$, then L_1 and L_2 have to add up to 4 mm. Therefore, we minimize R_{tot} by differentiating Equation (3.20) with respect to one variable—namely, L_1—and utilizing the constraint $L_1 + L_2 = 4\,\mathrm{mm}$.

$$\begin{aligned} R_{\mathrm{tot}} &= \frac{L_1}{D_1\Phi_1} + \frac{L_2}{D_2\Phi_2} + \frac{L_3}{D_3\Phi_3} \\ &= \frac{L_1}{D_1\Phi_1} + \frac{4\,\mathrm{mm} - L_1}{D_2\Phi_2} + \frac{L_3}{D_3\Phi_3} \\ &= \left(\frac{1}{D_1\Phi_1} - \frac{1}{D_2\Phi_2}\right)L_1 + \frac{4\,\mathrm{mm}}{D_2\Phi_2} + \frac{L_3}{D_3\Phi_3} \end{aligned}$$

Taking the derivative of R_{tot} with respect to L_1 in hopes of minimizing it,

$$\frac{\mathrm{d}R_{\mathrm{tot}}}{\mathrm{d}L_1} = \frac{1}{D_1\Phi_1} - \frac{1}{D_2\Phi_2} < 0 \qquad \forall L_1$$

we realize that the total resistance is strictly decreasing for all L_1. We compare the numbers from Equation (3.21) and Equation (3.22) to help determine the sign of $\mathrm{d}R_{\mathrm{tot}}/\mathrm{d}L_1$. Therefore, to minimize R_{tot}, we must set $L_1 = 3\,\mathrm{mm}$.

Therefore, we have the following values:

$$L_1 = 3\,\mathrm{mm};\, L_2 = L_3 = 1\,\mathrm{mm}$$

4 Problem 4

A drug delivery implant has been invented which consists of a 2.6 mm diameter sphere that maintains a constant concentration, C_0, of Doloxan (an anti-cancer drug) on its surface. The implant will be surgically placed in the brain of a patient, bypassing the blood-brain barrier. The following facts are known:

- The diffusivity of Doloxan in brain tissue is $4.7 \times 10^{-8}\,\mathrm{cm^2\,s^{-1}}$.
- According to the surgeon, the implant can be placed no closer than 18 mm to the primary tumor, and in that region, convection (due to blood flow) can be neglected.
- Far from the implant the drug will reach a blood vessel or cerebrospinal fluid which will quickly clear it – thus, far from the implant, the concentration of Doloxan will be ~ 0.
- Tumors are unaffected by Doloxan concentrations less than $8.5 \times 10^{-8}\,\mathrm{M}$.

What is the minimum concentration, C_0, of Doloxan that this implant needs to provide on its surface to ensure that this drug delivery system works? You may assume that the system quickly reaches a steady-state and that any rate of reaction of Doloxan (associated with, say, its enzymatic breakdown or its function as a drug) is negligible.

Hint: *Start by deriving $C(r)$ using Fick's laws in spherical coordinates.*

Assume a steady-state system with no reaction occurring. Fick's first and second laws can be expressed in spherical coordinates.

$$
\begin{aligned}
J_r &= -D\frac{\partial C}{\partial r} \qquad \text{[Fick's first law]} \\
\frac{\partial C}{\partial t} &= D\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C}{\partial r}\right) + \cancelto{0}{\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial C}{\partial\theta}} + \cancelto{0}{\frac{1}{r^2\sin^2\theta}\frac{\partial^2 C}{\partial\phi^2}}\right] + \cancelto{0}{R_i} \\
&= \frac{D}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C}{\partial r}\right) \qquad \text{[Fick's second law]}
\end{aligned} \tag{4.24}
$$

The heavy simplification comes from the fact that C does not vary through non-radial directions. Equation (4.24) can be heavily simplified using the steady-state and negligible reaction assumptions, making both $\partial C/\partial t$ and reaction rate R_{rxn} equal to zero.

$$
\begin{aligned}
0 &= \frac{D}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}C}{\mathrm{d}r}\right) \\
0 &= \frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}C}{\mathrm{d}r}\right)
\end{aligned}
$$

assuming we won't deal with the case where $r = 0$. Integrating twice, we get

$$\begin{aligned}
\int \frac{\mathrm{d}}{\mathrm{d}r}\left(r^2 \frac{\mathrm{d}C}{\mathrm{d}r}\right) \mathrm{d}r &= \int 0 \, \mathrm{d}r \\
r^2 \frac{\mathrm{d}C}{\mathrm{d}r} &= A \\
\int \frac{\mathrm{d}C}{\mathrm{d}r} \, \mathrm{d}r &= \int \frac{A}{r^2} \, \mathrm{d}r \\
C(r) &= -\frac{A}{r} + B \qquad (4.25)
\end{aligned}$$

where $A, B \in \mathbb{R}$ are integration constants. Since it is given that the concentration of Doloxan will converge to zero as the distance r goes off to infinity, we have to set $B = 0$ in the concentration profile (4.25).

$$\lim_{r\to\infty} C(r) = \lim_{r\to\infty} \left(-\frac{A}{r} + B\right) = B = 0 \implies C(r) = -\frac{A}{r}$$

