Transport Phenomena in Biological Systems
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Lecture-09
Shell balance approach

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Mass Flux –
Shell Balances Approach

Welcome back, let us continue, we started looking at mass flux in the previous class. We looked at some formulations for the flux itself in terms of rather fundamental quantities density, velocity concentration and let us take things further. In this class we are going to look at something called a shell balances approach to mass flux to get useful aspects from that analysis.

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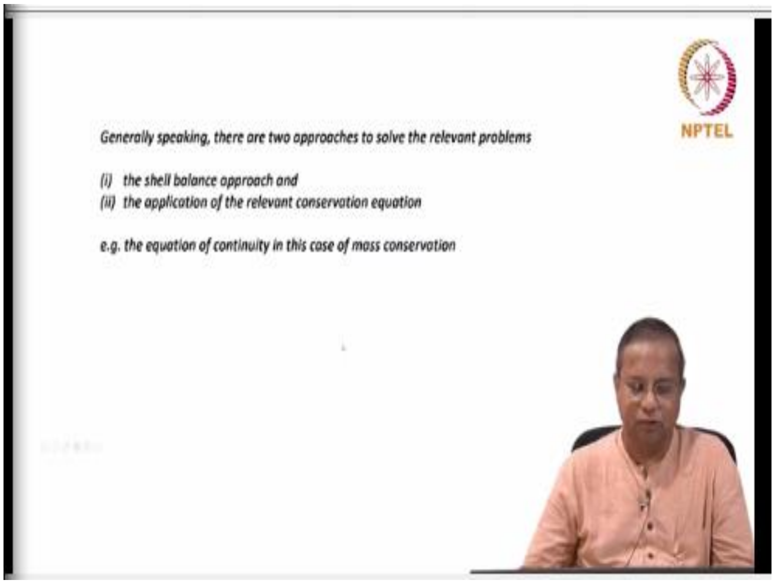

Generally speaking, there are two approaches to solve the relevant problems

(i) the shell balance approach and
(ii) the application of the relevant conservation equation

e.g. the equation of continuity in this case of mass conservation

Generally speaking, there are 2 approaches to solve these problems, the problems that involve motion of various substances which are plenty, plenty in engineering practice. There are two broad approaches, first is called the shell balance approach and second is the application of the relevant conservation equation directly. Both have good merit let us look at them and then we will talk about them.

The relevant conservation equation is nothing but the equation of continuity in the case of mass conservation. That is the only thing that we have seen so far and so I am going to look at that.

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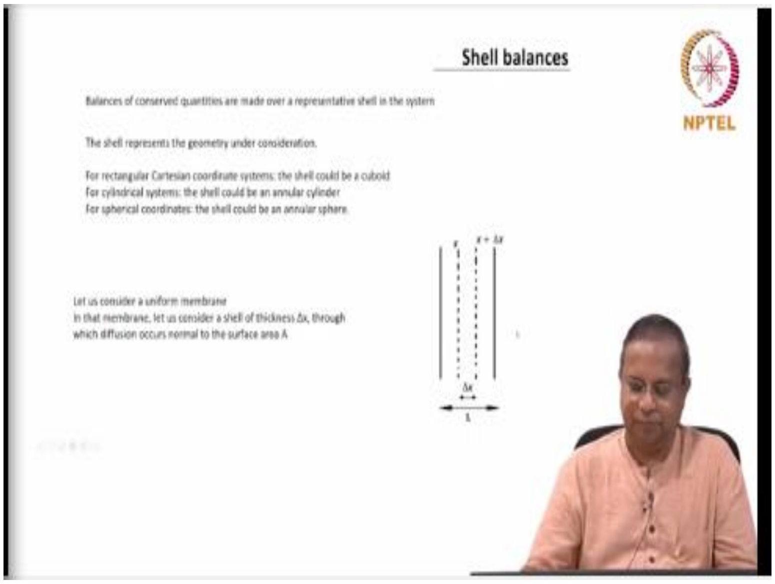

Shell balances

Balances of conserved quantities are made over a representative shell in the system

The shell represents the geometry under consideration.

For rectangular Cartesian coordinate systems: the shell could be a cuboid
For cylindrical systems: the shell could be an annular cylinder
For spherical coordinates: the shell could be an annular sphere

Let us consider a uniform membrane
In that membrane, let us consider a shell of thickness Δx, through which diffusion occurs normal to the surface area A

But first we look at the shell balance approach, what are shell balances. Look at the term, things will start falling into place. Shell balances, balances of conserved quantities are made over a representative shell in the system those are called shell balances. This representative shell what is that? The shell represents the geometry and a concentration, for rectangular Cartesian coordinate systems the shell could be a cuboid we will see this in detail next.

