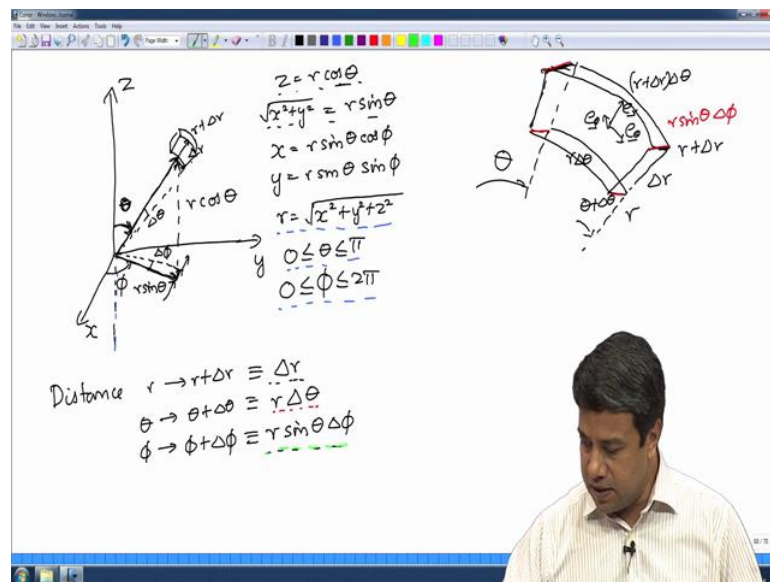


Transport Processes I: Heat and Mass Transfer
Prof. V. Kumaran
Department of Chemical Engineering
Indian Institute of Science, Bangalore

Lecture - 48
Mass and energy balance equations in spherical co-ordinates

In the previous lecture, I was deriving for you the balance equation in a spherical coordinate system. I told you earlier in a spherical coordinate system is used when you want to solve problems in which the boundaries have spherical symmetry. In those cases you would like the boundary to be a surface of constant coordinate and one of the surfaces in a spherical coordinate system is of course, at a constant distance from the origin you have a spherical shell as the boundary, the distance of every point on that from the origin is a constant and therefore, one would prefer to choose the distance from the origin as one of the coordinates and that is what is written as the radial coordinate over here the distance from the origin.

(Refer Slide Time: 01:13)



You need two other coordinates and these two are angles; the angle from the z axis any arbitrary axis can be chosen as the z axis depending upon the symmetry of the problem. The angle from the z axis is what is called theta, so theta is equal to 0 is the plus z axis. When you go through an angle of pi, you reach the minus z axis. So, theta is equal to pi is the minus z axis and theta varies from 0 to pi and phi goes from 0 to 2 pi because phi

is the angle made by the projection of the radius vector onto the x y plane, that projection makes an angle phi with respect to the x axis.

So, therefore, the projection is given by $r \sin \theta$ and the z axis is given by $r \cos \theta$ therefore, x is $r \sin \theta \cos \phi$ and y is equal to $r \sin \theta \sin \phi$. In this case, you choose a coordinate system in which the surfaces or surfaces of constant coordinate. So, there has to be one surface at r and one surface at r plus delta r, one surface at theta, the other surface at theta plus delta theta, one surface at phi and the other surface at phi plus delta phi. Along the r direction, if you increment by a small distance delta r; the actual distance moved is delta r itself.

In the theta direction, if you increment the angle theta by a small distance delta theta; the actual distance moved is r times delta theta and in the phi direction, if you increment the angle moved by a small increment delta phi, the actual distance moved is the radius times delta phi; radius in this case is r sin theta of the projection onto the x axis.

So, therefore, for this case you get r sin theta times delta phi which means that the surface areas of this are also functions of position. The surface at r is equal to the distance in the theta direction, times the difference in the phi direction and that does vary input radius because the surface area of a spherical shell is going to depend upon the distance from the center.

