Transport Phenomena in Biological Systems
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Lecture-10
Continuity Equation Approach

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Welcome back, in one of the earlier classes I said there are 2 approaches to solve these problems one was the shell balance approach that we saw in the previous class. Then this class we are going to see the conservation equation approach. The conservation equations that we have seen now is the continuity equation the mass conservation equation and we are going to apply it directly to get whatever we need.

I will tell you the reasons for doing that is much easier way of doing it although it has some limitations it could have some limitations.

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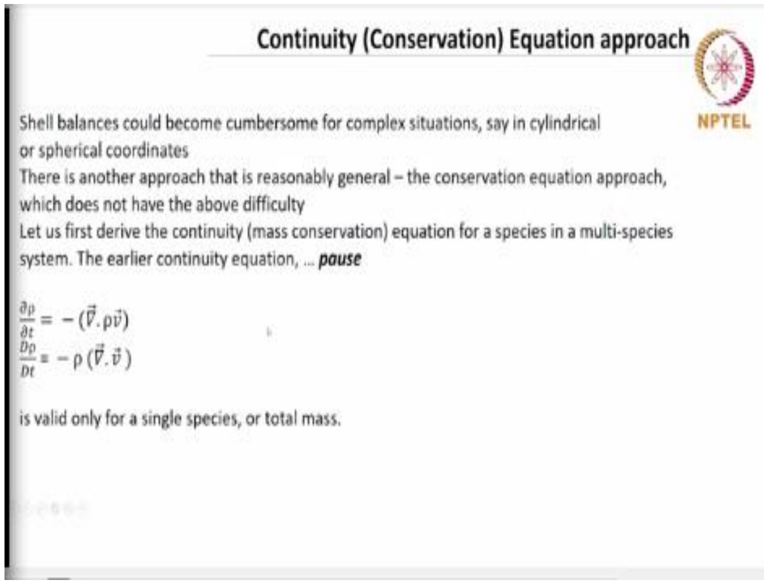

They shell balance approach is intuitive it gives you a very nice feel of what is going on, a physical feel of what is going on understanding is clear however it is a little cumbersome. The continuity equation approach overcomes that difficulty, that is the reason why we are looking at this. As I said the shell balances could become cumbersome for complex situations, here it was I took a simple case it was cuboid.

So, nice and easy dimensions to work with, are intuitive from an intuitive point of view because we are used to that. Suppose your system becomes a shellular and you will have to do balances over a differential shell with a cylindrical in shape. Then things become a little more complex, you take a spherical system, you have spheres let us say. And you take a spherical system then it will have to do balances over a spherical shell that can become even more difficult.

Let me say it could involve a lot more effort, it is not difficult but it would involve a lot more effort and for this reason or it becomes cumbersome. So, we look at this other approach which is reasonably general called the conservation equation approach. And of course this you can just apply the equation therefore it does not have that difficulty or the visualization is a lot less in this.

So, let us first derive the continuity equation or the mass conservation equation for a species in a multi species system. The earlier continuity equation that we derived was for what, you go back and check, pause the video here go back and check and let me know, why are we deriving the continuity equation again here, we have already done that. So, what is the difference between this and that, can you go back and check.

If you checked you would have found that this the earlier one was for a single species system or the total mass of multi component system. Here we are going to look at a species in a multi species system. This will make it applicable more generally and therefore we need to do this and this is different from the earlier expression and therefore we need to do this. The earlier continuity equation, this is nice to see many times therefore I am just writing both forms.

This is in terms of the derivative the regular derivative, partial derivative $\frac{\partial \rho}{\partial t} = -\nabla .(\rho\ v)$. And in terms of the substantial derivative it is - ρ times Δv nothing is constant here and so on in other words ρ is not a constant here. This is the continuity equation that we already seen, this is for a single component system or total mass.

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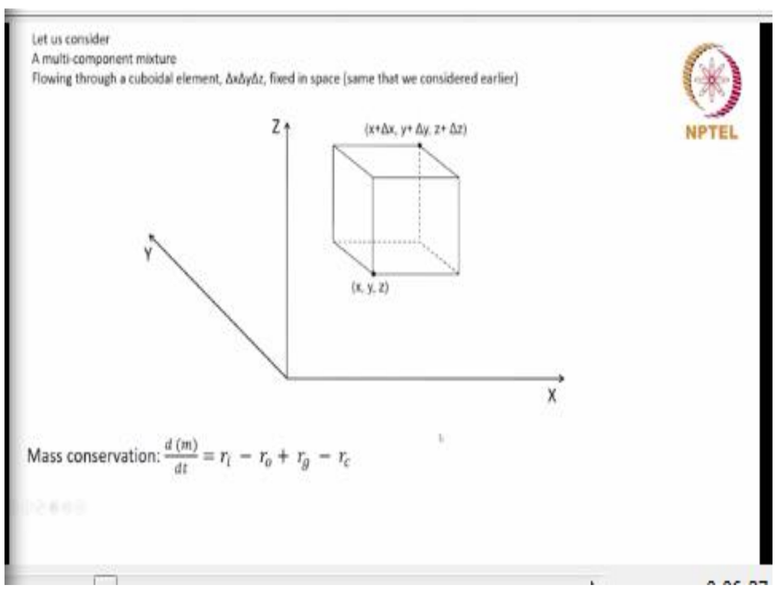

