Lecture 13

Steady State approximation for solving Diffusion equation (part I)

In the previous lecture we derived the Fick's second law (when there is no convection and no reaction to consume or generate materials):

$$\frac{\partial c}{\partial t} = D \nabla^2 c$$

Also in lecture two, we learned about different coordinate systems and for example how we can write the Laplalican operator in them:

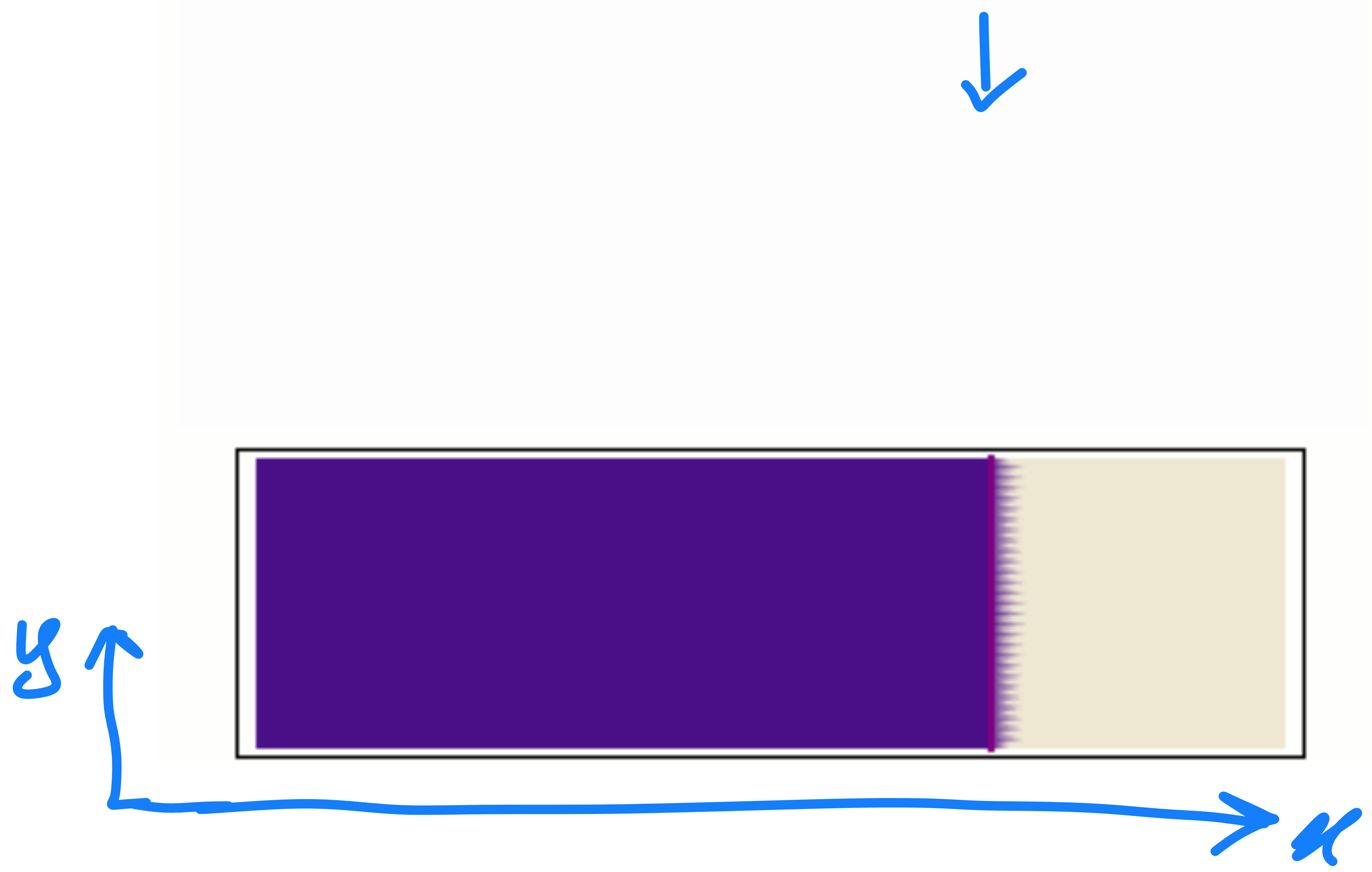
	Cartesian Coordinates	Cylindrical Coordinates	Spherical Coordinates
Laplacian $\nabla^2\phi$	$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial z^2}$	$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\phi}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2\phi}{\partial\varphi^2}+\frac{\partial^2\phi}{\partial z^2}$	$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\phi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\phi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\phi}{\partial\varphi^2}$

Which coordinate system to use, really depends on the shape and symmetries of the system that we want to study, coaching the right coordinate system can potentially make calculations easier.

We will discuss how we can apply this equation to particles that being diffused.

As you see on the left hand side of the equation we have time derivative and on the right hand side we have space. In principle this equation describes how the concentration C(x,t) changes over **time** and **space**.

non-steady state diffusion : Lets consider this closed system, we add ink to the left side and there is a wall, then we will remove the wall, soloing the diffusion equation can tell us how C changes in space and time



at time 0 we remove the wall, all blue particles (ink) are on the left, now how the concention C(x,y,t) changes over time.

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

Steady state diffusion : But not always C changes over time. In many cases, the concentration is at steady state, in this case, we can assume that dc/dt=0, this will significantly simplify solving the diffusion equation. Let's look at this example bellow, after some time the system reaches steady state!

Big reservoir with constant Concentrations

Steady State approximation for solving Diffusion equation (part I)

What is steady state (s.s)?

Refers to the condition when the properties of interest at a point in space do not change with time, i.e. are not functions of time, and thus the time derivatives can be set to zero. This will make our calculations way much easier.

$$\frac{\partial C(x,t)}{\partial t} = 0 \quad \text{or} \quad C(\vec{x})$$

$$\cancel{\frac{\partial C(\vec{x},t)}{\partial t}} = D\,\nabla^2 C(x,t) \Rightarrow D\,\nabla^2 C(\vec{x}) = 0$$

this process we will try to convert PDEs to ODEs...