For cylindrical systems, the shell is an annular cylinder. You have a cylindrical system you are going to use cylindrical set of coordinates. So, the shell over which you are going to do your balances is going to be an annular cylinder. And for spherical coordinates the shell could be an annular sphere, spherical coordinates - annular sphere. **So, essentially shell is the space over which we do balances and that space is differential.**

And therefore, the variations are captured nicely when you do balances over that shell and then when you integrate you get the entire picture, it is as simple as that. It will become clearer as we go along. Now, we are going to consider a uniform membrane, we will directly jump into systems of relevance to us, a uniform membrane.

(Refer to the diagram on the video).In that membrane let us consider a shell of thickness Δx through which diffusion occurs normal to the surface area. This is the membrane, indicated by these thick lines, of thickness L. And the area is perpendicular to the plane of the motion of the species. So, the area is somewhere here, we are going to consider a shell because this is to begin with a cuboid I have just drawn with 2 dimensions here, you could extend the third dimension and consider it a cuboid.

You take a thin shell of thickness Δx, so that is represented as x here and $x + \Delta x$ here, this is very thin, I have just expanded the Δx to show you, so, that you can see it. In reality, the Δx is very, very, very small. And in three dimensions this is going to be a cuboid of the same dimensions as that of the system or the membrane but with a thin thickness.

So, that is essentially the shell and we are going to do balances over the shell, mass balances over the shell, that becomes a system.

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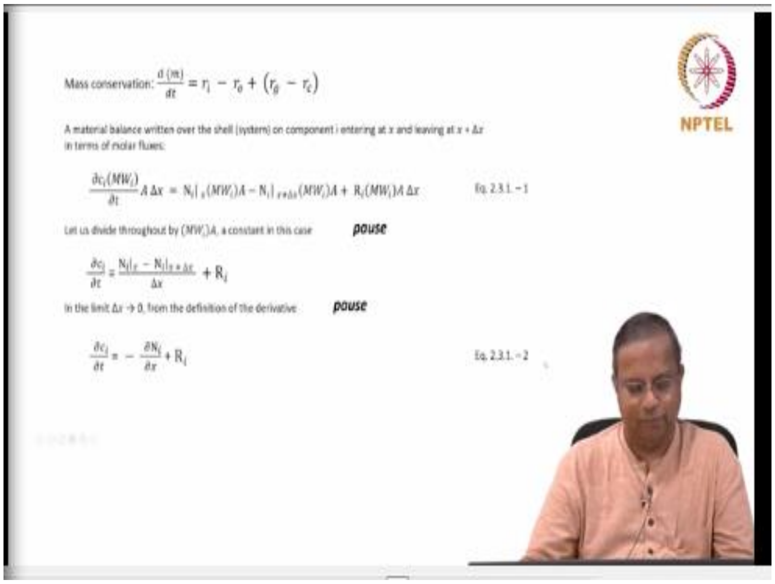

Mass conservation: $\frac{d(m)}{dt} = r_i - r_o + (r_g - r_c)$

A material balance written over the shell (system) on component i entering at x and leaving at $x + \Delta x$ in terms of molar fluxes:

$$\frac{\partial c_i (MW_i)}{\partial t} A\,\Delta x = N_i|_x (MW_i) A - N_i|_{x+\Delta x} (MW_i) A + R_i (MW_i) A\,\Delta x \qquad \text{Eq. 2.3.1.-1}$$

Let us divide throughout by $(MW_i)A$, a constant in this case **pause**

$$\frac{\partial c_i}{\partial t} = \frac{N_i|_x - N_i|_{x+\Delta x}}{\Delta x} + R_i$$

In the limit $\Delta x \to 0$, from the definition of the derivative **pause**

$$\frac{\partial c_i}{\partial t} = -\frac{\partial N_i}{\partial x} + R_i \qquad \text{Eq. 2.3.1.-2}$$

So, our mass conservation equation as you all know which can be used blindly is $\frac{dm}{dt}$ = r_i-r_o+r_g-r_c. You could consider both these together and call it the net production rate, $r_{generation}$ - $r_{consumption}$ as some sort of a net production rate. Now a material balance, if you write over the shell on the component i which is entering at x and leaving at x + Δx.

So, here is the shell you have x here, x + Δx here, the component i is entering in this direction at x and leaving at x + Δx that is the situation here. So, if you consider that in terms of the molar fluxes of i we could write this as $\frac{dm}{dt}$. So, $\frac{\partial m}{\partial t}$ you know since it could vary with time and space i have just given the more general partial derivative here.