For now we are looking at a species in a multi component system. So, let us consider a multi component mixture flowing through a cuboidal element Δx Δy Δz the same system as we saw earlier fixed in space. So, it is this, you have the x coordinate here, the y coordinate here, right handed coordinate system therefore this is the z. And this is the cuboidal element of thickness Δx Δy and Δz.

And therefore this point turns out to be x + Δx, y + Δy and z + Δz here. So, this is our control volume or the system control volume fixed volume and space through which a multi component mixture is flowing in three dimensions. Enters in the x direction, it enters the face at x leaves or the face at x + Δx, y direction it enters at the face at y as in this direction.

So, it enters the face at y which is this leaves at the face y + Δy which is that and in the z direction it enters at the face at z here and leaves at a face located at z + Δz which is this. So, this is the mass conservation equation $\frac{dm}{dt}$ = you have input rate - output rate + generation rate - consumption rate. This is a single species, so you could have generation, you could have consumption through appropriate reactions that happen.

Therefore all the terms are relevant here, earlier if you recall we did not consider generation and consumption because it was a single species nothing else going to happen to it or it was the total mass even in the case of total mass, there is no generation or consumption and therefore we did not consider these 2 terms earlier.

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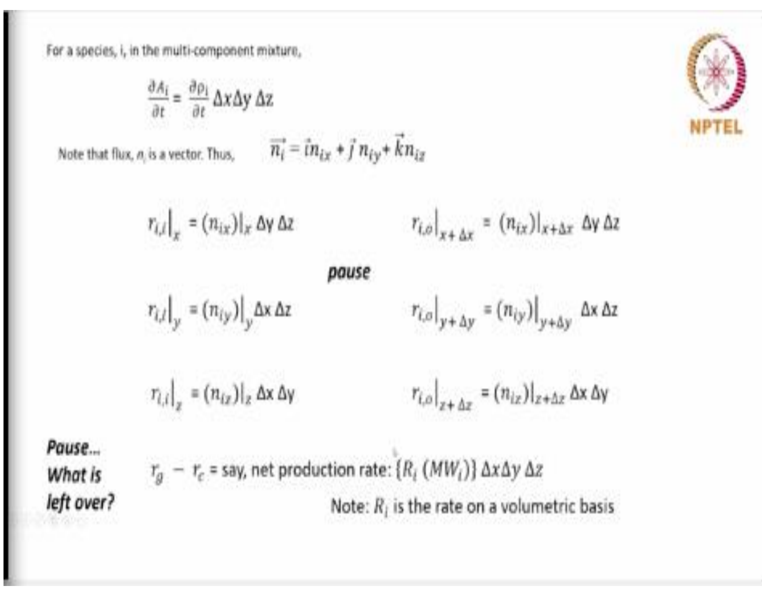

For a species i in a multi component mixture, $\frac{\partial m}{\partial t}$ which is the mass of i with respect to t, this is mass, mass is nothing but density times volume. So, density of i times the volume of the system is

Δx, Δy and Δz, it is a cuboid right. So, density times volume as mass and we have written in terms of density and volume, n is or n_i is a vector. And therefore n_i is nothing but in $_{ix}$+jn $_{iy}$+kn $_{iz}$.

So, n_{ix} is the flux in the x direction, n_{iy} is the flux in the y direction, n_{iz} is the flux in the z direction, components of the total of the flux n_i which happens to be a vector. So, input rate of i at x is nothing but the mass flux of i at x times the area because we need mass rate, flux times the area is the rate. And therefore mass flux times the area, what is the area again, this to recall, this is the x direction, this is the phase at which it enters the phase, area is nothing but $\Delta y\Delta z$ and therefore we have the flux times(n_i) $\Delta y\Delta z$.

Similarly the rate of the species i, leaving at the phase x + Δx is nothing but the flux of i in the x direction. At the phase located at x + Δx times $\Delta y\Delta z$, I hope you get the trend the way of writing this. We are looking at mass per time and we have fluxes, we have multiplied by the area to get rate.