(Refer Slide Time: 03:19)

Surface areas:

- Surface at $r = (r \Delta \theta)(r \sin \theta \Delta \phi)$
- Surface at $r + \Delta r = ((r + \Delta r) \Delta \theta)((r + \Delta r) \sin \theta \Delta \phi)$
- Surface at $\theta = (\Delta r)(r \sin \theta \Delta \phi)$
- Surface at $\theta + \Delta \theta = (\Delta r)(r \sin(\theta + \Delta \theta) \Delta \phi)$
- Surface at $\phi = (\Delta r)(r \Delta \theta)$
- Surface at $\phi + \Delta \phi = (\Delta r)(r \Delta \theta)$
- Volume $= (\Delta r)(r \Delta \theta)(r \sin \theta \Delta \phi)$

(Change in mass) = (Mass in) - (Mass out) + Accumulation

Flux = $\underline{u} \cdot \underline{c} + \underline{j}$

$\underline{u} = u_r \underline{e}_r + u_\theta \underline{e}_\theta + u_\phi \underline{e}_\phi$

The diagram shows a small 3D volume element in spherical coordinates, bounded by surfaces of constant r, theta, and phi. The element is a spherical shell segment with dimensions Delta r, r Delta theta, and r sin theta Delta phi. The unit vectors e_r, e_theta, and e_phi are shown at the corners of the element.

The surface that theta is equal to the distance moved in the r direction; times the distance moved in the phi direction, that is the surface area or the surface at the location theta.

Similarly, at theta plus delta theta and then you have two surfaces at phi and phi plus delta phi. The total volume is the increments in all three directions, the distances in all three directions and using these surfaces for this differential volume we will write down the balance equations.

(Refer Slide Time: 04:14)

$$\begin{aligned}
 & [C(r, \theta, \phi, t + \Delta t) - C(r, \theta, \phi, t)] \Delta r (r \Delta \theta) (r \sin \theta \Delta \phi) \\
 &= (u_r C + j_r) \Big|_r (r \Delta \theta) (r \sin \theta \Delta \phi) \Delta t - (u_r C + j_r) \Big|_{r+\Delta r} (r+\Delta r) \Delta \theta (r+\Delta r) \sin \theta \Delta \phi \Delta t \\
 &+ (u_\theta C + j_\theta) \Big|_\theta (\Delta r) (r \sin \theta \Delta \phi) \Delta t - (u_\theta C + j_\theta) \Big|_{\theta+\Delta \theta} (\Delta r) (r \sin(\theta+\Delta \theta)) \Delta t \\
 &+ (u_\phi C + j_\phi) \Big|_\phi \Delta r (r \Delta \theta) \Delta t - (u_\phi C + j_\phi) \Big|_{\phi+\Delta \phi} \Delta r (r \Delta \theta) \Delta t \\
 &+ S \Delta r (r \Delta \theta) (r \sin \theta \Delta \phi) \Delta t \\
 & \frac{C(r, \theta, \phi, t + \Delta t) - C(r, \theta, \phi, t)}{\Delta t} = \\
 & \frac{1}{(\Delta r) (r \Delta \theta) (r \sin \theta \Delta \phi)} \left[(u_r C + j_r) \Big|_r r^2 \sin \theta \Delta \theta \Delta \phi - (u_r C + j_r) \Big|_{r+\Delta r} (r+\Delta r)^2 \sin \theta \Delta \theta \Delta \phi \right. \\
 & \left. + (u_\theta C + j_\theta) \Big|_\theta \Delta r r \sin \theta \Delta \phi - (u_\theta C + j_\theta) \Big|_{\theta+\Delta \theta} \Delta r r \sin(\theta+\Delta \theta) \Delta \phi \right. \\
 & \left. + (u_\phi C + j_\phi) \Big|_\phi \Delta r r \Delta \theta - (u_\phi C + j_\phi) \Big|_{\phi+\Delta \phi} \Delta r r \Delta \theta \right]
 \end{aligned}$$

So I written down here, the change in concentration at time delta t, times the volume is equal to the flux in the r direction at r that is what is coming in, the flux in the r direction; at r times the surface area of the surface perpendicular to that direction which is basically the increment in the theta direction time increment in the phi direction minus what goes out at r plus delta r times, the distance in the theta direction times the distance in the phi direction is the surface area and all of these have to be multiplied by delta t to get the change in mass.

Similarly, in the theta direction; at theta the flux has to be multiplied by the surface area, the distance in the r direction times the distance in the phi direction and similarly a theta plus delta theta and similarly at phi and phi plus delta phi. We had taken this and we had divided throughout by the volume times the time and we had got an equation of this form.