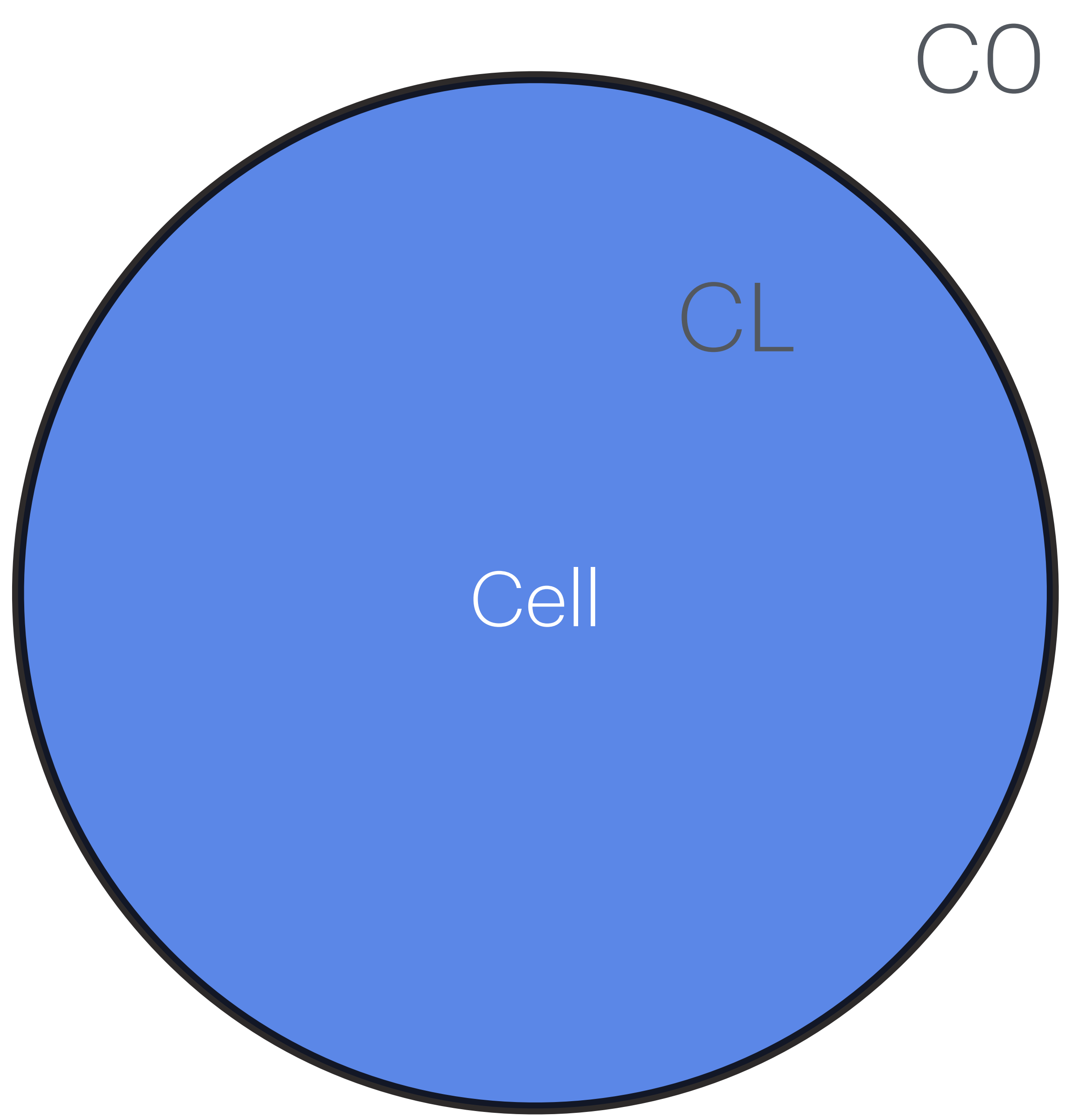
In the next couple of lectures we will study this equation

When the thickness of a biological structure, such as tissue or an organ, is significantly smaller compared to its length or breadth, we can make an important approximation: the diffusion across its surfaces can be treated as steady-state diffusion. This is relevant for example in tissues or even large organs like the skin or the kidney, where the diffusion process stabilizes quickly (will reach the steady state), allowing us to focus on the concentration gradient across the thin dimension in space.

Example 1: Steady State Diffusion Across a 'thin' Membranes with Dissolve-diffuse mechanism (The solute first dissolves in the membrane and then diffuses through it)

A nutrient species ***i*** diffuses across a membrane of thickness **d** through the dissolve- diffuse mechanism. The concentration of **i** outside the cell is CO and that inside the cell is CL (CL<CO).

Q1: Find the Concentration profile of i. For this you can assume the membrane thickness is very small in compare to cell radius (see if you can justify it). Also consider that the system is at S.S. What are your boundary conditions? Why can you justify them?



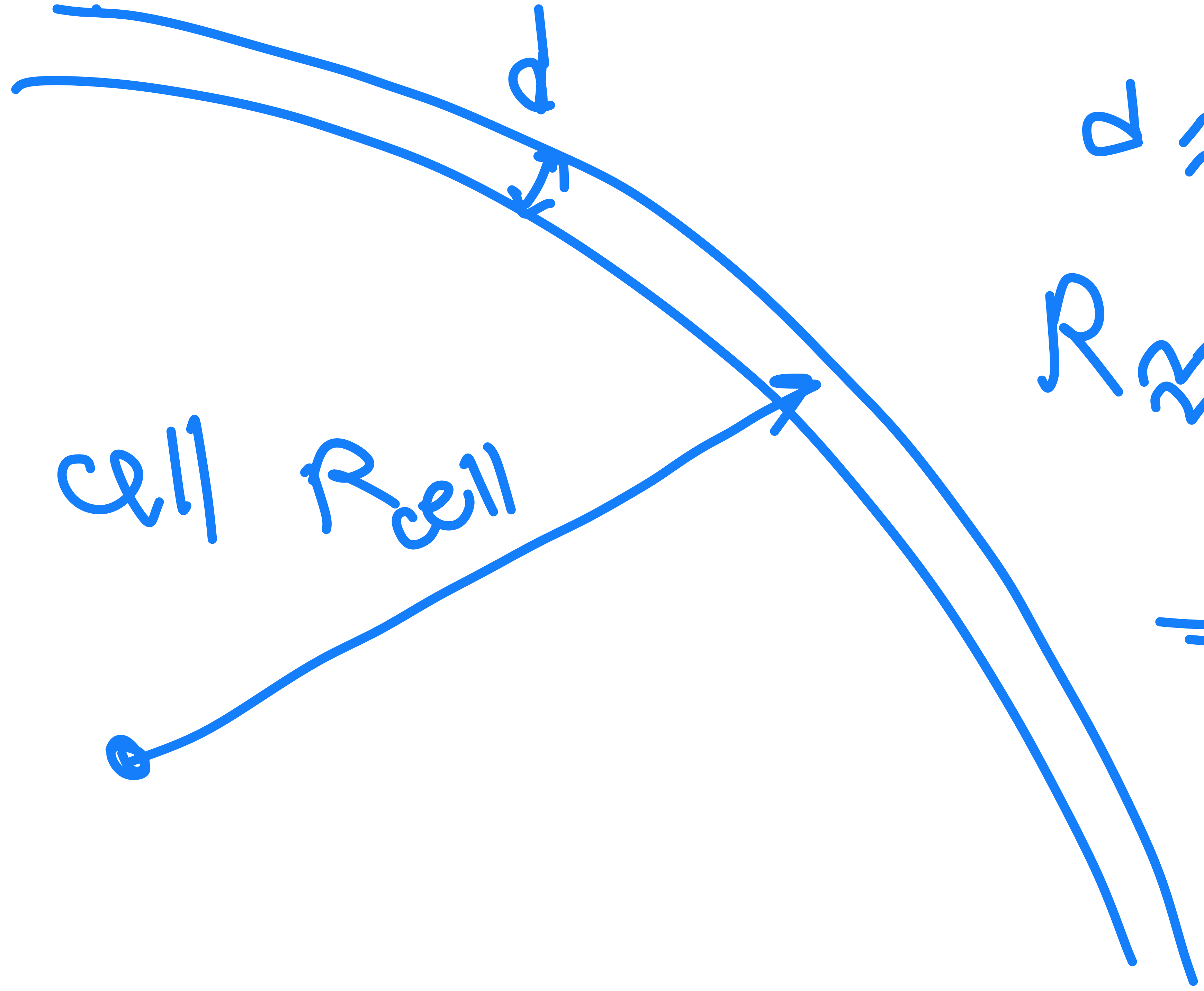
Solution :

a) let's write the diffusion law for concentration

$$\overset{S.S}{\overset{0}{\cancel{\frac{\partial C}{\partial t}}}} = D \nabla^2 C$$

b) now should we use cartesian coordinate or spherical ?