Can you write now similar expression for the input rate at of i at y and the output rate of i at y + Δy also do that for a z . Pause the video here, write those and then compare with whatever is being talked about go ahead please. The input rate of i at the phase located at y is n $_{iy}$ the flux of i at y at the phase located at y, this is the y direction, this is the phase located at y times the area which is Δx Δz this is y direction.

Similarly the rate output from the phase located at y + Δy is n $_{iy}$ in the y direction, the flux of i in the y direction output from the phase located at y + Δy times the same area Δx Δz. And hopefully you would have also gotten the z direction which is the input rate of i at z in terms of the flux of i in the z direction at the phase located at z times the area, the z area is Δx Δy.

And similarly, for output you have output rate of i at the phase z + Δz is the flux of i in the z direction at the phase z + Δx times Δx Δy. So, we have, what are we trying to do, we are trying to mass balance we had input rate, the output rate, generation rate, consumption rate. So, we have written the terms that will contribute to the input rate here, we have written the terms that will contribute to the output rate here, what is leftover.

Go back to the equation and find out, the r_g - r_c we will consider that together here net production rate. It is nothing but the reaction rate, to the reaction rate is typically in terms of mole per volume per time. Therefore, mole per volume times the molecular mass which will give you a mass per volume per time, times the volume will give you mass per time. So, this we had done earlier and we are doing the same thing here.

We want every term in that mass balance equation here in terms of mass per time. Our measurements are in terms of other quantities or usual measurements are in terms of other quantities, moles per volume per time, and therefore we are converting it into mass per time, so this is the net production rate. Now we put all these things input, output, $r_g - r_c$ into our mass balance equation which happens to be this $\frac{dm}{dt} = r_i - r_o + r_g - r_c$ is what do you get, you get an expression.

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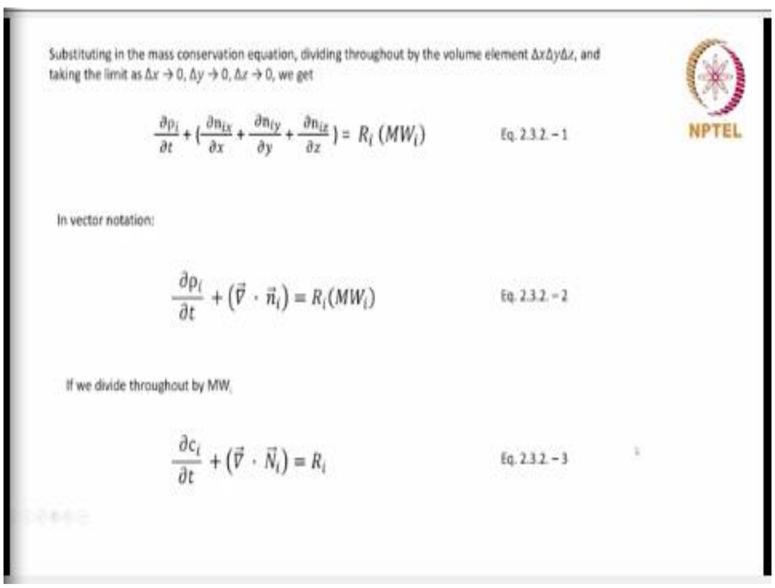

And if you divide throughout by the volume element Δx Δy Δz and take the limit as Δx tends to 0, Δy tends to 0, Δz tends to 0 you get this. We have seen the details already a couple of times, so I am not letting you work through the details, if you want you can do that to feel comfortable if you could do this. You can of course see here you know you have these various things input - output then you put that into that expression divided throughout by Δx Δy Δz.

Let us first consider a multi-component mixture. Let us take a cuboidal element, $\Delta x \Delta y \Delta z$, fixed in space (same as in Fig. 1.4.3-1) through which the multi-component mixture is flowing.

Let us apply the mass conservation principle to A, which is a species in the multi-component mixture. Recall that

$$\frac{dA}{dt} = \dot{I} - \dot{O} + \dot{P} \qquad (1.4.3\text{-}1)$$

Thus

$$\frac{\partial A}{\partial t} = \frac{\partial \rho_A}{\partial t} \Delta x \Delta y \Delta z$$

$$\dot{I}\,|_x = (n_{Ax})\,|_x\ \Delta y \Delta z$$

$$\dot{I}\,|_y = (n_{Ay})\,|_y\ \Delta x \Delta z$$

$$\dot{I}\,|_z = (n_{Az})\,|_z\ \Delta x \Delta y$$

$$\dot{O}\,|_{x+\Delta x} = (n_{Ax})\,|_{x+\Delta x}\ \Delta y \Delta z$$

$$\dot{O}\,|_{y+\Delta y} = (n_{Ay})\,|_{y+\Delta y}\ \Delta x \Delta z$$

$$\dot{O}\,|_{z+\Delta z} = (n_{Az})\,|_{z+\Delta z}\ \Delta x \Delta y$$

$$\dot{P} = r_A \Delta x \Delta y \Delta z$$

And so the terms that remain will form the expression for the derivative when the limit is taken as we saw earlier. And therefore, the mass balance equation would become