(Refer Slide Time: 05:37)

$$\frac{c(r, \theta, \phi, t + \Delta t) - c(r, \theta, \phi, t)}{\Delta t} = \frac{1}{r^2 \Delta r} \left[(u_r c + j_r) \Big|_{r-\Delta r}^{r+\Delta r} - (u_r c + j_r) \Big|_{r+\Delta r}^{r+\Delta r} \right] + \frac{1}{r \sin \theta \Delta \theta} \left[(u_\theta c + j_\theta) \Big|_{\theta-\Delta \theta}^{\theta+\Delta \theta} - (u_\theta c + j_\theta) \Big|_{\theta+\Delta \theta}^{\theta+\Delta \theta} \right] + \frac{1}{r \sin \theta \Delta \phi} \left[(u_\phi c + j_\phi) \Big|_{\phi-\Delta \phi}^{\phi+\Delta \phi} - (u_\phi c + j_\phi) \Big|_{\phi+\Delta \phi}^{\phi+\Delta \phi} \right]$$

$$\frac{\partial c}{\partial t} = -\frac{1}{r^2} \frac{\partial}{\partial r} [r^2 (u_r c + j_r)] - \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} [\sin \theta (u_\theta c + j_\theta)] - \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} (u_\phi c + j_\phi)$$

$$\frac{\partial c}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 u_r c) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta u_\theta c) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} (u_\phi c) = -\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 j_r) - \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta j_\theta) - \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} (j_\phi)$$

$$\frac{\partial c}{\partial t} + \nabla \cdot (u c) = -\nabla \cdot j$$

Now I will simplify this equation; the left side is as it is, keep the left side as it is. On the right hand side, if you look at the first term here I can cancel out the increments theta and sin theta delta phi because these do not vary as r varies, sin theta does not change as theta plus r varies and delta theta and delta phi do not change.

So, those I can cancel out and I will get if r times; r square minus whole square. I cancelled out sin theta, delta theta and delta phi; these do not change as I am varying r. The second term, I can cancel out delta r, so that the delta r does not change as theta changed and I can also cancelled out this delta phi here; delta phi can be cancelled out and then I have a factor of r here and this r once again it is not changing the theta changes; however, sin theta is changing therefore, I cannot just cancel out the sin theta terms.

So, if I do that I will get plus 1 by r sin theta, delta theta into u theta c plus j theta at theta times sin theta minus u theta c plus j theta; at theta plus delta theta sin of theta plus delta theta and on the final term on the left here, as you verify r does not change, delta r does not change, delta theta does not change. Therefore, I can cancel out all of these delta r; r delta theta delta r and r delta theta.

So, I will get into u phi c plus j phi at phi minus u phi c plus j phi, at phi plus delta phi. So, that is the difference equation simplified and now I take the limit delta t, delta r, delta theta, delta phi going to 0 and the differential equation you will get will be partial c by

partial t. I have u r c plus j r at r minus u r c plus j r at r plus delta r times r square. So, this is equal to minus 1 over r square; d by d r of r square into u r c plus j r. If it had been the value at r plus delta r minus the value at r I would have got a positive sign, this is the value at r minus the value at r plus delta r; so I have a negative sign here.

The second term is minus 1 over r sin theta d by d theta of I have a sin theta within the brackets times u theta c plus j theta and the last term I have plus 1 over r sin theta, delta by delta phi of u phi c plus j phi; this should also be with a negative sign. So, these are the three terms that I will get slightly more complicated differential operator. The reason for that is because those surface areas are changing with radius that is what gave you these terms over here the r square and r plus delta r square, the mass transport is equal to the flux times the surface area and as the surface area changes, you have to take that also into account to find out the total rate at which mass is being transported.

Once again I can take the convection terms to the left and the diffusion terms to the right; partial c by partial t plus 1 by r square; d by d r of r square c u r plus 1 by r sin theta; d by d t theta of sin theta, c u theta plus 1 by r sin theta; partial of c u phi by partial phi convection terms on the left, the diffusion terms on the right. If you recall, we had written the same equation in vector notation as partial c by partial t plus del dot u c is equal to minus del dot j. This equation has the same form as the concentration equation Cartesian coordinates.