lets look at the thickness of the membrane and compare it to cell radius:

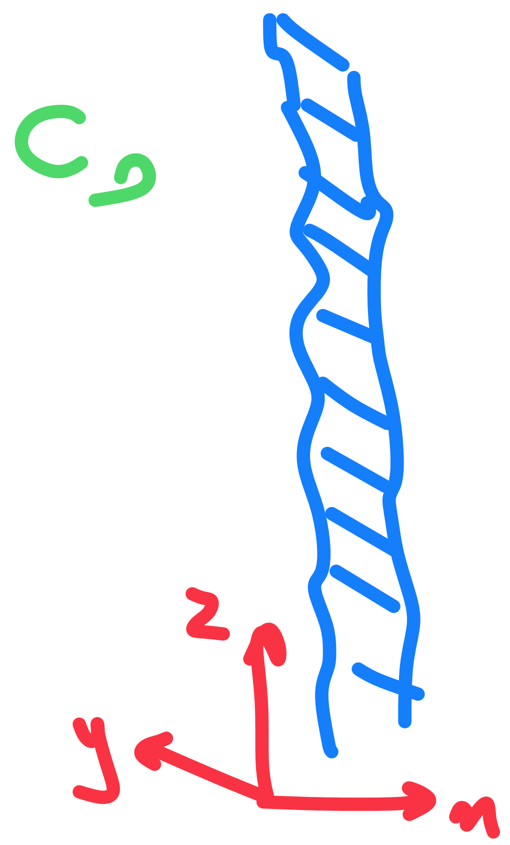


$d \approx 10\ nm \rightarrow 10^{-9} \times 10$

$R \approx 10\ \mu m \rightarrow 10^{-6} \times 10$

$\Rightarrow \frac{d}{R} \ll 1 \rightarrow$

c) now that it looks flat, we can use Cartesian coordinate:



$$\Rightarrow D\nabla^2 C(x,y,z) = 0 \Rightarrow \nabla^2 C(x,y,z) = 0$$

d) using symmetries: C should depend on y and z because membrane is very large and uniform

$$\Rightarrow \nabla^2 C = \frac{\partial^2 C}{\partial x^2} + \underbrace{\cancel{\frac{\partial^2 C}{\partial y^2}}}_{0} + \underbrace{\cancel{\frac{\partial^2 C}{\partial z^2}}}_{0} = 0 \Rightarrow \frac{\partial^2 C(x)}{\partial x^2} = 0$$

symmetry

e) this is a simple ODE, we integrate to solve:

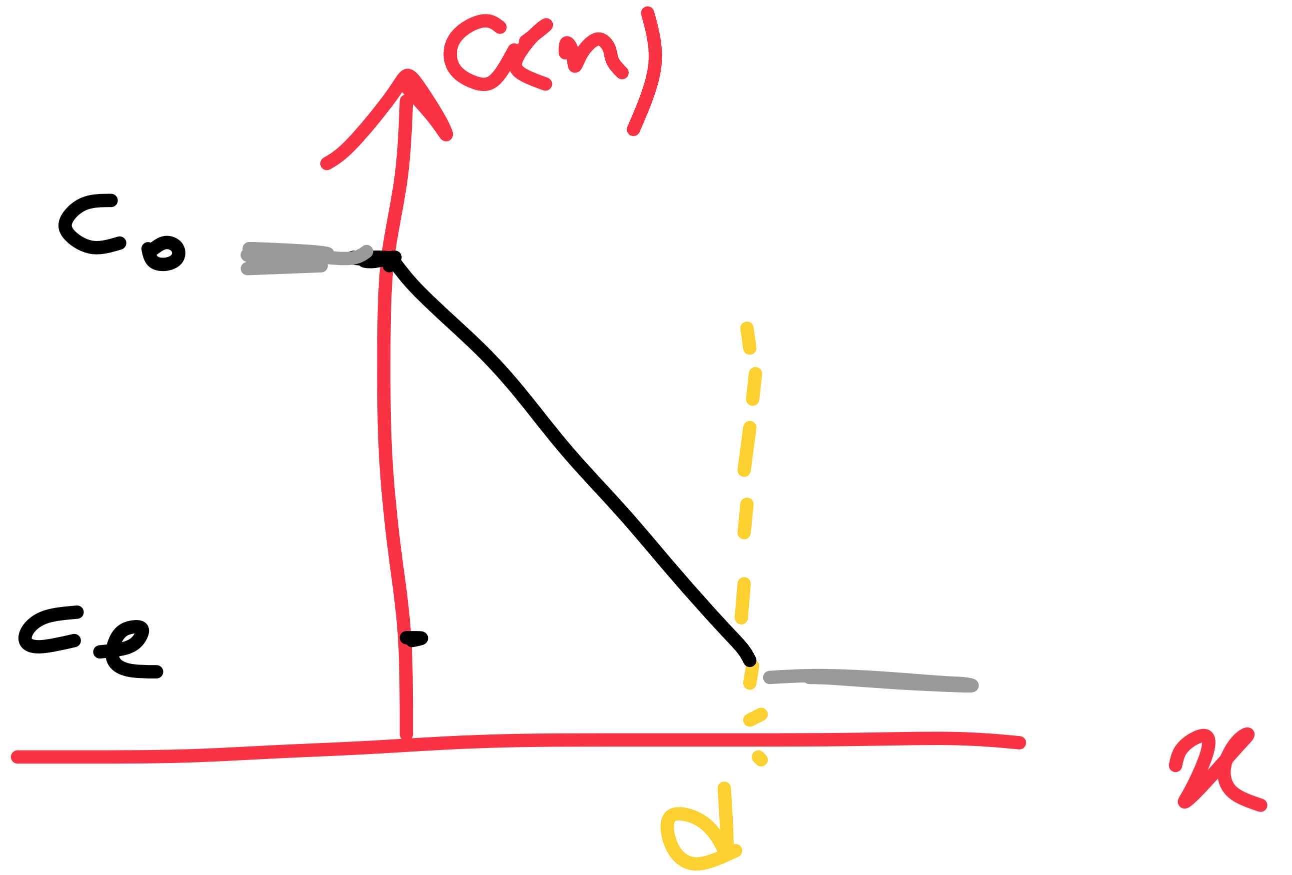
$$C(x) = C_1 x + C_2 \quad , \; C \text{ and } C_2 \text{ TBD by B.C}$$

f) determining B.C and finding the constants:

$$\begin{cases} C(x=0) = C_0 \\ C(x=d) = C_e \end{cases} \Rightarrow \begin{array}{l} C_0 = C_2 \\ C_e = C_1 d + C_2 \Rightarrow C_1 = -\dfrac{(C_0 - C_e)}{d} \end{array}$$

g) the full solution is:

$$C(x) = C_0 - \frac{(C_0 - C_e)}{d} x$$



Q2 :What are the fluxes at each side of membrane? Check if mass balance equation holds