$\frac{\partial \rho_i}{\partial t}$ + $\left(\frac{\partial n_{ix}}{\partial x} + \frac{\partial n_{iy}}{\partial y} + \frac{\partial n_{iz}}{\partial z}\right) = R_i(M.W)$ **2.3.2-1** (the volumetric basis rate times the molecular mass of i)

Vectorially, vector notation helps us write things in a compact fashion we can write this as $\frac{\partial \rho_i}{\partial t}$. This is nothing but you could recall $\nabla . n_i$ you could write down the individual terms take the dot product and see that it is actually reducing down to this,

$\frac{\partial \rho_i}{\partial t} + (\nabla . n_i) = R_i\ (M.W)$ **2.3.2 - 2.**

$$\dot{P} = r_A \Delta x \Delta y \Delta z$$

Substituting the terms in Eq. 1.4.3-1, dividing throughout by the volume element $\Delta x \Delta y \Delta z$, and taking the limit as $\Delta x \to 0$, $\Delta y \to 0$, $\Delta z \to 0$, we get

$$\frac{\partial \rho_A}{\partial t} + \left(\frac{\partial n_{Ax}}{\partial x} + \frac{\partial n_{Ay}}{\partial y} + \frac{\partial n_{Az}}{\partial z} \right) = r_A \qquad (2.3.2\text{-}1)$$

In a compact form

$$\frac{\partial \rho_A}{\partial t} + (\vec{\nabla} \, . \, \vec{n}_A) = r_A \qquad (2.3.2\text{-}2)$$

Note that $\vec{n}_A = \rho_A \vec{v}_A$.

Now, if we divide throughout by the molecular mass(MW), you know density divided by the molecular mass density is mass per volume. So, mass by molecular mass will turn out to be moles, moles per volume is concentration. i.e. $\frac{\frac{\partial \rho_i}{\partial t}}{MW} = \frac{\partial c_i}{\partial t}$

So, $\frac{\partial c_i}{\partial t}$ +(∇.N_i) = R_i **2.3.2-3**

(n_i is mass flux, mass flux divided by the molecular mass is mole flux N_i).

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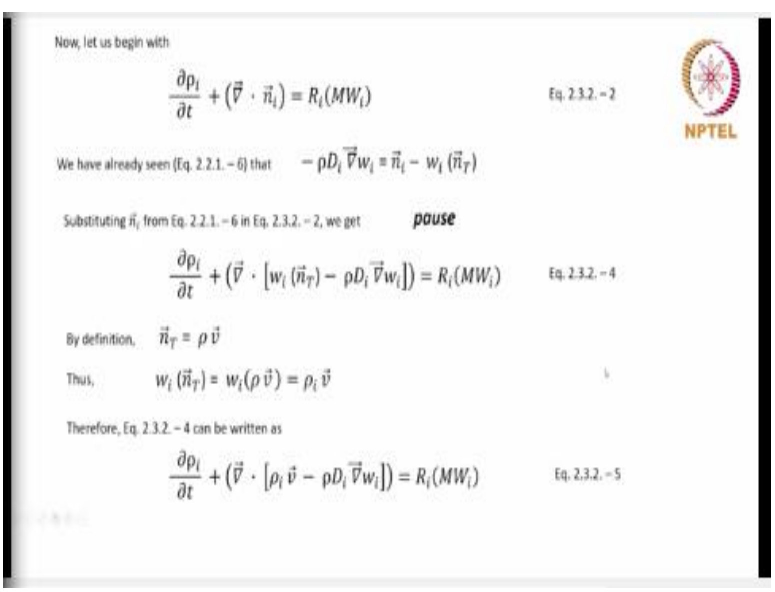

Now let us begin with this $\frac{\partial \rho_i}{\partial t}$ + **(∇.n_i) = R_i (M.W)** **2.3.2 - 2.**

We have already seen that this expression in a few classes earlier **$-\rho D_i \nabla w_i = n_i - w_i n_T$**, this is only general expression. Substituting n_i from this n_i is nothing but **$w_i n_T - \rho D_i \nabla w_i$** this if you substitute here (on equation 2.3.2-2) we are going to get what are you going to get, why do not you substitute and tell me, yeah it is a good thing to do it interactively you will pick up much more, pause the video here, go back do this substitute for n_i, from this expression on to this expression, tell me what you get, go ahead please. Hopefully you got

$$\frac{\partial \rho_i}{\partial t} + \nabla.(w_i n_T - \rho D_i \nabla w_i) = R_i(MW_i) \qquad \textbf{2.3.2 - 4}$$

