Transport Phenomena in Biological Systems
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Lecture - 19
Review of Mass Flux

Welcome. In towards the end of the last lecture, I mentioned that we have completed the second chapter on mass flux. Before we move forward, let us briefly review all that we have done so that it gives you things in perspective, the mass flux aspects in perspective, as well as it helps you revise some of the aspects. It improves the learning and so on so forth. So we will do this after every large chapter.

The first chapter was on mass conservation itself and that is part review, half of it was review. The application to microscopic systems was probably new. That is the reason why we did not spend an entire lecture reviewing that. Very briefly mass conservation, mass can neither be created nor destroyed that converted to a useful form was what we started using rate of input minus rate of output plus rate of generation minus rate of consumption equals the rate of accumulation.

$\frac{dm}{dt} = r_i - r_o + r_g - r_c$

We wrote it of a certain way that would be useful. Then we had shown the application to a humidifier, a macroscopic system. And then to a cell, a microscopic system. And that was pretty much what it was at that stage. And also I think we derived the equation of continuity for the total mass or a single component system, total mass. Now let us review the mass flux aspects, .

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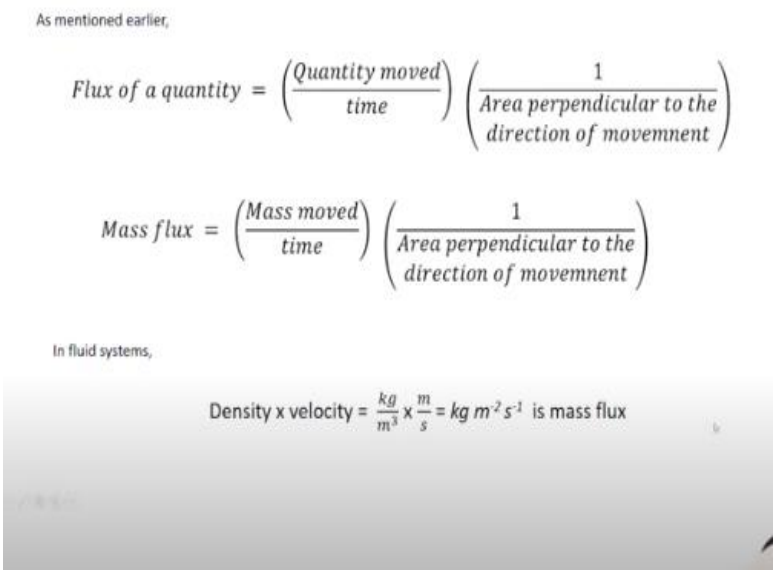

So, flux of any quantity we said was the quantity moved per time per unit area perpendicular to the direction of the motion itself. In this case mass flux is mass moved per time per area perpendicular to the direction of motion. And we also said that in fluid systems the density times velocity directly gives us mass flux. Density and velocity are measurable.

Mass flux formulation which helps us look at various things from the same perspective and that is why we are after a flux kind of a formulation, makes the things general, makes us see relationships between movement of various different conserved quantities and so on so forth. .

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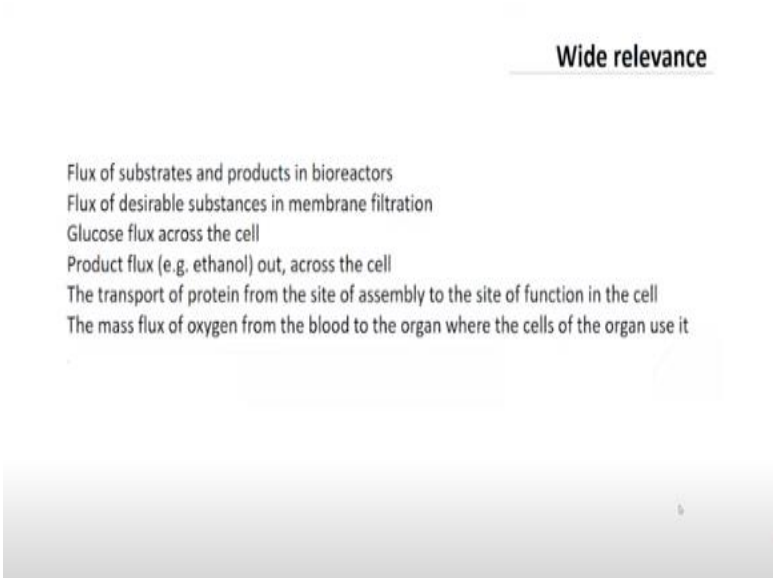

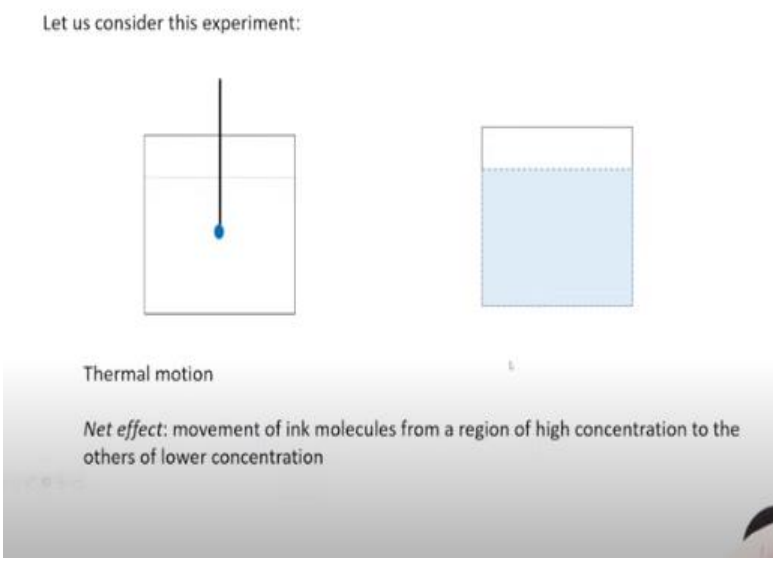

Then, we looked at the relevance of mass flux. And then we said how the mass flux comes into being when there is you know the thermal interaction between the various molecules, jiggle things around to effectively result in a motion of the species from a region of high concentration to a region of low concentration, till the concentrations are the same everywhere and in a particular phase.

We also said across phases it is the difference in chemical potential that drives it, but in a phase, the chemical potential can easily be replaced by concentration and that should work.

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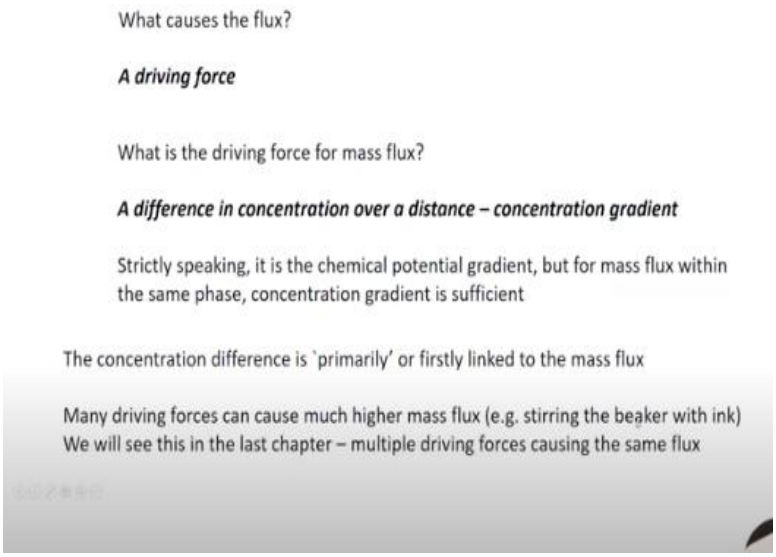

What causes the flux? That is what we have been talking about, the driving force. A difference in concentration over distance, a concentration gradient. So we also said that,

this is primarily associated with the mass flux and therefore, we call it the primary driving force. Although the primary driving force may not result in the maximum flux. We said that many different driving forces could cause a flux.

For example, many different driving forces could cause mass flux. Concentration gradient can cause bulk motion or convective motion of the fluid itself. If the fluid itself is moving, of course, the species would move along with the fluid much faster. The difference in temperatures or a temperature gradient can cause a mass flux as we will see later and so on so forth.

A difference in electrical potential, electrical potential gradient can cause a mass flux. And many of these driving forces can cause much higher mass fluxes. However, the one that is primarily associated with it is called the primary driving force, which is the concentration gradient here.