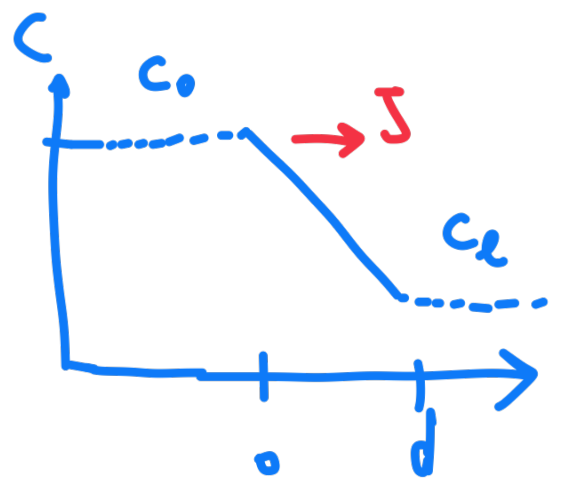
Solution: we have $C(x,t)$, how we can find J?

a) Fick's firs law: $J = -D\nabla C \xrightarrow{\text{in 1D}}$

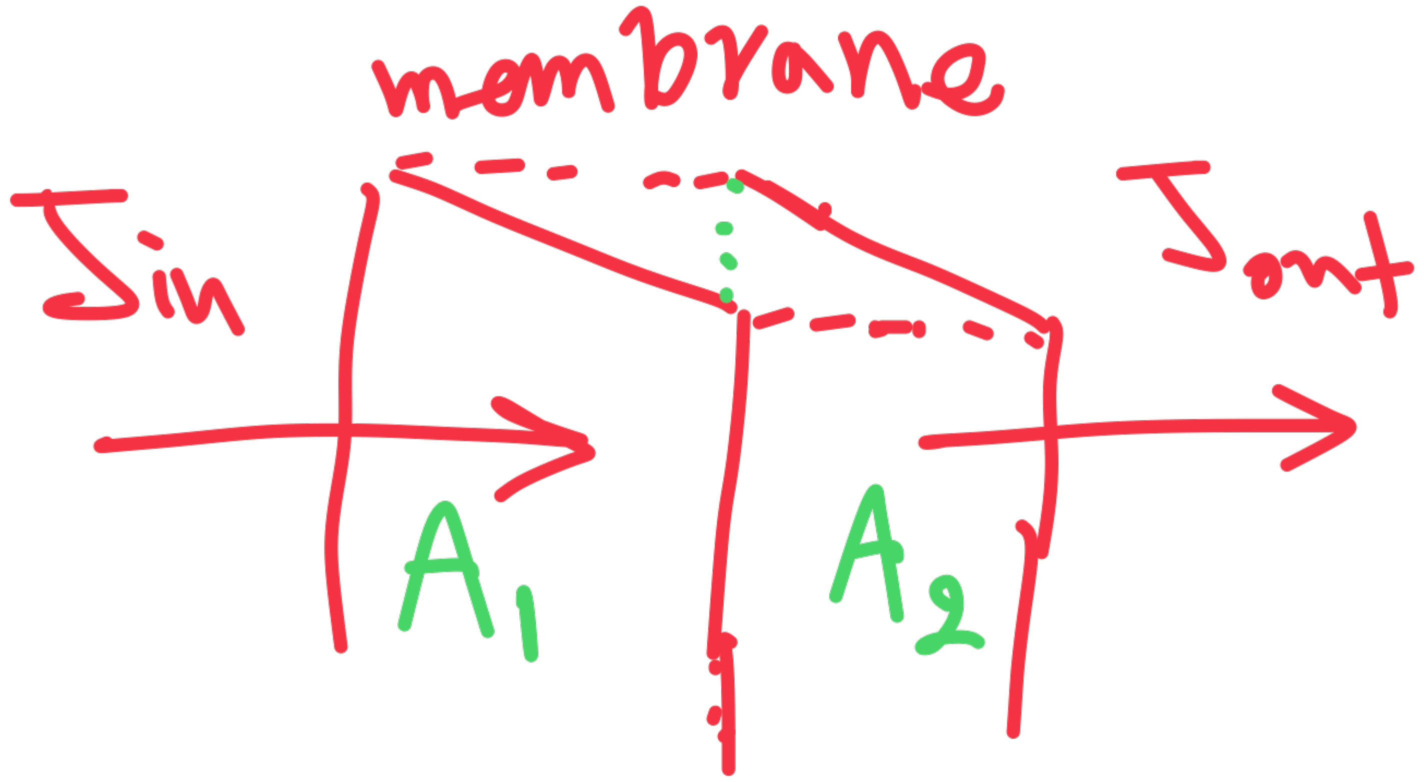
$$J(x) = -D\frac{\partial C}{\partial x} = +D\frac{(C_0 - C_\ell)}{d}$$

$J \propto \frac{1}{d} \Rightarrow$ the thicker the membrane the less the flux

now look at the direction, does it makes sense?



b) $\vec{J}$ is a constant flux on both sides of the membranes:



$$\frac{dm}{dt} = r_{in} - r_{out} = J(A_1) - J(A_2)$$

$A_1 = A_2 \equiv A_0$ rectangular $\longrightarrow$ $= JA_0 - JA_0 = 0$ ✓

Q3 (practice at home Example 2.4.1-1 in textbook) : Answer Q1 and Q2 in this case: there is a Partition coefficient for concentrations.

A species i diffuses across a membrane of thickness d through the dissolve-diffuse mechanism (Fig. 2.4.1-1). The concentration of i outside the cell is c_o and that inside the cell is c_L.

At $x = 0$, the concentration of i in the membrane is given by Kc_o, where K is the partition coefficient of i in the membrane. Partition coefficient is defined as the ratio of the solute concentrations in two phases at equilibrium, when a solute is partitioning across the two phases.

$$c_m|_{x=0} = Kc_o$$

and

$$c_m|_{x=d} = Kc_L$$

We have assumed that the partition coefficient is the same on both sides of the membrane. This is a reasonable assumption, but may not be applicable in situations where solutions on both sides of the membrane are widely different.