And by definition n_T is nothing but ρ v alright that is flux is nothing but density times velocity, that is what we saw in the very beginning. Therefore **$w_i n_T$** this term as **$w_i (\rho v)$** and w_i is the mass fraction, ρ is the total density. Therefore, total density times mass fraction is the density of i, so this becomes $\rho_i v$. And therefore, this equation can be written as

$$\frac{\partial \rho_i}{\partial t} + \nabla. [(\rho_i v) - \rho D_i \nabla w_i] = R_i(MW_i) \qquad \textbf{2.3.2 - 5.}$$

We are doing all this to set things up, so it is nice the way it is falling into place. We are deriving the equation the continuity equation that can be directly applied to solve problems. So, we are trying to do it as gently as possible, so that this would be applicable to a wide variety of situations.

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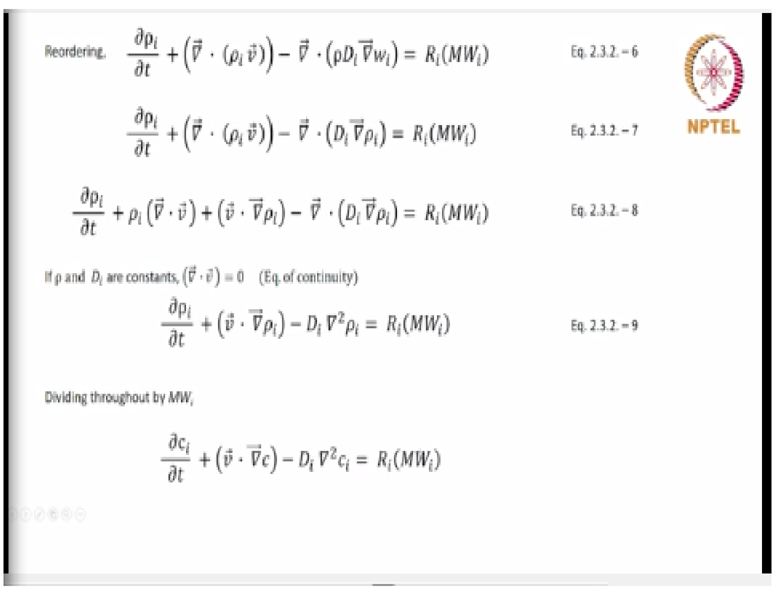

If you reorder this equation you know take the various terms you know the side, this is $\nabla.\rho_i$ times v, ρ_i is not a constant here. And therefore this is product of 2 functions, so we are taking the derivative in three dimensions therefore it is first function derivative of the second function + second function to the derivative of the first function and so on will turn out here.

And therefore we get that is the next step I have just split it up here

$$\frac{\partial\rho_i}{\partial t} + \boldsymbol{\nabla}.(\rho_i v) - \boldsymbol{\nabla}.(\rho D_i \boldsymbol{\nabla}) w_i = R_i (MW_i) \qquad 2.3.2\text{-}6$$

I have just expand just taking the derivative explicitly. These were together earlier I have separated out the terms. And here you could write this as

$$\frac{\partial\rho_i}{\partial t} + \boldsymbol{\nabla}.(\rho_i v) - \boldsymbol{\nabla}.(D_i \boldsymbol{\nabla} \rho_i) = R_i (MW_i) \qquad 2.3.2\text{-}7$$

As $\rho.\, w_i = \rho_i$

And now I am expanding, this is the product of 2 functions as I mentioned earlier they were derivative would be first function ρ_i times the derivative of the second function + the second function v times the derivative of the first function essentially split this up, the rest remain the same.

$$\boldsymbol{\frac{\partial\rho_i}{\partial t} + \rho i\, \nabla.(v) + v\, \nabla.(\rho_i) - \nabla.(D_i \nabla \rho_i) = R_i (MW_i)} \qquad \mathbf{2.3.2\text{-}8}$$

And now if we impose the condition till here it is very general we did not assume anything. Now if we impose the condition that the total density and the diffusivity of i are constants which is applicable in a wide variety of cases. If the density is a constant then we know that the equation of continuity reduces to $(\boldsymbol{\nabla}.v) = 0$ right this we already seen. So, if ρ and D_i are constants, this term will drop out $\boldsymbol{\nabla}\, v = 0$. Therefore this equation reduces to under these conditions.