Assuming the *center* of the implant can be placed no closer than 18 mm to the primary tumor, we are given the following condition that

$$C(R) = -\frac{A}{R} = C_0 \qquad (4.26)$$

$$C(D_{\text{sep}}) = -\frac{A}{D_{\text{sep}}} = C_{\text{min}} \qquad (4.27)$$

for $R = 1.3\,\text{mm}$ the radius of the spherical implant, $D_{\text{sep}} = 18\,\text{mm}$ the minimum separation distance between the implant and the tumor, and $C_{\text{min}} = 8.5 \times 10^{-8}\,\text{M}$ the minimum concentration under which the tumor can start being affected by the Doloxan. From Equation (4.27),

$$\begin{aligned}
A &= -C_{\text{min}} D_{\text{sep}} \\
C_0 &= \frac{C_{\text{min}} D_{\text{sep}}}{R}
\end{aligned}$$

and finally, substituting our values in,

$$C_0 = \frac{(8.5 \times 10^{-8}\,\text{M})(18\,\text{mm})}{1.3\,\text{mm}} = \boxed{1.18 \times 10^{-6}\,\text{M}}$$

5 Lab Questions

5.1 Problem 5

Verify that the sum of flow rates at the inlets is approximately equal to the sum of the flow rates at the outlet for your 3-D model.

According to COMSOL, the sum of flow rates at the inlets, when the mesh element size is set to Coarse, is equal to

$$(6.5338 \times 10^{-15}\,\mathrm{m^3\,s^{-1}}) + (6.5272 \times 10^{-15}\,\mathrm{m^3\,s^{-1}}) = \boxed{1.306\,10 \times 10^{-14}\,\mathrm{m^3\,s^{-1}}}$$

and the sum of the flow rate magnitudes at the outlets is equal to

$$(6.5346 \times 10^{-15}\,\mathrm{m^3\,s^{-1}}) + (6.5265 \times 10^{-15}\,\mathrm{m^3\,s^{-1}}) = \boxed{1.306\,11 \times 10^{-14}\,\mathrm{m^3\,s^{-1}}}$$

so they are approximately equal.

5.2 Problem 6

In Lab 3b, if you desire one outlet of the microfluidic device to have a concentration no more than 70% of the concentration in the other outlet, what is the maximum permissible solute diffusivity (in $\mathrm{m^2\,s^{-1}}$) for this device under these flow conditions? Describe briefly how you came to this result.

For one outlet to have at most 70% of the concentration of the other, then we must have

$$C_0 = C_1 + C_2$$

where $C_2 = 7C_1/10$. Thus,

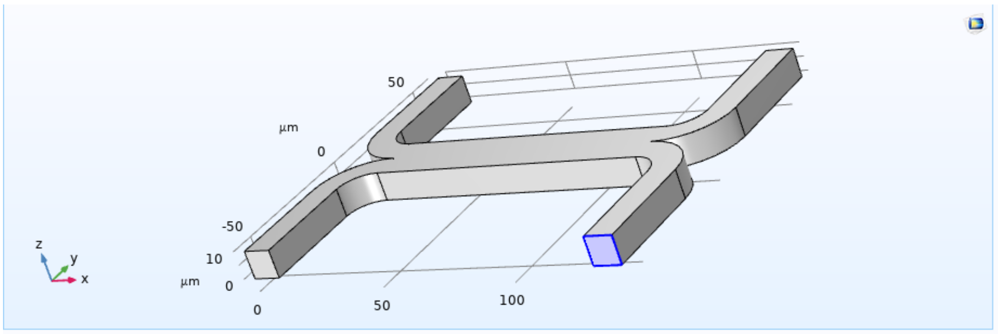
$$C_0 = \frac{17}{10}C_1 \implies C_1 = \frac{10}{17}C_0 = \frac{10}{17}(1 \times 10^{-6}\,\mathrm{mol\,m^{-3}}) = 5.88 \times 10^{-7}\,\mathrm{mol\,m^{-3}}$$

To achieve this concentration, a parametric sweep was ran on the model with a start value of 2.8×10^{-11} and a stop value of 3.1×10^{-11}, with the number of values set to 20 (see Figure 1).

We decided that the maximum solute diffusivity was

$$\boxed{D_{ij} = 3.0526 \times 10^{-11}}$$

with concentrations $C_1 = 5.8788 \times 10^{-7}\,\mathrm{mol\,m^{-3}}$ and $C_2 = 4.1240 \times 10^{-7}\,\mathrm{mol\,m^{-3}}$.



Dij	Concentration (mol/m^3)
2.8000E-11	5.9864E-7
2.8158E-11	5.9793E-7
2.8316E-11	5.9723E-7
2.8474E-11	5.9653E-7
2.8632E-11	5.9584E-7
2.8789E-11	5.9515E-7
2.8947E-11	5.9446E-7
2.9105E-11	5.9379E-7
2.9263E-11	5.9311E-7
2.9421E-11	5.9244E-7
2.9579E-11	5.9177E-7
2.9737E-11	5.9111E-7
2.9895E-11	5.9046E-7
3.0053E-11	5.8980E-7
3.0211E-11	5.8916E-7
3.0368E-11	5.8852E-7
3.0526E-11	5.8788E-7
3.0684E-11	5.8724E-7
3.0842E-11	5.8661E-7
3.1000E-11	5.8599E-7

Figure 1: The concentration at outlet 1 (C_1) plotted for several values of D_{ij} using a parametric sweep. The desired value of C_1 was no more than $5.88 \times 10^{-7}\,\mathrm{mol\,m^{-3}}$.