Concentration(c_i) = moles /volume,
moles= mass(m)/molecular mass(M.W) so we get mass(m)= moles*molecular mass(M.W)
Thus, Concentration(c_i)* molecular mass(M.W) = (moles *molecular mass(M.W))/Volume = mass/volume(which is nothing but mass(m) per volume.) So, if you multiply it by volume(A. Δx) throughout, we get mass alone. (Volume= area * thickness)
Mass(m) = Concentration(c_i)* molecular mass(M.W)*Volume
Thus , we get $\frac{\partial m}{\partial t} = \frac{\partial c_i *(M.W)}{\partial t} . A$. Δx on the LHS.

So, the molar flux(N_i) of species i at x times the molecular mass(M.W) will give you the mass flux (mass flux= molar flux * molecular mass) and that is the reason for this combination, (N_i) at x times area (A) and molecular weight(M.W) minus the output rate, (N_i) at x + Δx times area (A) and molecular weight(M.W). As mass rate = mass flux*area. Multiplying mass flux with area gives mass rate.

R_G - R_C in the regular reaction rate terms, is denoted by R_i. This is in terms of moles, typically we write it in terms of moles for reaction rates. Therefore, we need to multiply it by the molecular mass(M.W) times the volume(AΔx) because this rate R_i is normalized with respect to volume. And therefore, we need to multiply by the volume to get mass per time.

$$\boldsymbol{\frac{\partial c_i}{\partial t}\,(M.W)A\,\Delta x = N_i|_x\,(M.W)A \;-\; N_i|_{x+\Delta x}\,(M.W)A \;+\; R_i\,(M.W)A\,\Delta x} \qquad \textbf{2.3.1-1}$$

Where Ri= $N_i|_x$ (M.W)A , Ro= $N_i|_{x+\Delta x}$ (M.W)A and Rg-Rc= R_i (M.W)A Δx

Each of the terms above are in terms of mass per time.

The idea here is to get mass per time for each of these terms and therefore we took whatever we had concentration per time and converted that into mass per time by multiplying by the molecular mass and the volume here($\frac{\partial c_i}{\partial t}$ (M.W)A Δx). Here we had a flux, the molar flux $\mathbf{N_i}$, we converted it into mass flux first and then mass rate by multiplying it with M.W and A respectively. And then similar thing that we did here, for R_i we did the reaction rate which is in terms of the concentration on a volumetric basis multiplied by the molecular mass to get mass on a volumetric basis. Then we multiplied it by the volume of the system, A times the Δx, the cuboidal volume. So, that each of these terms is mass per time, that is the whole point. And that is what we normally do when we write balances make a note of that, this is equation 2.3.1 - 1.

Now if we divide the equation 2.3.1-1 throughout by molecular mass(M.W) and area(A), constants present on all the terms. So, you can divide throughout, can you divide throughout and tell me what you get, pause the video here come back after you get the expression then will continue ego ahead please. And now if you divide by Δx throughout here you are left with $\frac{\partial c_i}{\partial t}$ on LHS. Here you are left with ($N_i|_x$ - $N_i|_{x+\Delta x}$ / Δx) and R_i on the RHS. Do you recall something familiar here you soon well I give you a hint plus of course only R_i remains here ok. This if you recall is nothing but the definition of a derivative when the **limit of Δx tending to 0** is taken.

$\frac{\partial c_i}{\partial t} = (\frac{Ni|x - Ni|x + \Delta x\ )}{\Delta x}) + R_i$

If you do that we get go ahead please, pause, do that and get back. If you do that you get $\frac{\partial c_i}{\partial t}$ equals minus because the definition of the derivative is (x + Δx)- x divided by Δx. Here you have just the negative of that therefore - $\frac{\partial N_i}{\partial x}$ + R_i ok, we will call this equation 2.3.1 - 2.

$$\frac{\partial c_i}{\partial t} = -\frac{\partial N_i}{\partial x} + R_i \qquad (2.3.1\text{-}2)$$