(Refer Slide Time: 13:11)

The slide contains the following mathematical derivations:

$$\nabla \cdot \mathbf{j} = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 j_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta j_\theta) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} (j_\phi)$$

$$\nabla \cdot (u c) = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 c u_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta c u_\theta) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} (c u_\phi)$$

$$j_x = -D \frac{\partial c}{\partial x} \quad j_y = -D \frac{\partial c}{\partial y} \quad j_z = -D \frac{\partial c}{\partial z}$$

$$j_r = -D \frac{\partial c}{\partial r} \quad j_\theta = -D \frac{1}{r} \frac{\partial c}{\partial \theta} \quad j_\phi = -D \frac{1}{r \sin \theta} \frac{\partial c}{\partial \phi}$$

$$\frac{\partial c}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 c u_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta c u_\theta) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} (c u_\phi)$$

$$= D \left[\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial c}{\partial r}) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \frac{\partial c}{\partial \theta}) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 c}{\partial \phi^2} \right]$$

$$\frac{\partial c}{\partial t} + \nabla \cdot (u c) = D \nabla^2 c$$

If I want to define the divergence operator; give the divergence operator $\text{del} \cdot \mathbf{j}$ in this case is equal to $\frac{1}{r^2} \frac{d}{dr} (r^2 j_r) + \frac{1}{r \sin \theta} \frac{d}{d\theta} (\sin \theta j_\theta) + \frac{1}{r \sin \theta} \frac{d}{d\phi} (j_\phi \sin \theta)$ by this is the divergence of the flux vector, if you define it this way and similarly for the velocity times concentration for the convective flux, you get the same relation and this $\text{del} \cdot \mathbf{u} c$ is to find as; note that as I expected, this divergence operator has dimensions of 1 over length, each term in this divergence operator has dimensions of 1 over length because it is a divergence; it is one derivative with respect to spatial position.

Now this flux can be written once again in a spherical coordinate system, in a Cartesian coordinate system if you recall this was quite easy; $\text{div} \mathbf{j} = \frac{\partial j_x}{\partial x} + \frac{\partial j_y}{\partial y} + \frac{\partial j_z}{\partial z}$ in the Cartesian coordinate system. In a spherical coordinate system, it will not be just derivatives with respect to the angles because the derivative with respect to an angle does not have dimensions of inverse of length whereas it should expect all terms in the flux to be a diffusion coefficient terms a derivative with respect to position.

So, you actually take the actual distance moved, so therefore, j_r will be equal to $-\text{D} \frac{\partial c}{\partial r}$ because the actual distance moved this Δr when you go from r to $r + \Delta r$, the actual distance moved is Δr . The flux in the θ direction is going to be equal to $-\text{D} \frac{\partial c}{\partial \theta}$, when you go a small distance in the θ a small increment in the θ direction from θ to $\theta + \Delta \theta$, the distance moved is $r \Delta \theta$ therefore, you will get $\frac{1}{r} \frac{\partial c}{\partial \theta}$.

Similarly, in the ϕ direction when I move a small distance; when I change the ϕ angle by from ϕ to $\phi + \Delta \phi$, the distance moved is actually $r \sin \theta \Delta \phi$ as I showed you the distance moved is $r \sin \theta \Delta \phi$ because the length of the projection is $r \sin \theta$ that times the angle. So, I will get $-\text{D} \frac{\partial c}{\partial \phi}$ and these expressions I can insert into the differential equation on the right side. So, on the left side I had $\frac{\partial c}{\partial t} + \text{div}(\mathbf{u} c)$, on the right side I had minus the divergence of the flux. So, I have the $-\frac{1}{r^2} \frac{d}{dr} (r^2 j_r)$ into $-\text{D} \frac{\partial c}{\partial r}$; that is j_r and minus the second term is $\frac{1}{r \sin \theta} \frac{d}{d\theta} (\sin \theta j_\theta)$ into j_θ which is $-\text{D} \frac{\partial c}{\partial \theta}$ and the third term is $\frac{1}{r \sin \theta} \frac{d}{d\phi} (j_\phi \sin \theta)$ into j_ϕ which is $-\text{D} \frac{\partial c}{\partial \phi}$.

theta, d by d phi of j phi which is given by this minus D by sin theta, r sin theta partial c by partial phi.

You can simplify each of these terms, if you assume that the diffusion coefficient is independent of position So, this first term just becomes equal to I take the D out; the minus and minus cancels and I will get D into 1 by r square d by d r of r square times d c by d r minus, I have a d by r here, if I have taken the D out and they canceled the negative sign, so I will get a plus here this D has come out over here and I can take this r outside, I get 1 over r square sin theta, if sin theta partial c by partial theta and once again I take the D out on the last term; I get a plus sign here and 1 over r square sin square theta comes out; sin squared theta. So, remove this and this term becomes partial square c by partial phi square.