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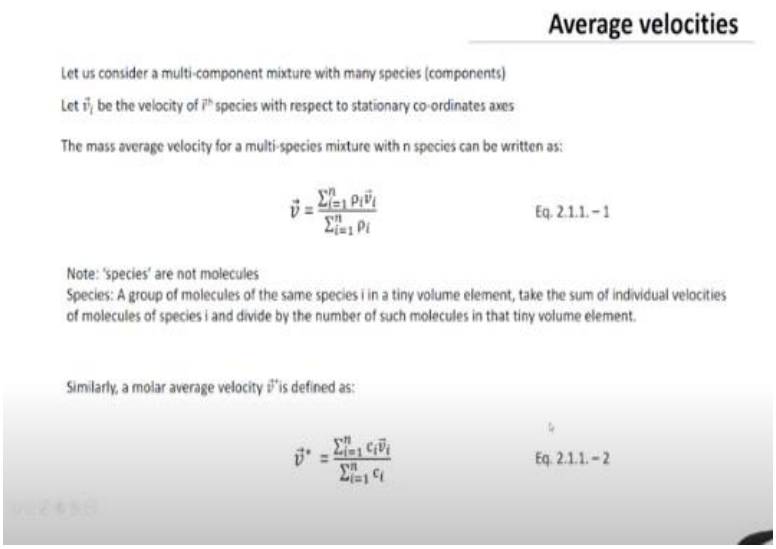

Then we talked of average velocities, the mass average velocity, the molar average velocity.

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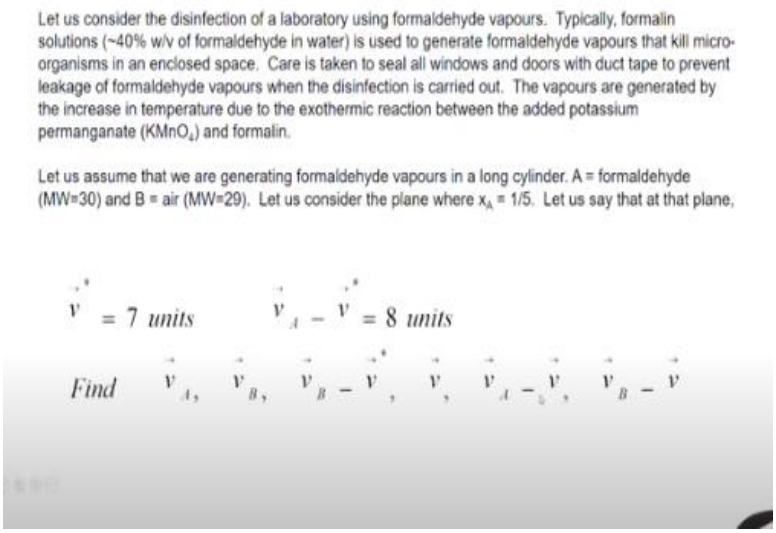

Then we worked out a problem to understand these various velocities.

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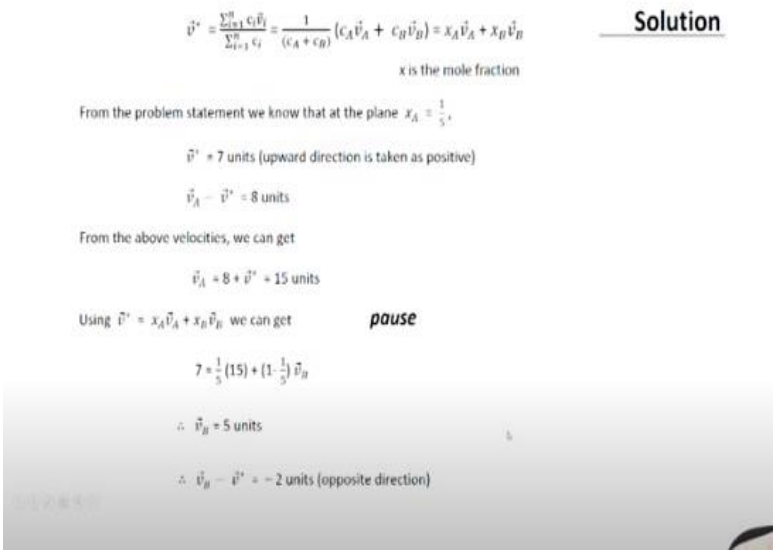

Essentially a substance moving. Therefore, there is a velocity associated with it. We are trying to get to fluxes. So, flux needs to be written in terms of velocities. That is the reason why we looked at velocities in some detail. And this was the problem that we worked out.

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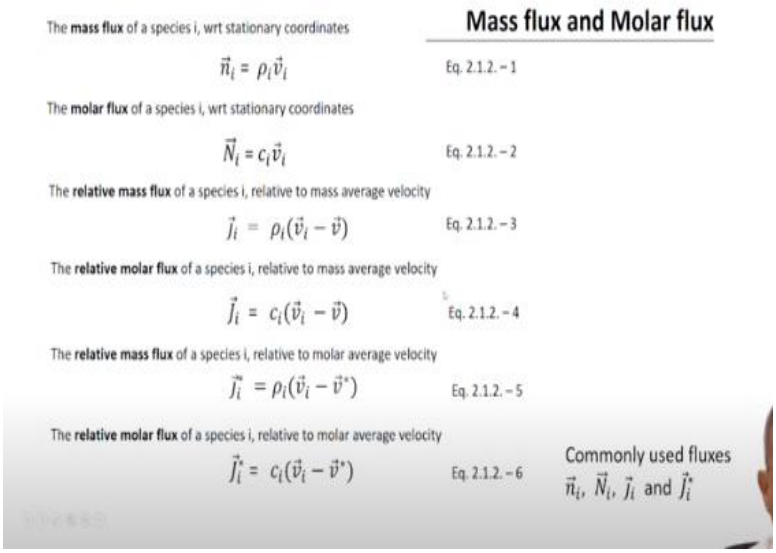

And then the expressions for mass and molar flux in terms of very fundamental quantities, density, velocity and so on so forth. The mass flux and the molar flux capital N_i, they are vectors. **Molar flux is concentration times velocity whereas mass flux is density times velocity**. Then we said that we are typically interested in the motion with respect to other species, not with respect to stationary coordinates.

And therefore, we brought in the relative mass flux $\rho_i v_i$ minus the average velocity, mass average velocity. And then the relative molar flux with respect to the mass average velocity for completeness. Relative mass flux and relative molar flux relative to the molar average velocity.

Of these we said we commonly would be using the mass flux, the molar flux, and the relative mass flux relative to the mass average velocity as well as the last one, the relative molar flux relative to the mass average velocity. These are the ones that are commonly used. There are many other fluxes that are available. You can define and so on so forth. We will not be getting into those.

To know about some of those fluxes that are not covered here, you could look at Bird, Stewart and Lightfoot, one of your main reference books to get an idea of a molal average and so on so forth; molal flux.

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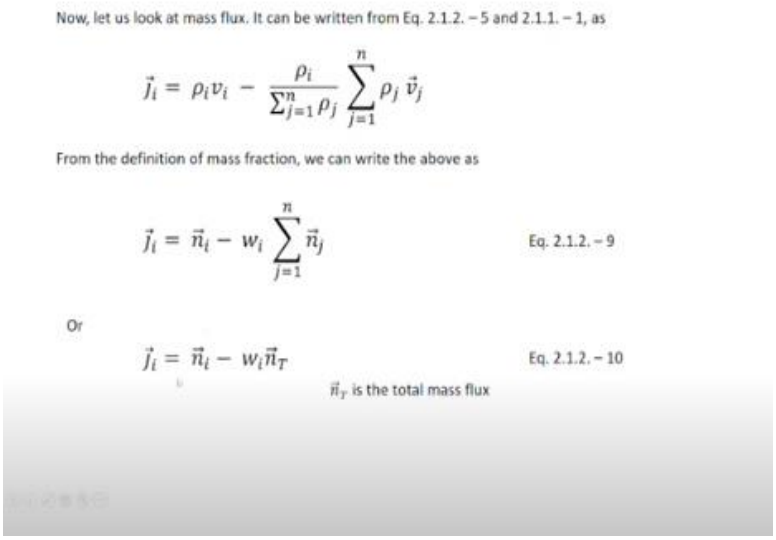

Then, we started finding out the relationships between these various quantities to make sense. We got to some important relationship. This was $\mathbf{j_i = n_i - w_i n_T}$ was one of them.

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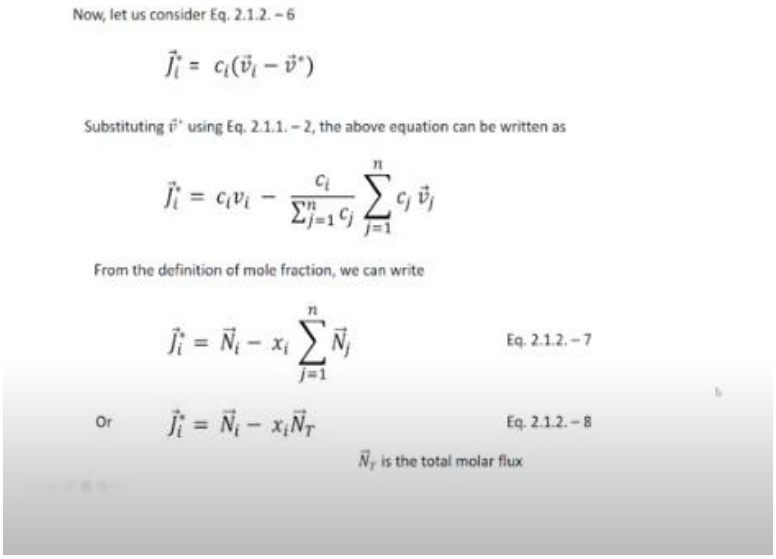

Earlier we $\mathbf{J_i^* = N_i - x_i N_T}$, . These two are important relationships where the link between a total flux and the diffusive flux is given. However, we said in throughout this chapter, we will consider only diffusive flux, only the flux that arises out of its primary driving force, a concentration gradient. And therefore, you do not have to worry about the convective bulk motion and so on and so forth.