Now we have conditions ρ and D_i are constants and $(\boldsymbol{\nabla}.v) = 0$

$$\boldsymbol{\frac{\partial\rho_i}{\partial t} + v.\nabla.\rho_i - D_i\ \nabla^2.\, \rho i = R_i(MW_i)} \qquad \mathbf{2.3.2 - 9.}$$

$\left(\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$. If you are uncomfortable with it, just go and check the appendix in the book, it would give you how those things come about.

And now if we divide throughout by the molecular mass, we get this density divided by the molecular mass is concentration. **(Video Starts: 20:46)** Let us get just write here can take care of this little later. **(Video Ends: 21:19)** So, we are dividing by the molecular mass, so that term should not be there and this equation 2.3.2 - 10, let me go to the full screen mode.

$$\frac{\partial c_i}{\partial t} + (v.\nabla c) - D_i\ \nabla^2 .\, c = R_i \qquad \textbf{2.3.2 - 10.}$$

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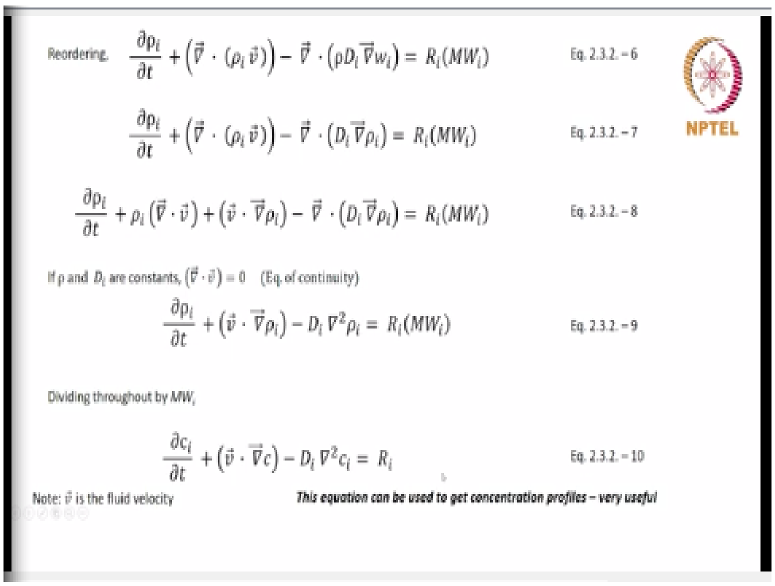

This equation can be use to get concentration profiles and that turns out to be very useful as you will realize as we go through the various examples and you work out the various exercises. So, this equation is applicable if the **density and the diffusivity are constants**, this equation is applicable in general, so remember this, here of course the v is the fluid velocity.

So, here I have a set of tables which give you first in the equation of continuity for a species i in a multi component mixture. In general terms and when c and D_i are constant or ρ and D_i are constant both are the same. And c and D_i are constant it reduces to this easier to use in many different situations. So, the general case is ai which is a little difficult to use because it is in terms of the molar fluxes difficult to measure. Whereas here this is in terms of c and diffusivity and velocities which are much easier to measure.

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Cylindrical coordinates:

$$\frac{\partial c_i}{\partial t} + \left(\frac{1}{r}\frac{\partial}{\partial r}(rN_{ir}) + \frac{1}{r}\frac{\partial N_{i\theta}}{\partial \theta} + \frac{\partial N_{iz}}{\partial z}\right) = R_i \qquad \text{(B1)}$$

When c and D_i are constant,

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

(B2)

So, that is what the table consists of first for a rectangular coordinates then cylindrical coordinates, conversion has happened non trivial conversion is happened from rectangular to cylindrical.

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Spherical coordinates:

$$\frac{\partial c_i}{\partial t} + \left(\frac{1}{r^2}\frac{\partial}{\partial r}(r^2N_{ir}) + \frac{1}{r\sin\theta}\frac{\partial}{\partial \theta}(N_{i\theta}\sin\theta) + \frac{1}{r\sin\theta}\frac{\partial N_{i\phi}}{\partial \phi}\right) = R_i \qquad \text{(C1)}$$

When c and D_i are constant,

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

(C2)

And then in spherical coordinates and as mentioned earlier I would like you to make a copy either a hard copy or a soft copy of table 2.3.2 - 1 which is in these three tables consisting of equations A1, A2, B1, B2 and C1, C2 . And keep it aside at a place where you can easily refer to, we are going to use these equations very often.