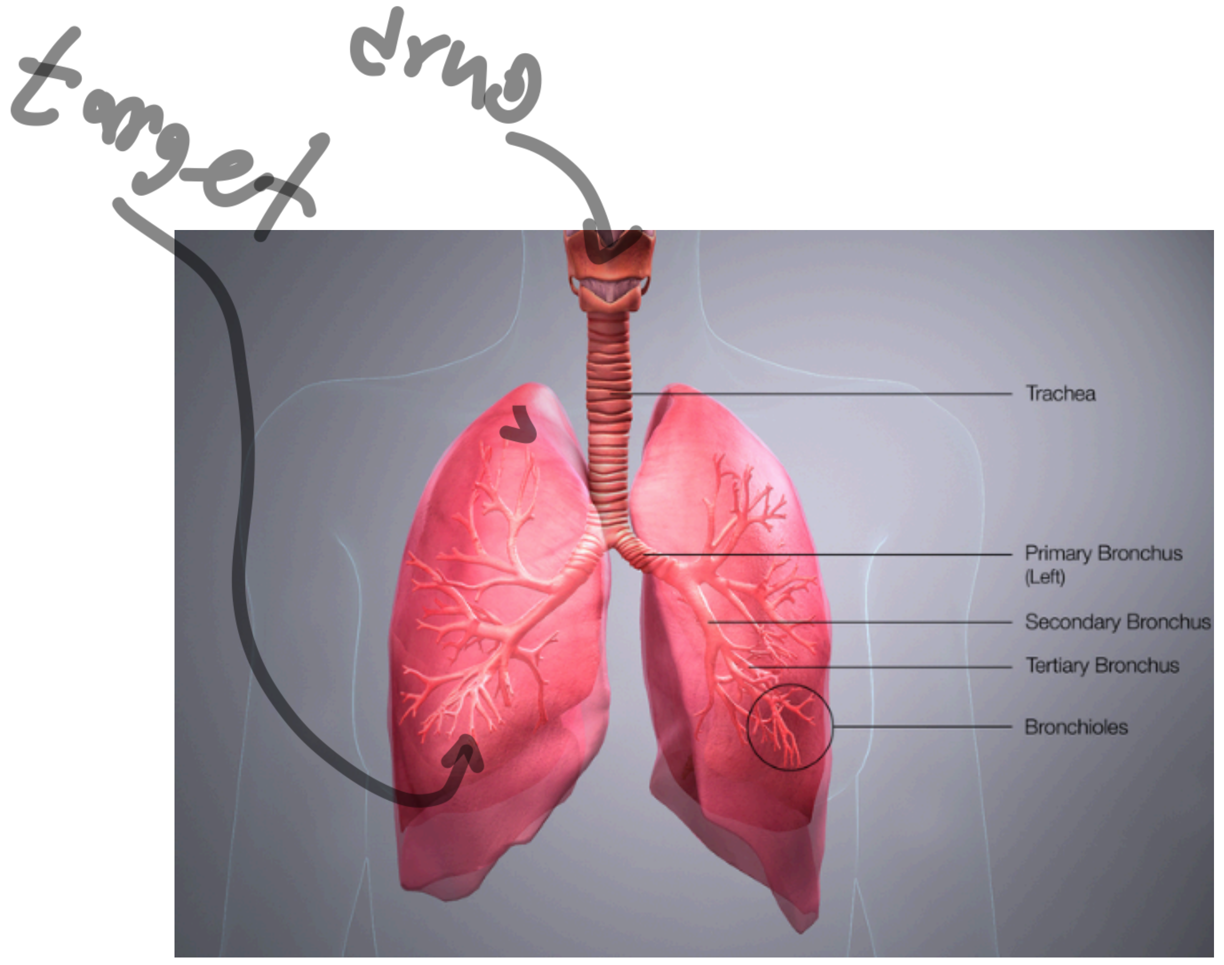
Pause point

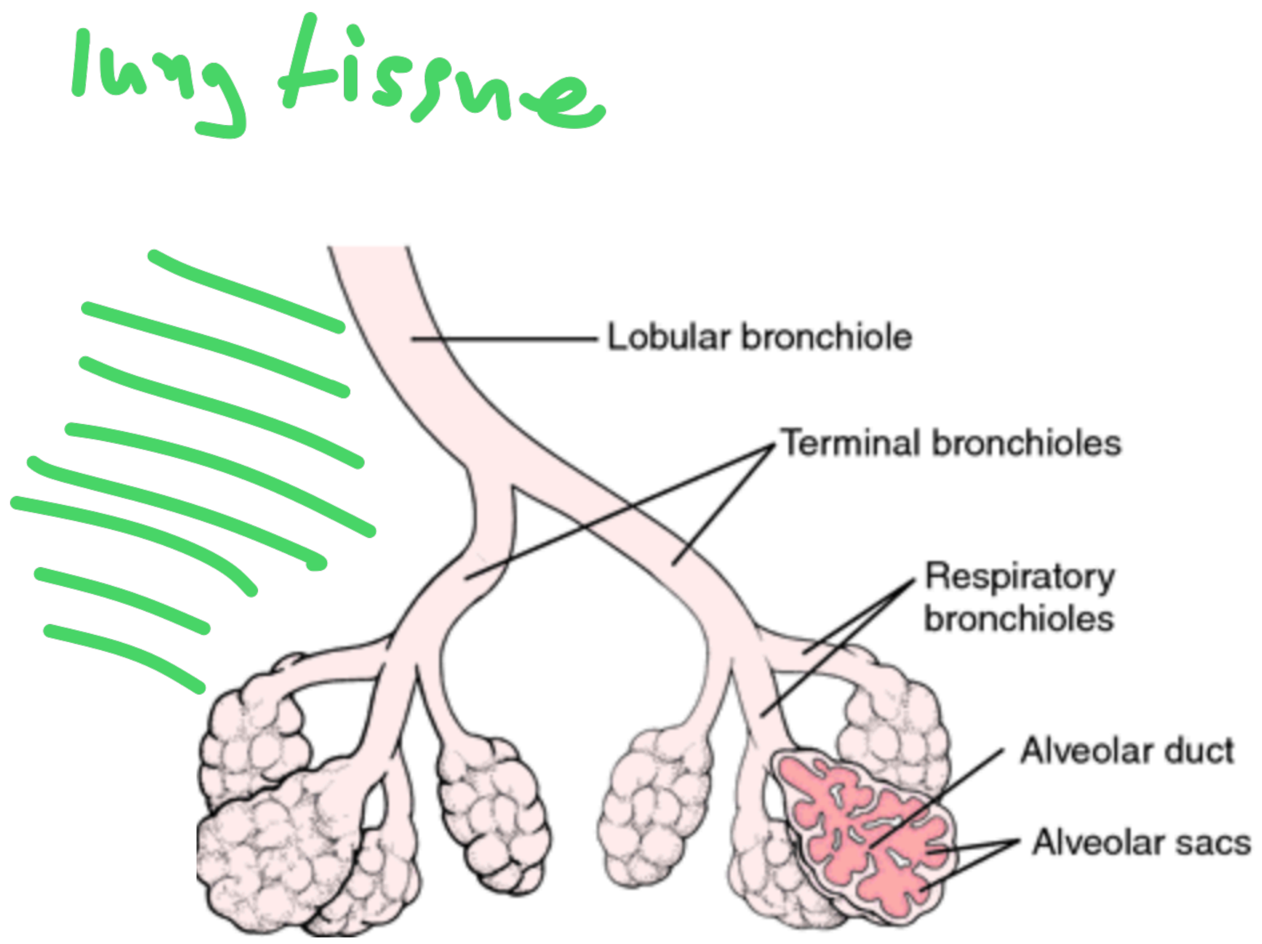
Questions?