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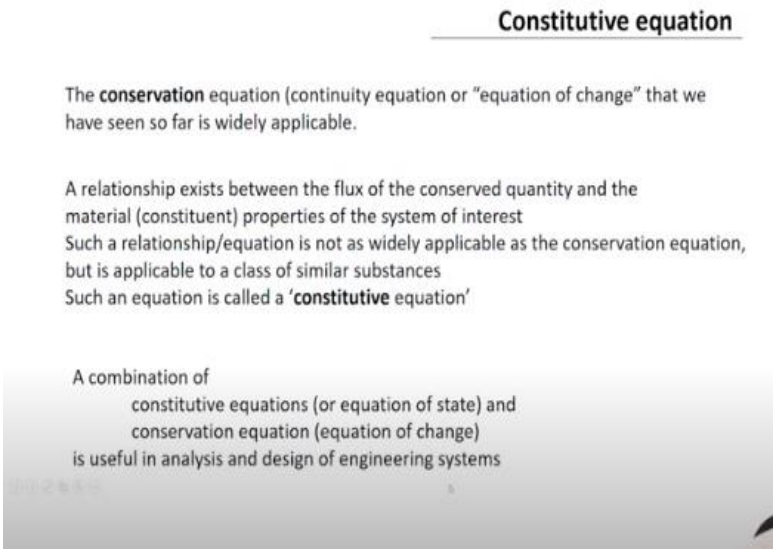

Then, we looked at something called the constitutive equation. We said a conservation equation is applicable in general pretty much throughout, the for all practical purposes, pretty universal. And whereas a constitutive equation which depends on the constituent nature of the substance. There are, there is a relationship between flux of a conserved quantity and the material properties of the system of interest.

Such a relationship is the constitutive equation. And a combination of the constitutive equations or equations of state as they are called, as well as the conservation equations are very helpful in the analysis and design of engineering systems.

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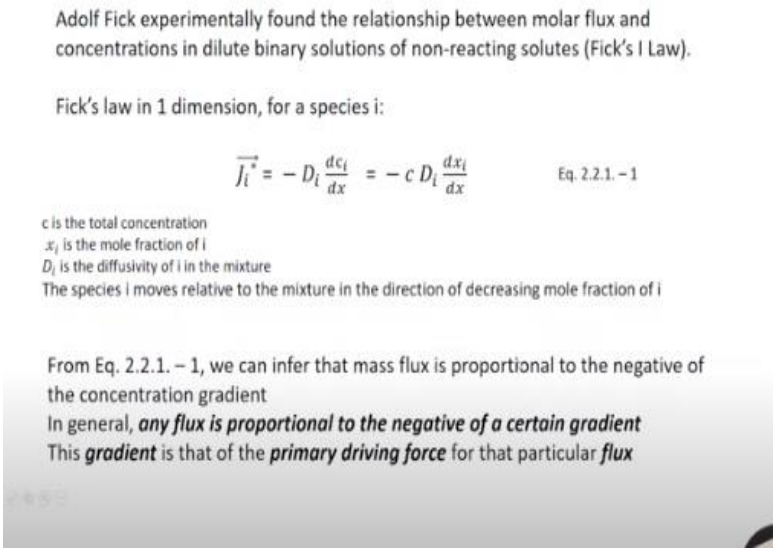

We saw the Fick's first law which provides us with a way of getting estimates of the flux in terms of a diffusivity coefficient and so on so forth. This is in one dimension.

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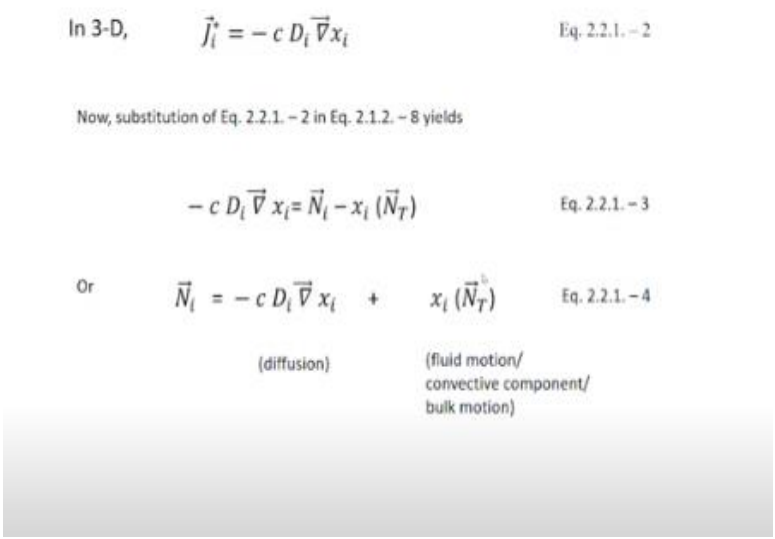

You could have it in three dimensions. You know the derivative, one derivative gets replaced by a ∇, which is derivative in all three dimensions. Then yeah this is the total flux as a diffusive flux plus the flux due to fluid motion, convective component, bulk motion. There could be many other things as well, we will see later. Here in this chapter, we are not going to consider this at all.

The aspects have been carefully chosen such that this does not come into the picture for understanding the subject better. In the last chapter, we will bring this up.

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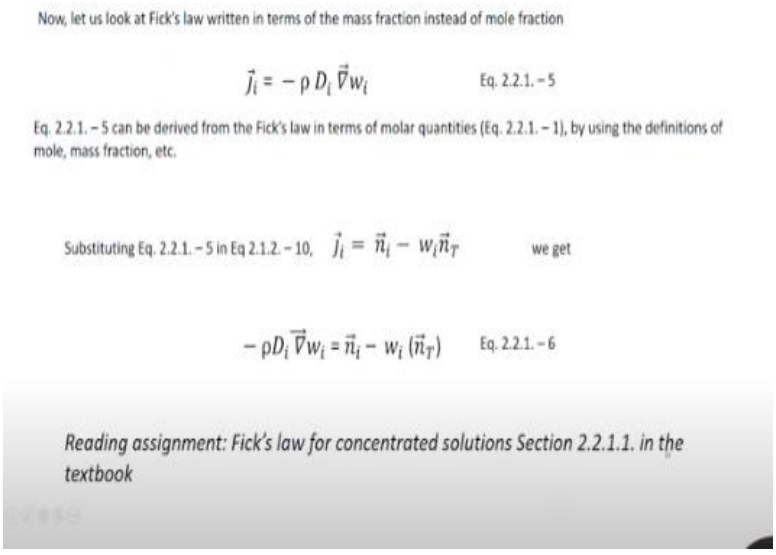

Then the mass, the Fick's law written in terms of the mass fraction is where we finished up with the, with that part. And then let me get to wherever I am getting to. Yes, this is

the, we said that you could approach these problems in two different ways. One is a shell balanced approach.

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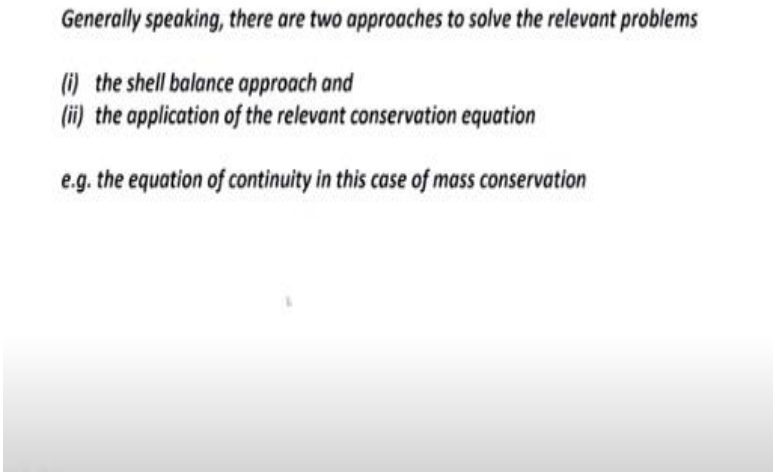

And the other one is application of the relevant conservation equation. A shell balance approach means that you, we apply the material balance or we do a material balance over a thin representative shell. That shell depends on the geometry of the system if it is a rectangular Cartesian coordinate kind of a system. Rather, if it is a rectangular system, then we use a rectangular Cartesian coordinate geometry cuboidal system.