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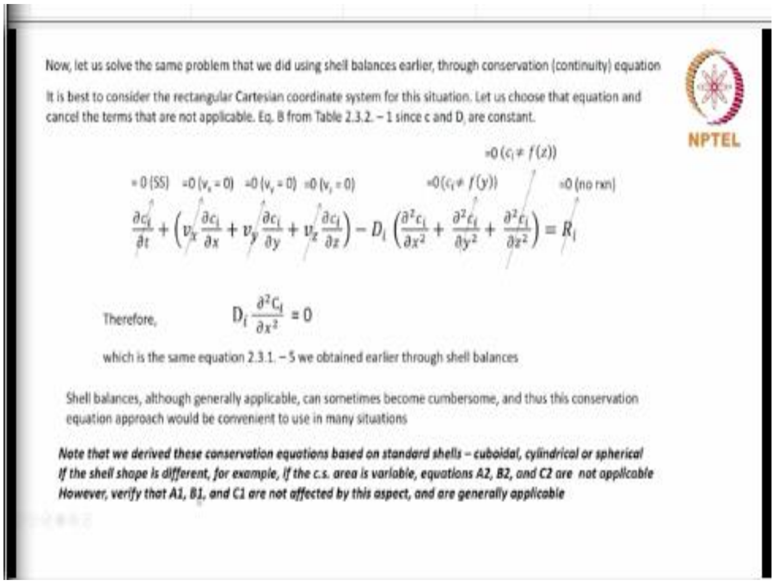

Now let us solve the same problem that we did using shell balances earlier we are remember shell balance is we had written at representative shell or we had considered as a representative shell. We had written our material balance over the representative shell and come up with useful expressions Earlier the problem that we did with the shell balance method was the diffusion of species i through a membrane which again has various applications it could be a shell membrane it could be various other membranes that we use and biological engineering.

So, whatever we did using shell balances let us do using the conservation equation, you will see that it happens in one step. So, we will consider the Cartesian coordinate system because this happens to be the system that best fits the geometry of the membrane. And let us choose that equation and cancel the terms that are not applicable. In this case when we consider C or ρ and D to be constants then we could use equation B from table 2.3.2 - 1 which is this.

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Table 2.3.2. – 1
The equation of continuity for a species, say i, in a multi-component mixture

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Rectangular coordinates:

$$\frac{\partial c_i}{\partial t} + \left(\frac{\partial N_{ix}}{\partial x} + \frac{\partial N_{iy}}{\partial y} + \frac{\partial N_{iz}}{\partial z}\right) = R_i \qquad \text{(A1)}$$

When c and D_i are constant,

$$\frac{\partial c_i}{\partial t} + \left(v_x \frac{\partial c_i}{\partial x} + v_y \frac{\partial c_i}{\partial y} + v_z \frac{\partial c_i}{\partial z}\right) - D_i\left(\frac{\partial^2 c_i}{\partial x^2} + \frac{\partial^2 c_i}{\partial y^2} + \frac{\partial^2 c_i}{\partial z^2}\right) = R_i \qquad \text{(A2)}$$

Refer the above figure:

Yeah, I think it is A2, I need to convert it to A2. So, we are going to choose equation A2 from here because it is rectangular coordinates which fits the geometry c and D_i are constants. Therefore this equation can directly be used this is much easier to use. So, this is the equation here $\frac{\partial c_i}{\partial t}$ and this is the velocity times the concentration gradient and this is the second order term here and the reaction rate term here.

Now you see how easy it becomes, it is steady state and therefore the time derivatives are set to 0. There is no convective or stirring bulk motion and only in the case of bulk motion will these velocities come into being. Therefore we can cancel this there is no velocity component in the x direction, there is no velocity component in the y direction, there is no bulk velocity component in the z direction.

There is no equivalent of the whole liquid moving, it is only the species that is moving in the liquid. That movement is taken care of in the diffusive terms and there is no bulk motion here the liquid is stationary or the system is stationary right. So, all these terms go to 0 and here again the motion is only in the x direction therefore there is no movement in the y direction. Because the concentration does not vary with y, y is in this direction, the concentration does not vary with y.

Here again x equal to 0 because the concentration is not a function and the z direction and there is no reaction that is taking place therefore this goes to 0. So, in one single step just by taking the comprehensive equation, cutting out the various terms that are not applicable, you do not have to remember this, just write down from the table. And in one step we got this equation that we derived through shell balance over various different steps in the previous case.

So, that is the ease of working with this, although there is some caution that you need to exercise here when using this. So, we got this equation which is the same equation that we got earlier through shell balances $\mathbf{D_i}\,\boldsymbol{\frac{\partial^2 c_i}{\partial x^2} = 0}$. Now we come to the caution, shell balances although generally applicable can sometimes become cumbersome and thus this conservation equation approach would be convenient to use in many situations, that is the reason why we got into this.