In this case, the flux N_i results only from diffusion. Thus

$$\vec{N}_i = \vec{J}_i^* = -D_i \frac{\partial c_i}{\partial x}$$

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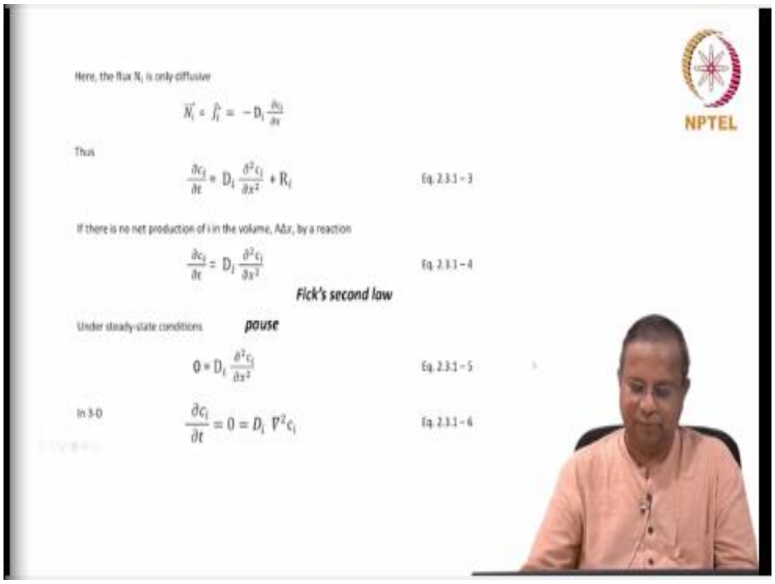


Here, the flux N_i is only diffusive

$$\vec{N}_i = \vec{J}_i^* = -D_i \frac{\partial c_i}{\partial x}$$

Thus

$$\frac{\partial c_i}{\partial t} = D_i \frac{\partial^2 c_i}{\partial x^2} + R_i \qquad \text{Eq. 2.3.1 - 3}$$

If there is no net production of i in the volume, AΔx, by a reaction

$$\frac{\partial c_i}{\partial t} = D_i \frac{\partial^2 c_i}{\partial x^2} \qquad \text{Eq. 2.3.1 - 4}$$

Fick's second law

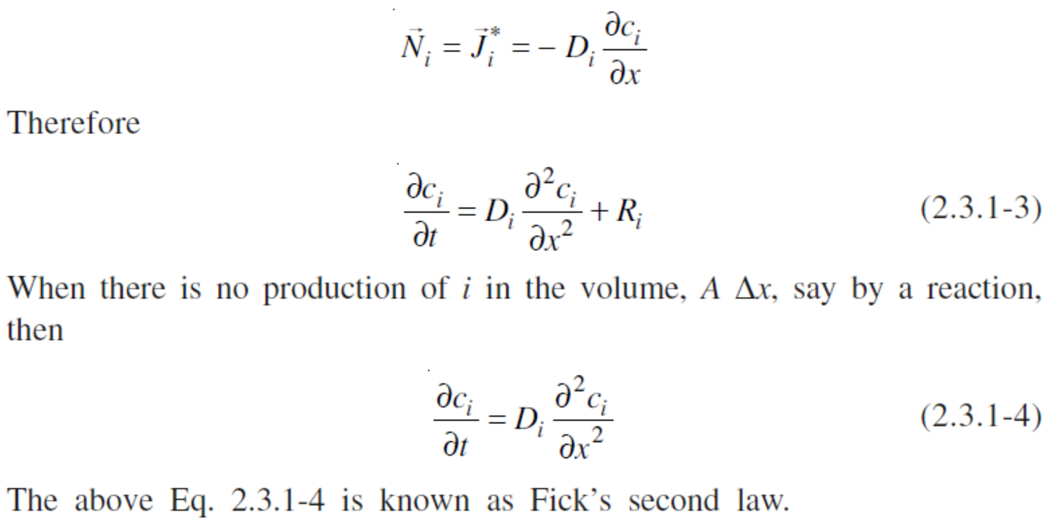
Under steady-state conditions *pause*

$$0 = D_i \frac{\partial^2 c_i}{\partial x^2} \qquad \text{Eq. 2.3.1 - 5}$$

In 3-D

$$\frac{\partial c_i}{\partial t} = 0 = D_i \nabla^2 c_i \qquad \text{Eq. 2.3.1 - 6}$$

Here the flux is purely diffusive, it is just diffusing, there is no other driving force that is causing this motion. Therefore, N_i is nothing but J_i star only the molar flux and we have an expression for molar flux in terms of Fick's first law, molar flux is - $D_i \frac{\partial c_i}{\partial X}$. Strictly speaking, it is $D_i(-\frac{\partial c_i}{\partial X})$ but by writing this we understand what we mean by - $D_i \frac{\partial c_i}{\partial X}$



$$\vec{N}_i = \vec{J}_i^* = -D_i \frac{\partial c_i}{\partial x}$$

Therefore

$$\frac{\partial c_i}{\partial t} = D_i \frac{\partial^2 c_i}{\partial x^2} + R_i \qquad (2.3.1\text{-}3)$$