If it is a cylindrical system, we can use cylindrical coordinates. If it is a spherical system, we can use spherical coordinates. Then the equation of continuity is what we get in the case of mass conservation.

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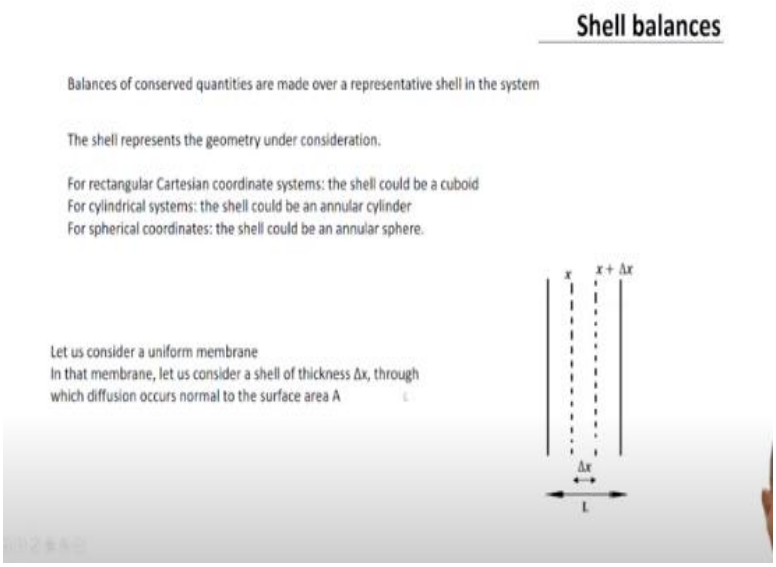

I showed you how to do shell balances for a uniform membrane. We chose a shell. And then we wrote our balances over it.

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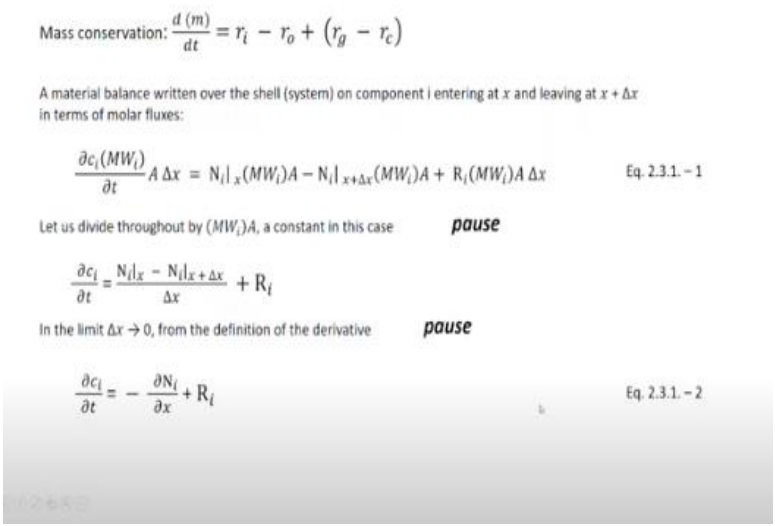

To arrive at some very useful relationships for a membrane, which we used much repeatedly in fact.

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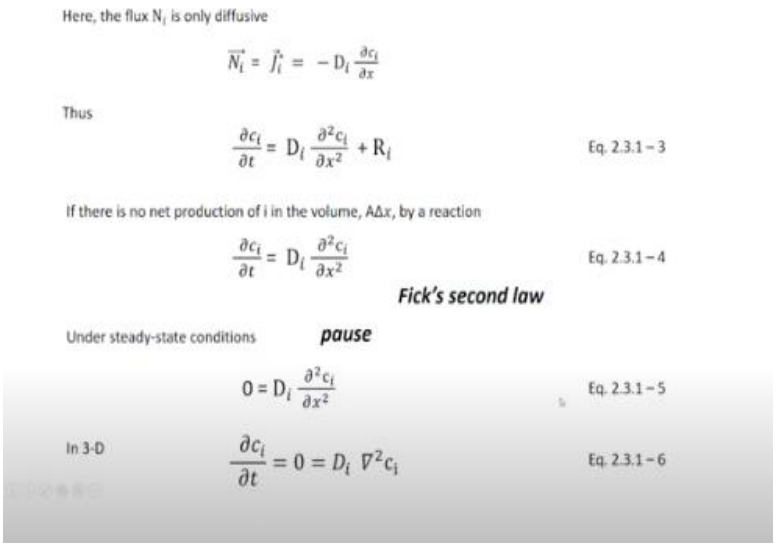

You know this relationship could have been used many times. And then we looked at, we derived the Fick's second law from this relationship. This is the variation of time and the variation of space both given the same relationship here, that is the niceness of it. And under steady state conditions, we get a nice compact relationship using Fick's second law that can be used to analyze it.

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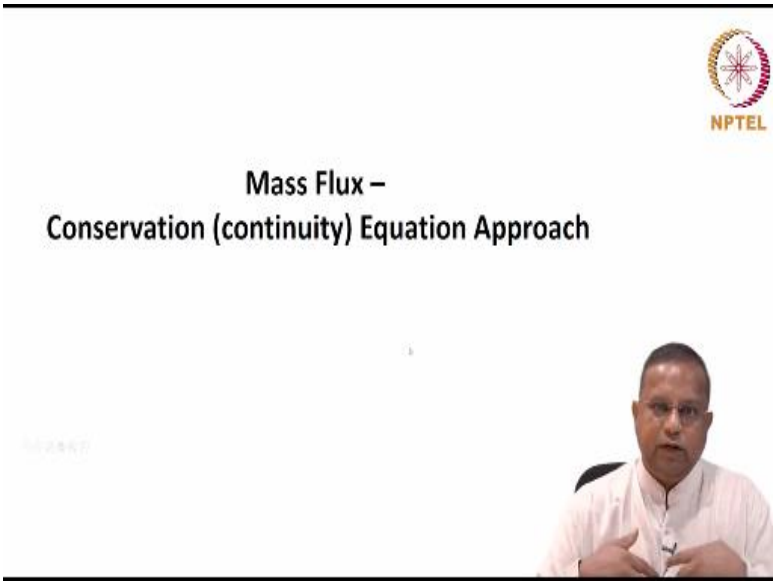

Then we looked at the conservation equation approach a continuity equation approach. We derived the conservation equation because we said shell balances could get cumbersome, especially with cylindrical and spherical coordinate systems it could get very cumbersome. Therefore, we derived a reasonably general equation, one very general equation and another at constant c, D_{AB} which is reasonably general as long as there is no change in geometry.

You can, that is one of the limitations. If there is a change in geometry of the system, you cannot use that. Otherwise you can use that. And so we have derived it. We have an equation. All we need to do is take that equation see what terms are relevant and go forward with it, . Let me not show you the derivation here because we are, it is a review. So you can go back and check how we derived it and so on so forth.

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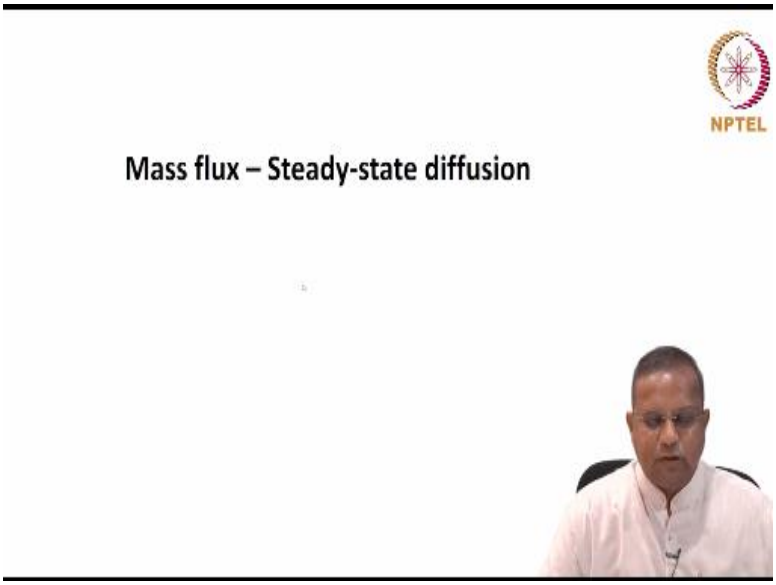

Then, we looked at steady state diffusion. We started applying the conservation equation because we have derived the relationship directly. I asked you to make a copy of these tables, soft copy, hard copy whatever it is and keep it for ready reference because we will be using it many different times as you have already seen. We directly go to those tables pick up the relevant equation and use it, cancel the irrelevant terms and whatever remains is what gives us the basis for analysis.