The below equation for binary components:

$$\overset{=0\ (SS)}{\cancel{\frac{\partial c_A}{\partial t}}} + \left(v_x \overset{=0\ (v_x=0)}{\cancel{\frac{\partial c_A}{\partial x}}} + v_y \overset{=0\ (v_y=0)}{\cancel{\frac{\partial c_A}{\partial y}}} + v_z \overset{=0\ (v_z=0)}{\cancel{\frac{\partial c_A}{\partial z}}} \right) - D_{AB}\left(\frac{\partial^2 c_A}{\partial x^2} + \overset{=0\ (c_A \neq f(y))}{\cancel{\frac{\partial^2 c_A}{\partial y^2}}} + \overset{=0\ (c_A \neq f(z))}{\cancel{\frac{\partial^2 c_A}{\partial z^2}}} \right) = \overset{=0\ (\text{no } rxn)}{\cancel{R_A}}$$

Hence

$$D_{AB}\frac{\partial^2 C_A}{\partial x^2} = 0$$

However, note that we derive these conservation equations based on standard shells, cuboidal shells, cylindrical shells, spherical shells. If the shell shape happens to be different, for example if we have a cone. The cone there is a gradual change in the cross sectional area, there could be various situations where the area changes. For example if the cross section area is variable.

Equation A2, B2, C2 are not applicable you know that those constants c, D_{AB} we derived by taking the area to be a constant if you go back and check. You would have implicitly assumed that the area does not vary there, and we cancel the areas. And if that is not applicable, those equations will not be applicable. So, be very careful whenever you deal with variable area you cannot use A2, B2, C2, you can use A1, B1, C1 they are not based on the area, that is what is mentioned here. However verify that A1, B1 and C1 you are asked to verify are not affected by this aspect and are generally applicable. Go back check this convince yourself that this is indeed the case or understand that this is indeed the case, if you are not able to understand get back to me I will talk to you on a one on one basis through email. That is what we have here, we had derived the conservation or we have shown the conservation equation approach to solve problems to get concentration profiles which are important in many cases. To do that we first derived the continuity equation for a single species in a multi component mixture to make it generally applicable, that is what we did in this class. Let us stop here, we will continue in the next class, see you.

The below equation are for binary systems.

Rectangular coordinates

$$\frac{\partial c_A}{\partial t} + \left(\frac{\partial N_{Ax}}{\partial x} + \frac{\partial N_{Ay}}{\partial y} + \frac{\partial N_{Az}}{\partial z} \right) = R_A \qquad \text{(A1)}$$

When c and D_{AB} are constant

$$\frac{\partial c_A}{\partial t} + \left(v_x \frac{\partial c_A}{\partial x} + v_y \frac{\partial c_A}{\partial y} + v_z \frac{\partial c_A}{\partial z} \right) - D_{AB} \left(\frac{\partial^2 c_A}{\partial x^2} + \frac{\partial^2 c_A}{\partial y^2} + \frac{\partial^2 c_A}{\partial z^2} \right) = R_A \qquad \text{(A2)}$$

Cylindrical coordinates

$$\frac{\partial c_A}{\partial t} + \left(\frac{1}{r} \frac{\partial}{\partial r}(r N_{Ar}) + \frac{1}{r} \frac{\partial N_{A\theta}}{\partial \theta} + \frac{\partial N_{Az}}{\partial z} \right) = R_A \qquad \text{(B1)}$$

When c and D_{AB} are constant

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$$\begin{aligned} &\frac{\partial c_A}{\partial t} + \left(v_r \frac{\partial c_A}{\partial r} + v_\theta \frac{1}{r} \frac{\partial c_A}{\partial \theta} + v_z \frac{\partial c_A}{\partial z} \right) \\ &- D_{AB} \left(\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial c_A}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 c_A}{\partial \theta^2} + \frac{\partial^2 c_A}{\partial z^2} \right) = R_A \end{aligned} \qquad \text{(B2)}$$

Spherical coordinates

$$\frac{\partial c_A}{\partial t} + \left(\frac{1}{r^2} \frac{\partial}{\partial r}(r^2 N_{Ar}) + \frac{1}{r \sin\theta} \frac{\partial}{\partial \theta}(N_{A\theta} \sin\theta) + \frac{1}{r \sin\theta} \frac{\partial N_{A\phi}}{\partial \phi} \right) = R_A \qquad \text{(C1)}$$

When c and D_{AB} are constant

$$\begin{aligned} &\frac{\partial c_A}{\partial t} + \left(v_r \frac{\partial c_A}{\partial r} + v_\theta \frac{1}{r} \frac{\partial c_A}{\partial \theta} + v_\phi \frac{1}{r \sin\theta} \frac{\partial c_A}{\partial \phi} \right) \\ &- D_{AB} \left(\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial c_A}{\partial r} \right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial c_A}{\partial \theta} \right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2 c_A}{\partial \phi^2} \right) = R_A \end{aligned} \qquad \text{(C2)}$$