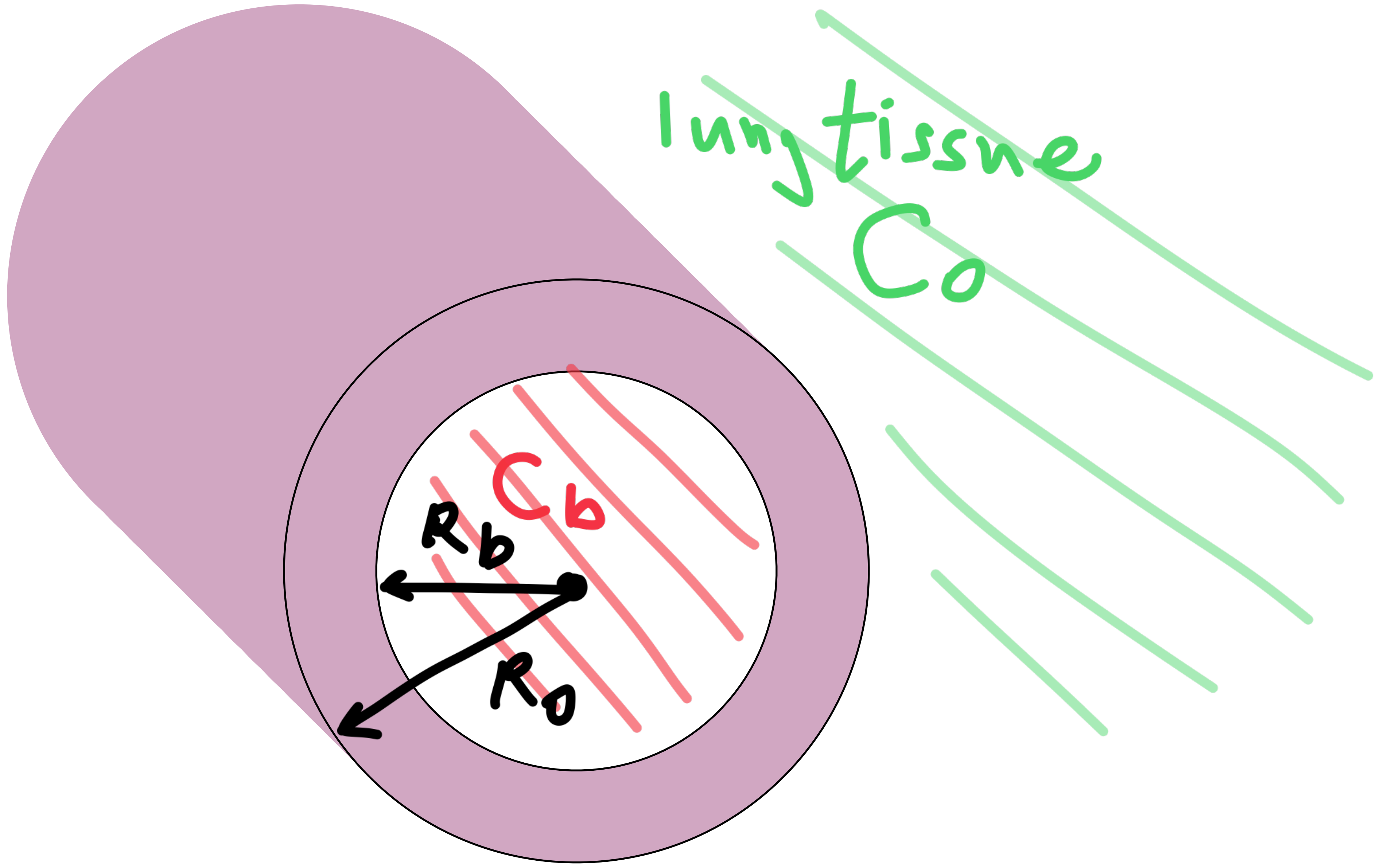
Example 2: Steady State Radial Diffusion Across Tubular Walls:

A drug is administered continuously through the nasal cavity, at an appropriate dose, to reach the lung tissue by passing across the bronchiole wall. The concentration of the drug in the air present in the lumen of the bronchiole is Cb at steady state. The drug concentration in the lung tissue on the other side of the bronchiolar wall is needed to be C0 for effectiveness. The inner and outer radii of the bronchiole are Rb and R0.

Q1: Find the Concentration profile of drug in the bronchiole wall. Find the best coordinate system. Also consider that the system is at S.S. What are your boundary conditions?







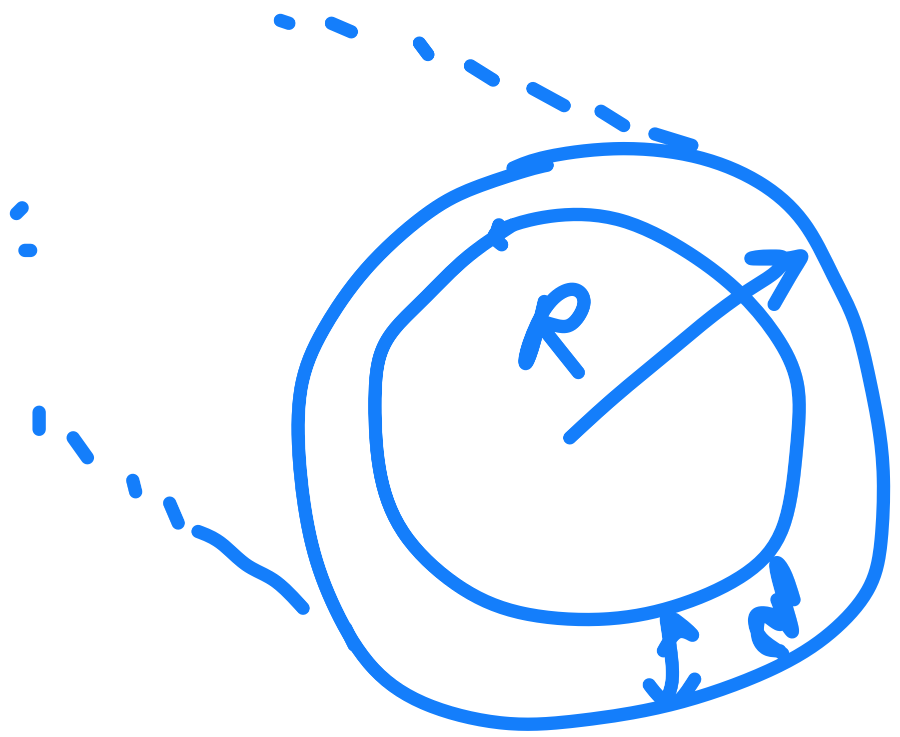
Solution:

a) s.s? $\longrightarrow$ yes $\Rightarrow$ $\cancel{\dfrac{\partial C}{\partial t}}^{0} = D\,\nabla^2 C$

b) coordinate system? two options $\longrightarrow$ Cartesian: low curvature

$\hookrightarrow$ cylindrical: high curvature

let's check it:



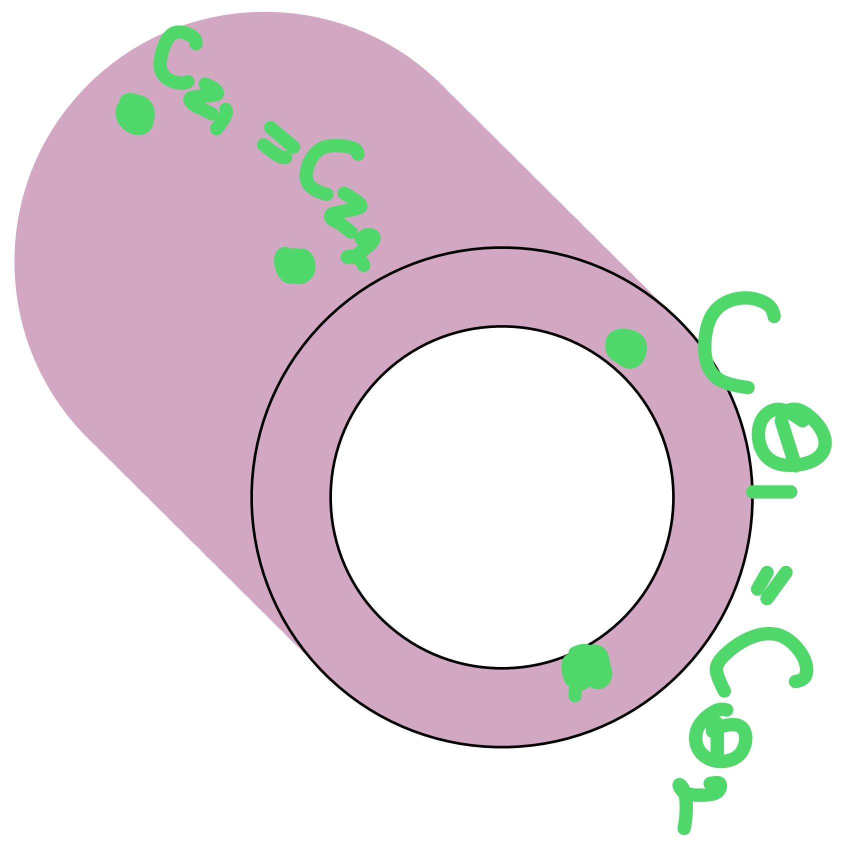
$d \approx 0.3\,mm$

$R \approx 1.5\,mm$ $\Rightarrow$ $\dfrac{d}{R} \simeq 0.2$ is high

$\Rightarrow$ Cylindrical

c) now the equation ($\nabla^2 C = 0$).

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right)+\underbrace{\cancel{\frac{1}{r^2}\frac{\partial^2 C}{\partial \theta^2}}}_{0}+\underbrace{\cancel{\frac{\partial^2 C}{\partial z^2}}}_{0}$$



d) using symmetries, c should not depend on θ or z:

e) now this is an ODE (C only depends on r):

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{dc}{dr}\right)=0 \Rightarrow \frac{d}{dr}\left(r\frac{dc}{dr}\right)=0 \xrightarrow{\text{integrate}} r\frac{dc}{dr}=C_1$$

$$\frac{dc}{dr}=\frac{C_1}{r} \xrightarrow{\text{integrate}} C(r)=C_1\ln(r)+C_2$$

, C_1 and C_2 TBD by B.C

f) B.C:

$$\begin{cases} C(R_b) = C_b \Rightarrow C_b = C_1 \ln R_b + C_2 \rightarrow C_2 = C_b - C_1 \ln R_b \\ C(R_o) = C_o \Rightarrow C_o = C_1 \ln R_o + C_2 \end{cases}$$

$$\Rightarrow C_o = C_1 \ln R_o + C_b - C_1 \ln R_b \Rightarrow C_1(\ln R_o - R_b) = C_o - C_b$$

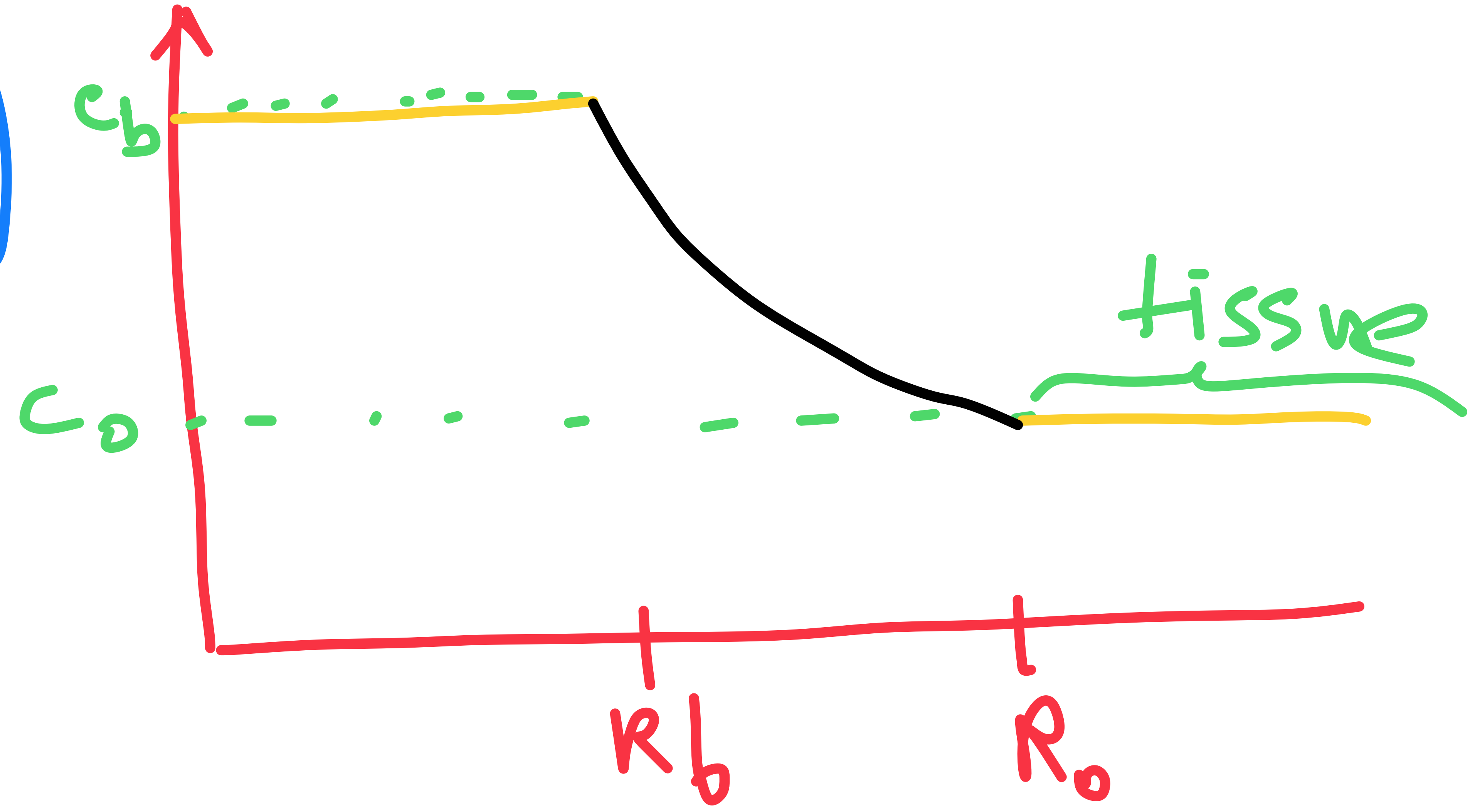
$$\Rightarrow C_1 = \frac{(C_o - C_b)}{\ln\left(\frac{R_o}{R_b}\right)} \quad \bullet \text{ Similarly} \Rightarrow C_2 = C_b - (C_b - C_o)\frac{\ln R_b}{\ln\left(\frac{R_b}{R_o}\right)}$$