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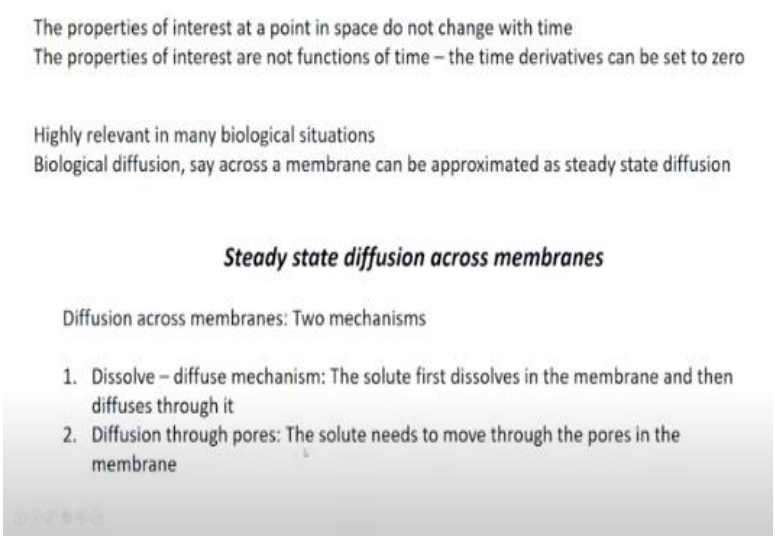

So steady state flux when steady state is when the properties of interest at a time do not change, at a point in space do not change with time and that is relevant for many biological processes. Many biological processes take place at steady state. Here we derived the steady state diffusion across membranes which is highly useful in many different cases.

So, we said that the diffusion occurs due to two mechanisms. One a dissolve diffuse mechanism and then diffusion through pores. We spent a good amount of time on the dissolve diffuse mechanism to arrive at.

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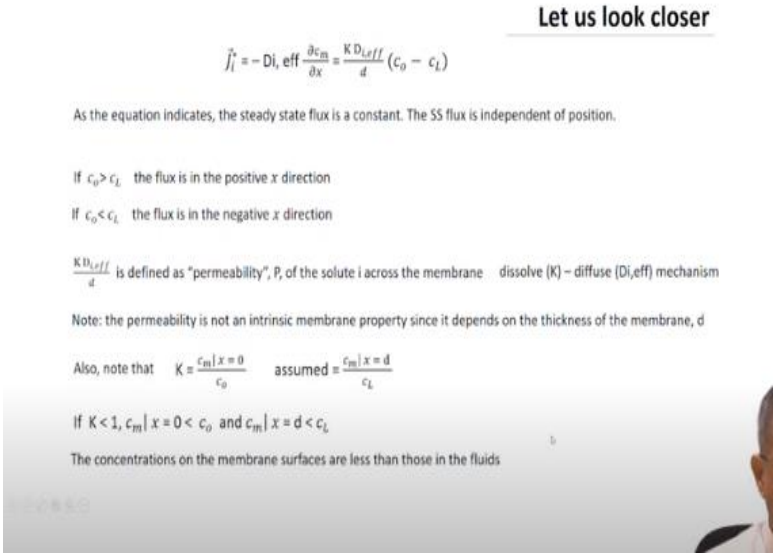

This relationship the molar flux is - $\mathbf{D_{i\ effective}}\ \frac{\partial c_m}{\partial x}$ **or** $\frac{k\, D_{i\ effective}}{d}$**(c0- cL)** which gives the flux across a thin, across a membrane, across a uniform membrane. Then we said that

$\frac{k D_{i\,effective}}{d}$, K is the partition coefficient. $D_{i\ effective}$ is the diffusion coefficient. So the dissolved diffuse mechanism divided by the thickness of the membrane(d) is the permeability.

Permeability is an important parameter for any membrane. And then we looked at some insights .

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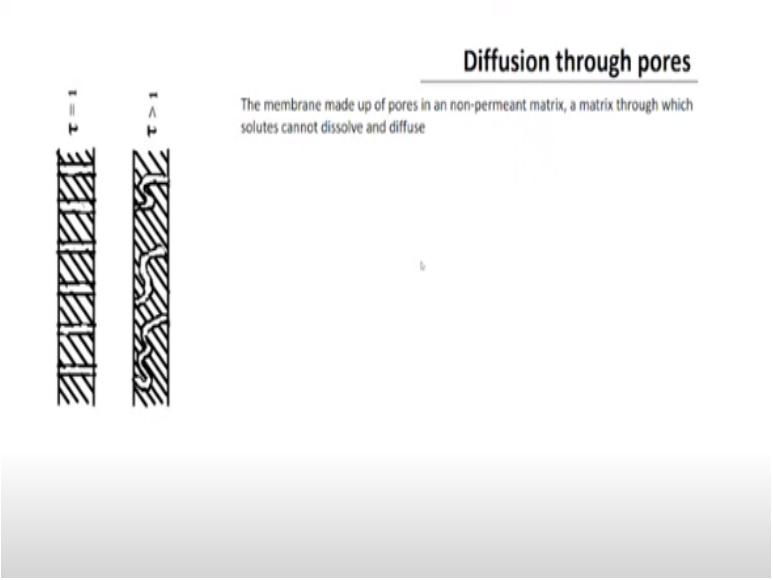

Then I directly gave you some relationships for the diffusion through pores without the derivation. I had given you a source for the derivation of these equations. We considered two cases there. One is when the pores are large enough compared to the size of the solute. Whereas, the other case was the size of the pores are comparable to the size of the solute. We had two different expressions for that.

Then we looked at a different geometry right. This was to show you how you could apply the conservation equation, equation of continuity to a cylindrical to a system with cylindrical geometry. So steady state diffusion radial diffusion across tubular walls. We had looked at a problem to understand how to use it because just application of the equation.

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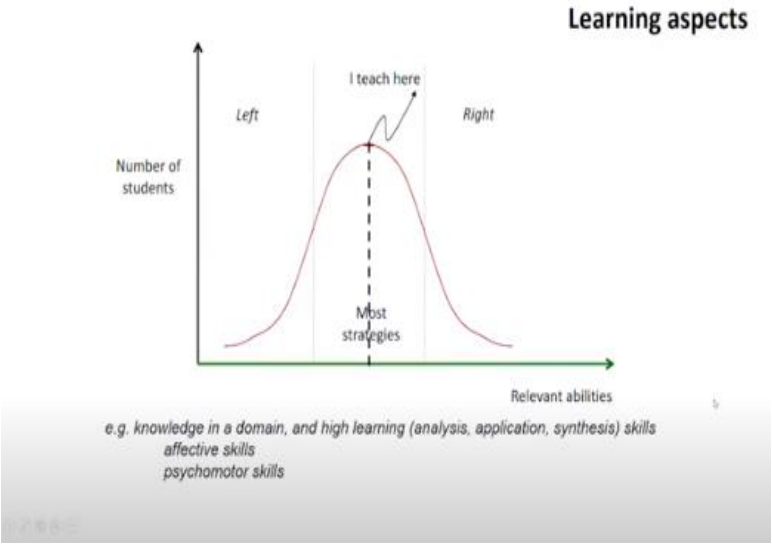

So I gave you the problem first. But before I, before that I talked about learning aspects. I said, usually there is a distribution, a normal or a Gaussian distribution in terms of relevant abilities. I typically teach in the middle, somewhere here. And if you are here, you might feel a little bored, you could probably go through it faster.

If you are here, you might feel a little lost, which means you will have to look at it a few more times. And then you should be able to get it. Because I have worked out every single step, every single mathematical step, which is usually one of the major difficulties for people here or here, sometimes even here because many textbooks do not give you the intervening steps.

Then you spend a lot of time trying to figure out how we went from one step to another. But that we obviate in this particular presentation as well as the book.

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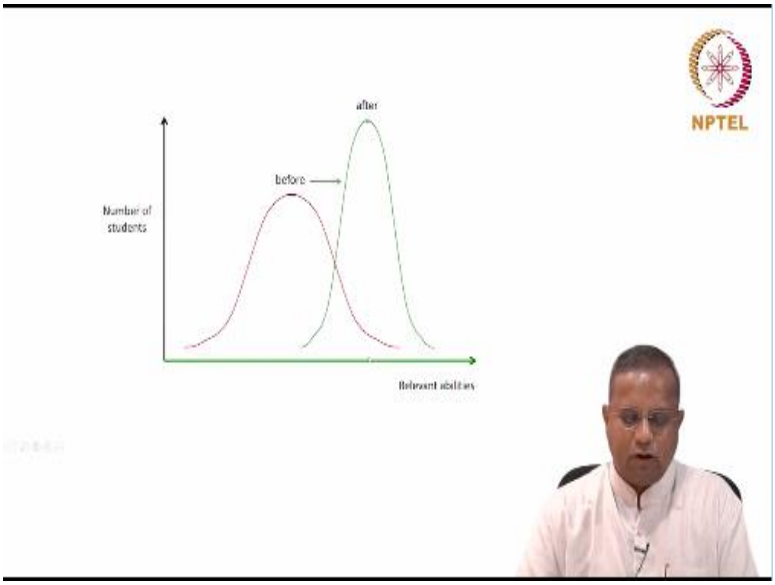

And then I talked about going from a distribution like this before the course began to a distribution that is much narrower and taller at the end of the course. This is what we are after. That is for the learning aspect.