So, this is the right side simplified it by just inserting the expression for the fluxes and once again if you compare it with the equation partial c by partial t plus del dot u c is equal to D del square c; this gives me the expression for the Laplacian operator.

(Refer Slide Time: 21:03)

The image shows a series of handwritten mathematical derivations on a whiteboard background. The equations are as follows:

$$\nabla^2 c = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial c}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial c}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 c}{\partial \phi^2}$$

$$\nabla(u \cdot c) = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 u_r c) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta u_\theta c) + \frac{1}{r \sin \theta} \frac{\partial (u_\phi c)}{\partial \phi}$$

$$j = -D \nabla c = -D \left[\frac{\partial c}{\partial r} e_r + \frac{1}{r} \frac{\partial c}{\partial \theta} e_\theta + \frac{1}{r \sin \theta} \frac{\partial c}{\partial \phi} e_\phi \right]$$

$$\frac{\partial c}{\partial t} + \nabla(u \cdot c) = D \nabla^2 c + S$$

$$\frac{\partial c}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 u_r c) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta u_\theta c) + \frac{1}{r \sin \theta} \frac{\partial (u_\phi c)}{\partial \phi} = D \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial c}{\partial r} \right) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial c}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 c}{\partial \phi^2} \right] + S$$

In a spherical coordinate system; del square is equal to 1 by r square d by d r, that is the Laplacian of the concentration; del dot u c is equal to 1 by r square d by d r of r square u c r and the equation for the gradient, j is equal to minus D grade c is equal to minus D into partial c by partial r plus sorry with these definitions I can write the conservation equation as partial c by partial t plus. So, the equation when written in this vector

notation looks the same, only thing is of the definitions of these; the Laplacian here the divergence here and this gradient here, these have changed in this spherical coordinate system.

So, this is the conservation equation in the spherical coordinate system. So, if I write it again for you partial c by partial t plus; so that is the conservation equation in a Cartesian coordinate system; seems a little complicated, but the procedure for deriving this is exactly the same as a Cartesian coordinate system. You have to identify what are the three coordinates, what are the surfaces of constant coordinate, what are the distances moved along the three directions when these coordinates are incremented by a small amount.

Construct a differential volume whose surfaces are surfaces of constant coordinate, identify the surface area of each surface there will be six surfaces in three dimensions and where the surface area of each surface; the total volume, change in mass is equal to mass in minus mass out plus sources, take the limit as the increment in each coordinate goes to 0; you will get a differential equation. One has to be careful when the surface area depends upon the coordinate, in that case you cannot just cancel the coordinates themselves because the surface area is varying as the coordinate changes, for where did you do that correctly, you will get the correct differential equation; from that you can get back what are the definitions of the divergence, the gradient and the Laplacian in this coordinate system.

So, I have shown you how to get balance equations in Cartesian in a cylindrical; cylindrical is slightly complicated procedures exactly the same. Next we will look at how to solve these balance equations; in limiting cases that convection is dominant, the diffusion is dominant. First when diffusion is dominant, if you recall the diffusion term is the Laplacian of the concentration field. So when diffusion is dominant, the Laplacian of the concentration field is just equal to the sources. So, the procedures for solution basically reduce to procedures solving the Laplacian.

Convection dominated regime, this you would expect to be 0. You can neglect diffusion, but I showed you in the last lecture even when convection is dominant, diffusion will be important near surfaces. We have to identify the length scale of the region near the surface where convection is important and then find out what is the concentration field

within that region. We will start looking at diffusion dominated flows in the next lecture, where we can neglect the convective terms.

So, that we will start in the next lecture, solution of the Laplacian equation in most cases just is done by separation of variables. I have shown you previously how to do separation of variables in the Cartesian coordinate in one direction. In three directions, the procedure is very similar; I had shown you how to do it in a cylindrical coordinate system. In this series of lectures, I will show you how to do it in a spherical coordinate system and physically what do those separation of variables solutions physically mean and then we will go on to convection dominated flows, where we will use boundary layer theory to solve for the concentration field in ten regions near surfaces where diffusion and convection are comparable. So, we will start solving problems; diffusion dominated flows in the next lecture, I will see you then.