g) the full solution is:

$$C(r) = \underbrace{\frac{(C_o - C_b)}{\ln \frac{R_o}{R_b}}}_{-} \ln(r) + \underbrace{\left(C_b - (C_b - C_o)\frac{\ln R_b}{\ln\left(\frac{R_b}{R_o}\right)}\right)}_{+}$$

$C_o < C_b$

$R_o > R_b$



Q2 :What are the fluxes at each side of the walls? Check if mass balance equation holds

Solution:

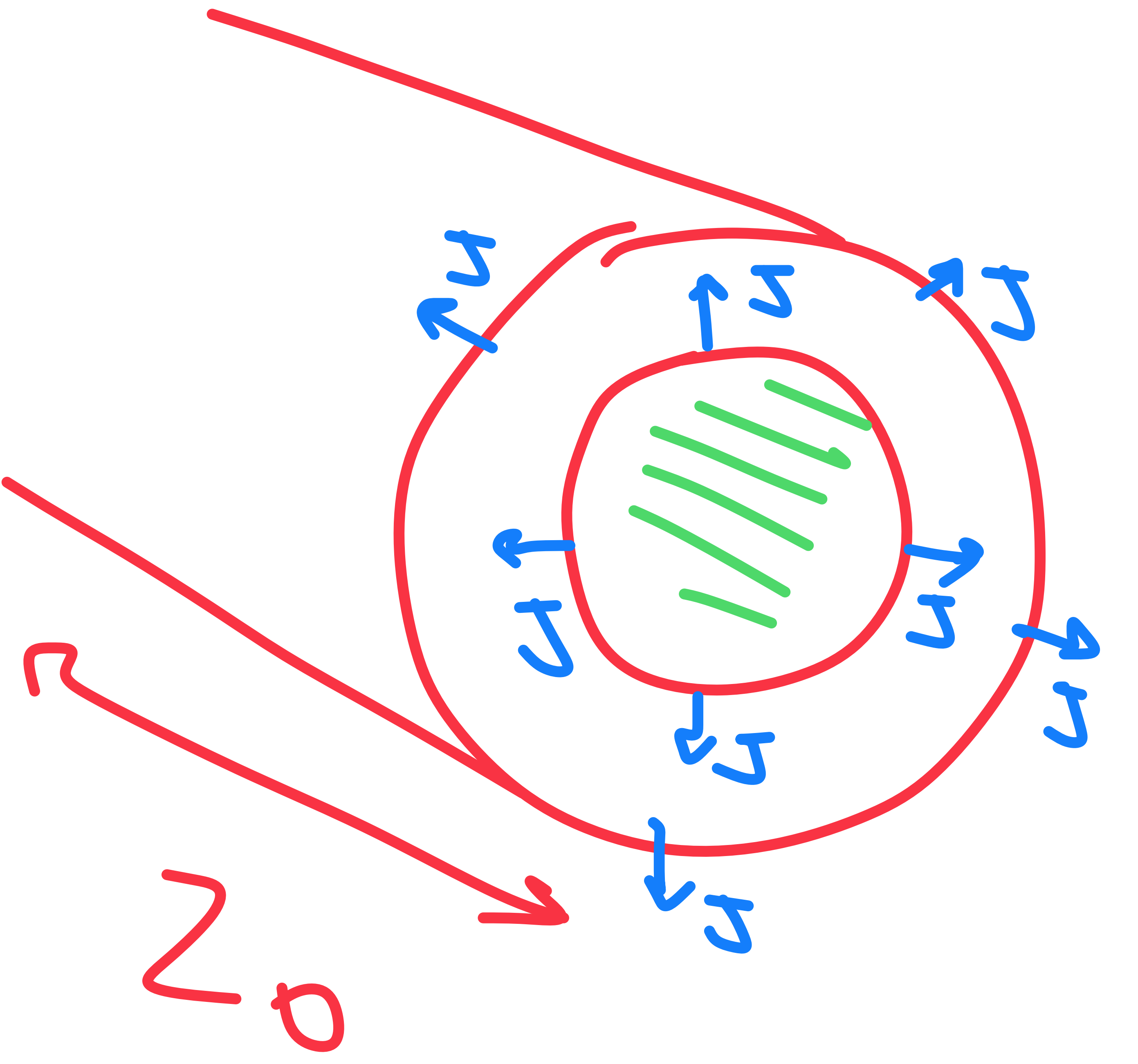
a) $\vec{J} = -D\nabla C$

$$\frac{\partial\phi}{\partial\rho}\hat{\rho} + \frac{1}{\rho}\frac{\partial\phi}{\partial\varphi}\hat{\varphi} + \frac{\partial\phi}{\partial z}\hat{z}$$

$$\vec{J} = -D\left(\frac{\partial C}{\partial r}\hat{r} + \frac{1}{r}\cancel{\frac{\partial C}{\partial\theta}}^{\,0}\hat{\theta} + \cancel{\frac{\partial C}{\partial z}}^{\,0}\hat{z}\right) \Rightarrow \vec{J}(r) = D\frac{(C_b - C_o)}{\ln\left(\frac{R_b}{R_o}\right)}\frac{1}{r}$$

function of r

b) lets write the mass balance for the wall of the tube with length Z_o



$$\frac{dm_{\text{storing in wall}}}{dt} = r_{in} - r_{out} = \underset{r=R_b}{J_{in}} \times A_{in} - \underset{r=R_o}{J_{out}} A_{out}$$

$$= \frac{D(C_b - C_o)}{\ln\left(\frac{R_b}{R_o}\right)}\frac{1}{R_b} \times (2\pi R_b Z_o) - \frac{D(C_b - C_o)}{\ln\left(\frac{R_b}{R_o}\right)}\frac{1}{R_o}(2\pi R_o Z_o)$$

$= 0$ ✓

Q3 (practice at home Example 2.4.2 in textbook) : Answer Q1 and Q2 in this case: there is a Partition coefficient for concentrations.