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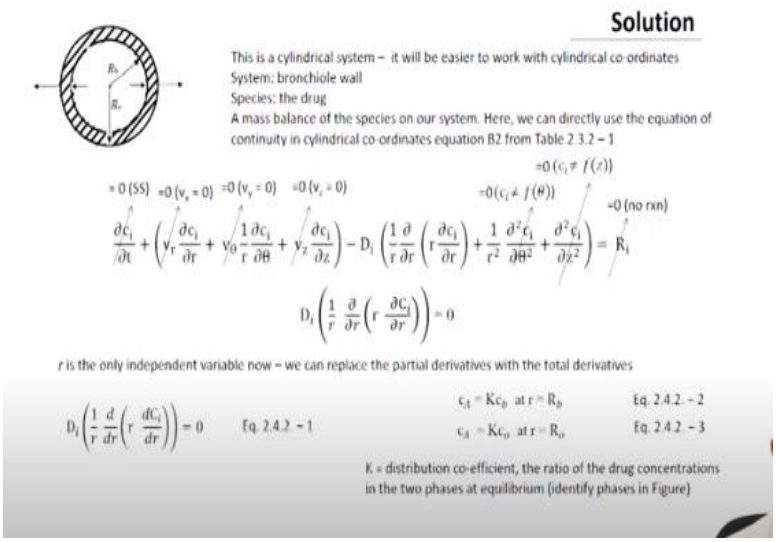

And then I showed you how to apply the equation of continuity to a cylindrical system which is again applied to a very relevant situation that of a drug diffusion across a bronchiole wall.

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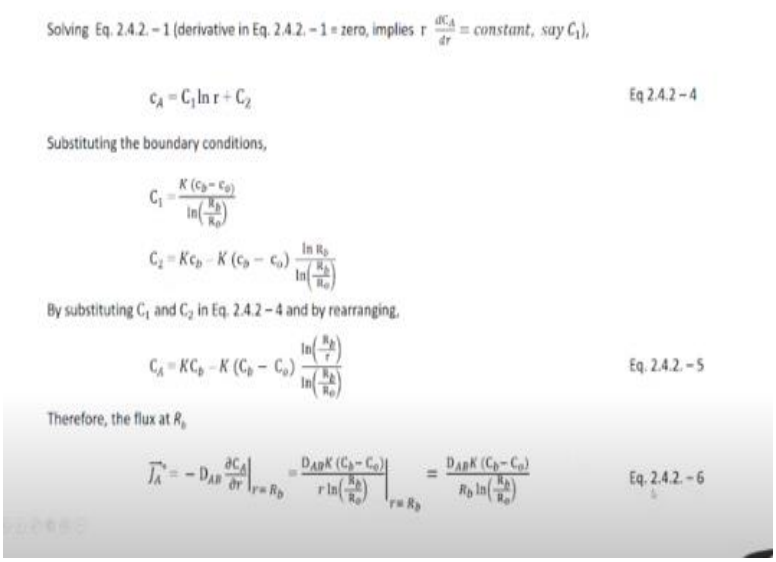

We got relationships that give us the concentration profile in the wall of the bronchiole of the drug as well as an expression for the flux at the wall. After this, I showed you the application to a spherical system.

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That was this aspect. Spherical pellets. Radial, steady state radial diffusion in spherical aspects. We had used the spherical coordinate, the equation of continuity in spherical coordinates to solve this problem.

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To improve yields of ornamental plants, certain growth factors are released from porous, spherical, ceramic pellets embedded in the soil near the roots, in a time-dependent fashion. At the surface of the pellet (r = R), the growth factor concentration in the soil is KC_0. Far from the surface, the growth factor concentration drops to zero. Develop an expression for the steady-state release rate (moles time^{-1}) of the growth factor from the pellet.

Diffusion out from a sphere, equally in all directions
Spherical geometry, thus, spherical co-ordinates

Consider a 'sphere of influence' of the growth factor as our system. Note: the roots where the growth factor is consumed are not a part of the system.
Let us do a material balance on the growth factor over the above system
We can directly use equation C2 in Table 2.3.2 – 1

$$\frac{\partial c_i}{\partial t} + \left(v_r \frac{\partial c_i}{\partial r} + v_\theta \frac{1}{r}\frac{\partial c_i}{\partial \theta} + v_\emptyset \frac{1}{r\sin\theta}\frac{\partial c_i}{\partial \emptyset}\right) - D_i\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_i}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial c_i}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 c_i}{\partial \emptyset^2}\right) = R_i$$

= 0 (SS); =0 (v_r = 0); =0 (v_θ = 0); =0 ($v_\emptyset$ = 0); =0 ($c_i \neq f(\theta)$); =0 ($c_i \neq f(\emptyset)$); =0 (no rxn)

Thus

$$D_i\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_i}{\partial r}\right)\right] = 0$$

r is the only independent variable here. Partial derivatives can be replaced with the total derivatives.

$$D_i\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dc_i}{dr}\right)\right] = 0 \qquad \text{Eq. 2.4.3. – 1}$$

And thereby we picked up how the concentration of the growth factor varies in the sphere of influence of the pellet that is releasing the growth factor.

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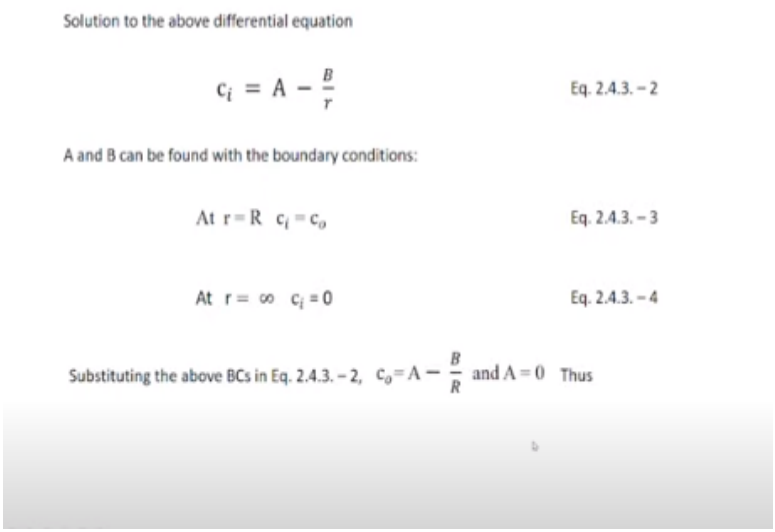

And that is what we did. I do not think I need to get into details. You can look at the details. Then, after that, we looked at steady state. Yeah. No I think I still have a reaction term.

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We took a spherical pellet and then we looked at inside the pellet. The only difference between the previous times is that the previous times there was no reaction term. And here there is a reaction term. We had looked at the case of an immobilized enzyme and the reaction occurring there and the relevant aspects.

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Let us consider an enzyme reaction for which the enzyme is immobilized on a porous spherical pellet. The pores could have a high surface area say 250 m^2g^{-1}. The pellet itself is placed in a fluid environment. Since the enzyme is immobilized inside the pores of the pellet, the transfer of substrate to the site of the immobilized enzyme through the pores, and the transport of product out of the pores are expected to play a major role in determining the process kinetics. Thus, the transport inside the pores needs to be considered rather than the transport to and from the surface of the pellet.

Derive an expression for the 'effectiveness factor', which gives a measure of how much the reaction is hindered due to immobilization.

So this is the immobilized enzyme pellet and the substrate needs to go through the various pores to reach the point of the enzyme and the product needs to move out.

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Spherical geometry – so, let us use spherical co-ordinates

System: spherical pellet
Let us do a material balance on the substrate (concentration = s) over the above system
We can directly use equation C2 in Table 2.3.2 – 1

$$\frac{\partial c_i}{\partial t} + \left(v_r \frac{\partial c_i}{\partial r} + v_\theta \frac{1}{r}\frac{\partial c_i}{\partial \theta} + v_\phi \frac{1}{r\sin\theta}\frac{\partial c_i}{\partial \phi}\right) - D_i\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_i}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial c_i}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 c_i}{\partial \phi^2}\right) = R_i$$

$= 0$ (SS); $= 0$ ($v_r = 0$); $= 0$ ($v_\theta = 0$); $= 0$ ($v_\phi = 0$); $= 0$ ($c_i \neq f(\theta)$); $= 0$ ($c_i \neq f(\phi)$)

For an enzyme catalyzed reaction, the Michaelis Menten equation is a good first approximation for the reaction rate
Also, r is the only variable. Thus, the partial derivatives can be replaced with total derivatives

$$D_{eff}\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{ds}{dr}\right)\right] = \frac{v'_{max}s}{K'_m + s}$$

' used to indicate immobilized parameters
D_{eff} = effective diffusivity

$$-D_{eff}\left[\frac{d^2s}{dr^2} + \frac{2}{r}\frac{ds}{dr}\right] = \frac{v'_{max}s}{K'_m + s}$$

Eq. 2.4.3.1 – 1

We looked at those movements, the concentration profiles of the substrate and so on so forth along with the assumption that a Michaelis Menten equation gives us the reaction rates.