When there is no production of *i* in the volume, $A\ \Delta x$, say by a reaction, then

$$\frac{\partial c_i}{\partial t} = D_i \frac{\partial^2 c_i}{\partial x^2} \qquad (2.3.1\text{-}4)$$

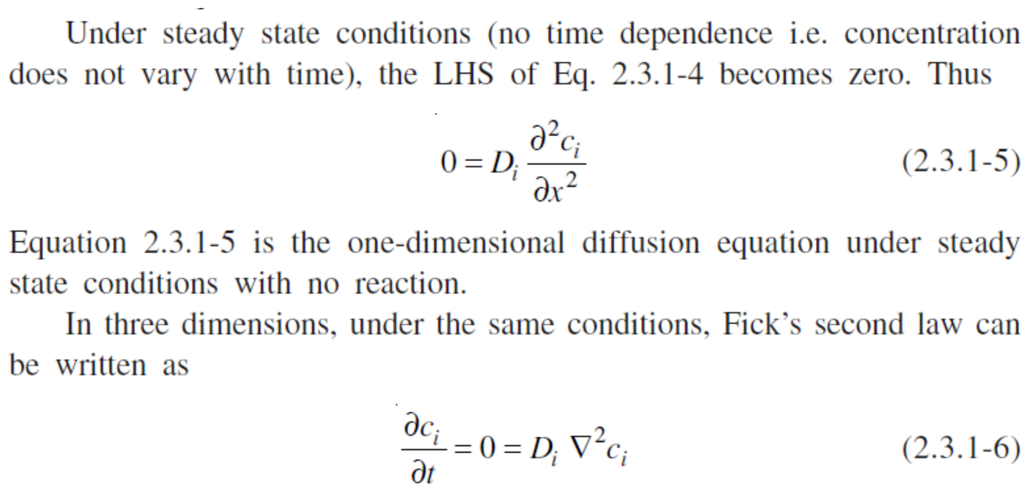
The above Eq. 2.3.1-4 is known as Fick's second law.

If you consider that there is no reaction, that term R_i disappears indicating $\frac{\partial c_i}{\partial t} = D_i \frac{\partial^2 c_i}{\partial x^2}$, we will call this 2.3.1 - 4. And this is Fick's second law, Fick's first law is the constitutive equation, the relationship between mass flux and the concentration gradient. This the variation of concentration with time on this side(LHS) and the variation of concentration with space on the RHS. So, that way it is very powerful variation with time is related to variation in space through this diffusion coefficient or diffusivity D_i.

Under steady state conditions you know what steady state the properties of interest at a point do not vary with time, which means effectively any time derivative goes to 0. So, this time derivative goes to 0 and what do you get? pause, do that and get back, yeah you would get $D_i \frac{\partial^2 c_i}{\partial x^2} = 0$. Very simple, beautiful expression, **$D_i \frac{\partial^2 c_i}{\partial x^2} = 0$ and this is equation 2.3.1 - 5.**

In three dimensions we looked at one dimension to get a physical feel of things, we can extend this very easily to three dimensions. It is going to be **$\frac{\partial c_i}{\partial t} = 0 = D_i \nabla^2 c_i$**, where

$\nabla^2 c_i = \frac{\partial^2 c_i}{\partial x^2} + \frac{\partial^2 c_i}{\partial Y^2} + \frac{\partial^2 c_i}{\partial Z^2}$ ok. So, three-dimensional variation is brought in here, so this is Fick's second law in three dimensions, equation 2.3.1 - 6 ok.



Under steady state conditions (no time dependence i.e. concentration does not vary with time), the LHS of Eq. 2.3.1-4 becomes zero. Thus

$$0 = D_i \frac{\partial^2 c_i}{\partial x^2} \qquad (2.3.1\text{-}5)$$

Equation 2.3.1-5 is the one-dimensional diffusion equation under steady state conditions with no reaction.

In three dimensions, under the same conditions, Fick's second law can be written as

$$\frac{\partial c_i}{\partial t} = 0 = D_i \nabla^2 c_i \qquad (2.3.1\text{-}6)$$

So, we will stop here we have covered quite a bit of new information here, constitutive equation, Fick's first law is an example. Then we looked at that was previous class, in this class we looked at shell balances and shell balances we wrote for membrane. Then representative shell which turns out to be a cuboidal shell in a membrane. And then we derived the Fick's second law which is a relationship between it is the time variation of concentration. And the space variation of concentration in the system ok, we will continue in the next class, see you in the next class.