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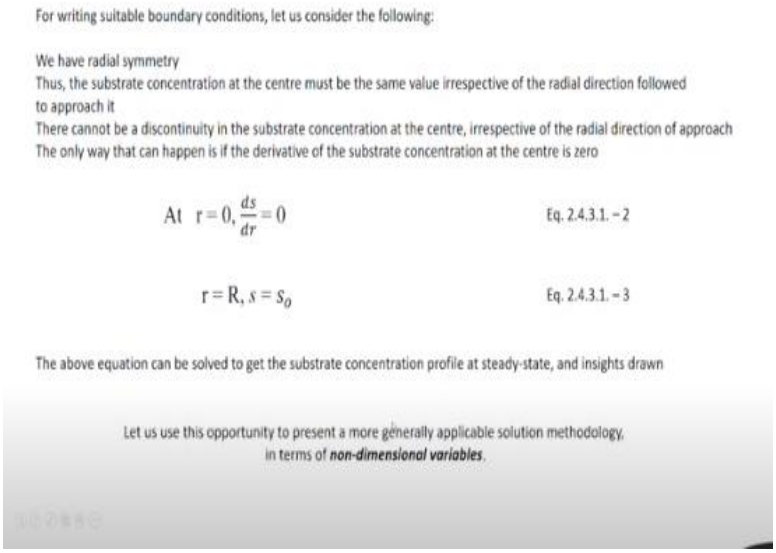

And then we looked at something called an effectiveness factor, which is what we derived as a part, which is what we have found as a part of this exercise, this problem that is.

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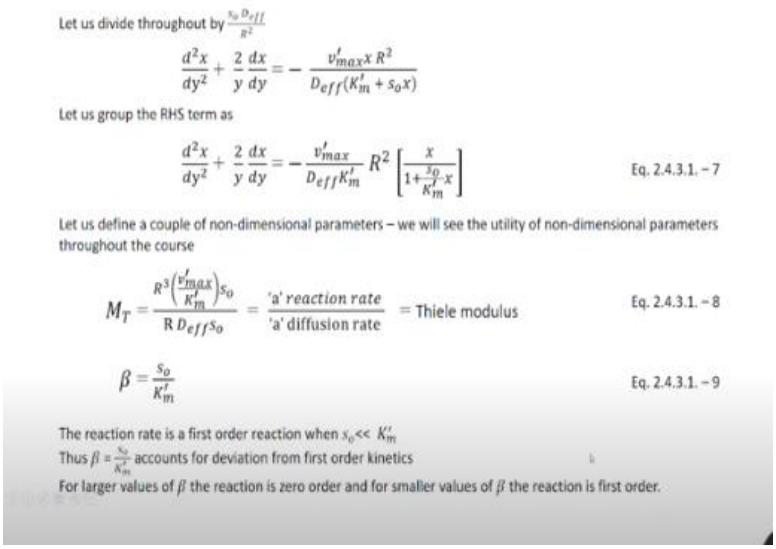

And also we looked at the use of non-dimensional variables to generalize the solution.

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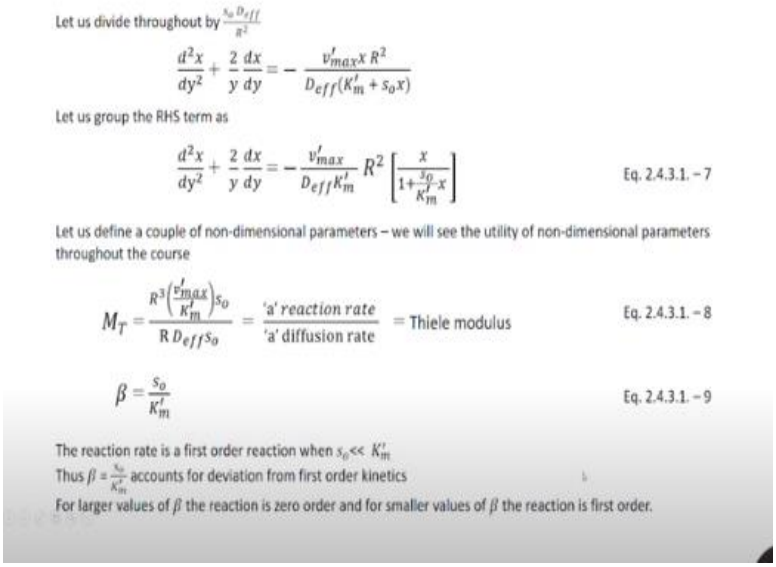

And coming to the, a Thiele modulus is also very generally used, widely used. It is nothing but the ratio of a reaction rate to a diffusion rate, which lets us compare these two rates in a system, the Thiele modulus.

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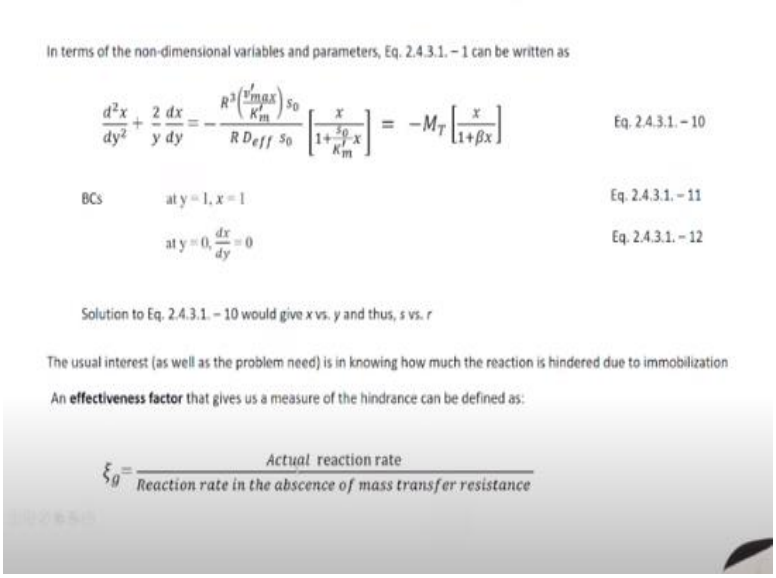

And then where are we with the effectiveness factor? Yeah, it is an actual reaction rate divided by the reaction rate in the absence of mass transfer resistance. We said that when we immobilize an enzyme we could lose the speed aspects, the kinetic aspects because of the immobilization. However, there are very many advantages to immobilization. That is why we immobilize it.

And therefore, when we immobilize it, we would like to know how much of loss is occurring. And the effectiveness factor is one of the parameters that gives us that. It is

the ratio of the actual reaction rate which is actually happening to a hypothetical reaction rate which is the reaction rate in the absence of mass transfer resistance.

For example, if there is no mass transfer resistance, then the concentration of the substrate would be the same as that in the solution throughout. So that gives us the limiting case. So that gives us a parameter by which we can assess the effectiveness of our design maybe if you are designing the immobilized enzyme pellet. And you can use it in many different ways.

And then we looked at the unsteady state case, unsteady state diffusion spherical pellets yes.

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Unsteady state is this. Yes. Unsteady state diffusion. The only difference here is you have an additional time variation term. And that term complicated the mathematics significantly. We went through all the details.

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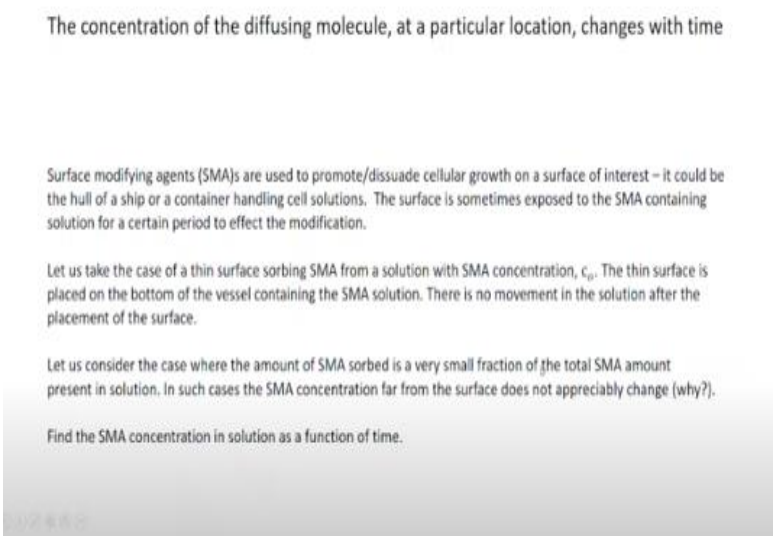

We were looking at the concentration profiles in solution of a surface modifying agent when you place a surface to be modified at the bottom and then you allow the surface modifying agent to move through the liquid to react at the surface and modify it. We had considered an appropriate system to allow us for the analysis to get the various concentration profiles of the surface modifying agent variation with time different curve for different times.

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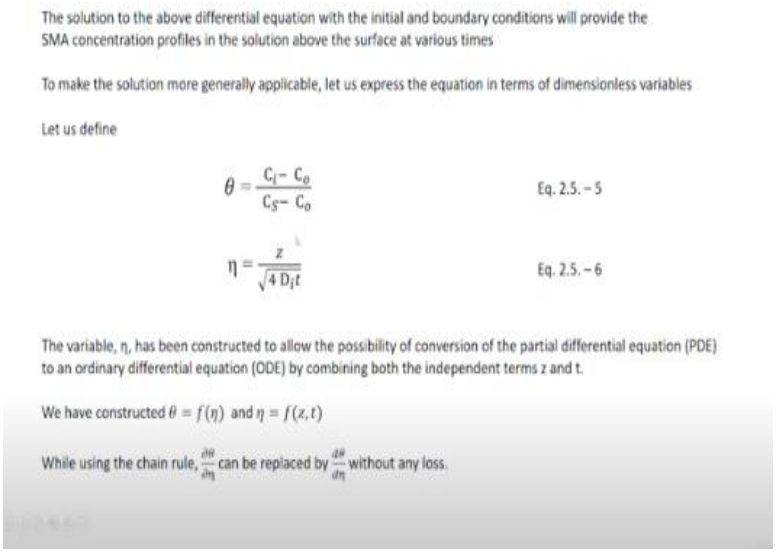

And we had also used non-dimensional variables to solve it. The solution, the analytical solution that we usually prefer is very involved. We also used non-dimensional variables. I showed you that. Let us go quickly to yeah, that was our solution which is involved.

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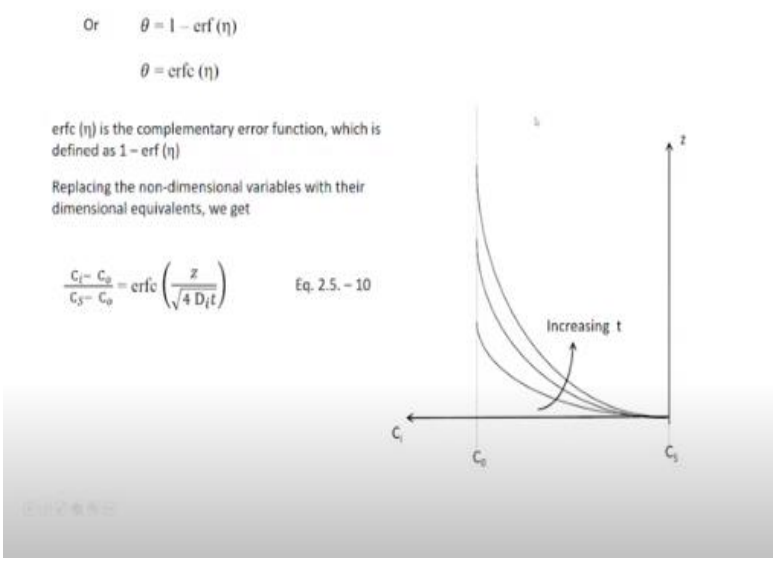

Yeah, this is if you look at this as the concentration axis and this as the distance axis in the liquid. So here it is close to 0 and then at time 1 is this. At time 2, which is greater than time 1, it is this. Time 3, which is greater than both, other two, it is this and so on so forth. So, at various different times this profile evolves, . So that is what we found.

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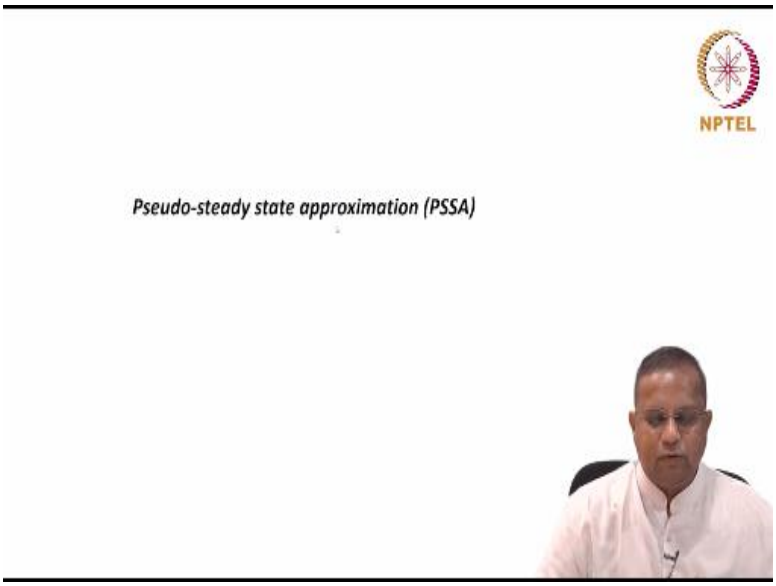

Then, we finally looked at the pseudo steady state approximation. We said when you have two processes,

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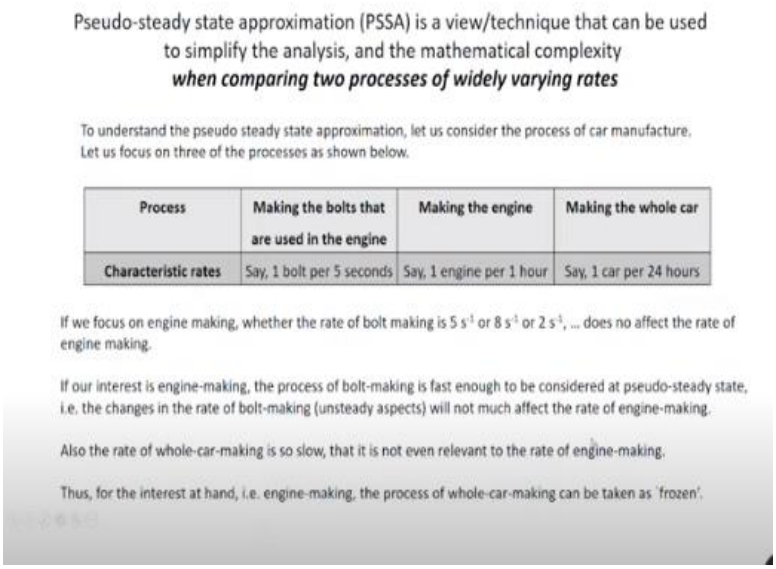

I think I should spend a little bit of time on this new concept, maybe. A pseudo steady state approximation PSSA is a view or a technique that can be used to simplify the analysis and mathematical complexity when comparing two processes of widely varying rates, . This is important, this is the only place we could use this. And then I gave you an example of bolt making and engine making.

The variation in the rate of bolt making does not impinge the rate of engine making. If our interest is in the rate of engine making, we could assume that the bolt making process is at steady state or is at pseudo steady state. It does not really matter whether it is actually at steady state or not. It is at pseudo steady state and that significantly simplifies the analysis.

We can, we do not have to consider the time variation. And that as you can see, as we have already seen, simplifies the analysis significantly.

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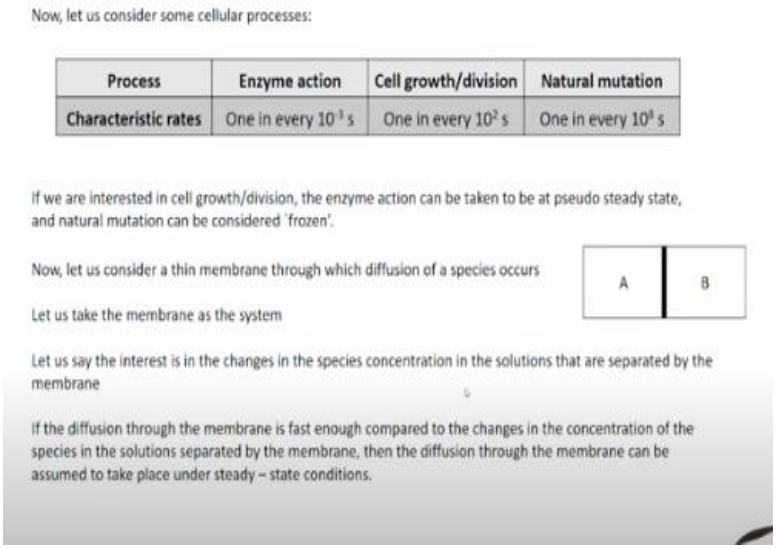

We looked at the application of that to a particular problem of determining the permeability of a coating layer to a certain model, protein albumin, . We saw the strategy of getting to the permeability is quite involved. We looked at it over two classes, . So that is what we looked at in terms of mass flux. When we begin the next class, we will start looking at momentum flux. See you then.