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

Lecture – 45
Mass and energy balance equations in Cartesian co-ordinates

Welcome to our continuing discussion on fundamentals of transport processes. In the previous few lectures, we have been looking at shell balances and how to use these to get conservation equations for the concentration or the temperature field these conservation equations containing the flux entering and leaving the differential volume and then we substitute for the flux using the constitutive relations. The Fourier's law for heat conduction or the Fick's law for diffusion to get an unsteady diffusion equation for that particular configuration, we have looked at a specific configurations one is a flux surface where we used a Cartesian coordinate system. Surface which has a cylindrical boundary like a pipe for example, where we had used a cylindrical coordinate system and done a similar balance equation, the form of the differential operator in that balance equation was slightly more complicated than a Cartesian coordinate system because these were curved surfaces and we had also looked at a spherical coordinate system, where the surfaces of constant coordinate are spherical shells.

In this lecture I will start deriving conservation equations for a general differential volume where there could be variations in all three spatial directions as well as in time. I will start with the Cartesian coordinate system and get a balance equation that includes both convection and diffusion. For a given coordinate system, if you get the balance equation then for specific applications you can solve that balance equation in order to determine the temperature, the concentration of the velocity fields.

So, we will derive general balance equations which have variations in three spatial dimensions as well as in time and we will do that here first for the Cartesian coordinate system and then we will do it for the spherical coordinate system. I will leave it to you for an assignment to do the same thing for a cylindrical coordinate system and once we have derived those balance equations, we will then see how to solve them in limiting cases such as diffusion dominated flows and convection dominated transport problems.

So, we start balance equation.

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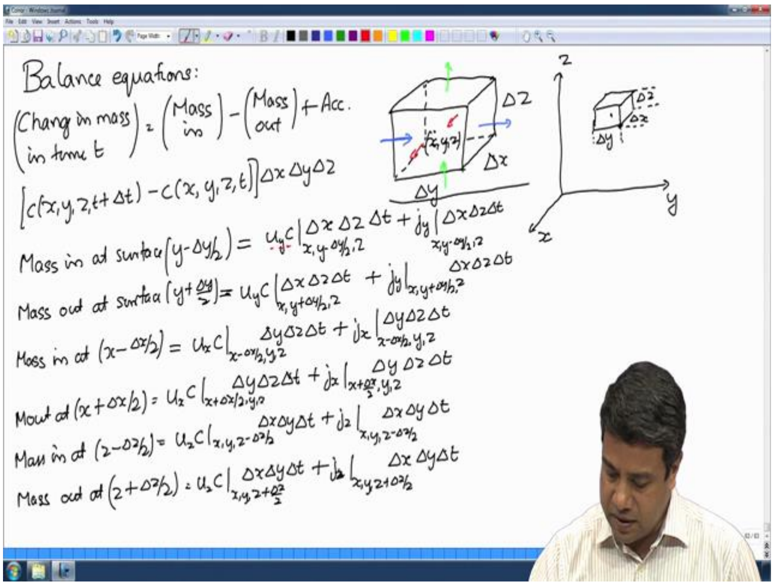

First in a Cartesian coordinate system we have to choose a differential volume whose surfaces are surfaces of constant coordinate. So, in a Cartesian coordinate system that differential volume will be cuboidial volume with dimensions delta x in the x direction, delta y in the y direction and delta z in z direction. So, that is going to be the volume that I choose I will increase it a little bit over here just to amplify the volume. So, this is delta y, delta x and delta z; if I were to write the mass balance equation for this particular differential volume, the mass balance equation has the form, the change in mass in time t is equal to mass in minus mass out plus any accumulation mass due to reactions or some other reason, so that is the balance equation.

What was the change in mass in time t, the change in mass in time t is equal to the difference in concentration at time t plus delta t minus the concentration times the volume delta x, delta y, delta z. So, that is the first one to change in mass in time t, on the right side we have the mass coming in and the mass going out this volume has six surfaces two of which are perpendicular to the x axis, if two of which are perpendicular to the x axis; that is the front and the rear surfaces two of which are perpendicular to the y axis; that is on the left and the right and two of which are perpendicular to the z axis at the top and the bottom and the two perpendicular to the x axis are the front and the rear surfaces right there could be mass coming in and going out at each of these surfaces.

Let us take the left and the right surfaces first, I will put the center of the differential volume at x, y, z; you can put the center of the differential volume at x, y, z therefore, the surface on the left is the surface at x y minus delta y by 2 and z because I will put the center of the differential volume at x y and z. So, mass in at surface; now y minus delta y by 2. I will first take this left surface here is a mass in at the surface y minus delta y by 2, mass is coming in for two reasons; one is due to convection and the other is due to diffusion. The mass per unit area per unit time coming in due to convection, if you recall it is just equal to the velocity perpendicular to the surface times the concentration at that location the mass coming in at that surface is the velocity perpendicular to the surface times the concentration that is the mass per unit area per unit time, that is the flux and I have to multiply that by the area and by time.

So, due to diffusion the mass coming in at the surface at y minus delta y by 2 is going to be equal to the perpendicular velocity; velocity perpendicular to the surface that is u y times c times the concentration at the location y, x, y minus delta y by 2 and z that is the mass coming in due to convection, the perpendicular velocity times the concentration gives you a mass per unit area per unit time. Now I have to multiply this by the surface area and by time; the surface area in this case the surface that is perpendicular to the y axis, the surface area of the surface is going to be equal to delta x times delta z.

That is the mass coming in at the left the phase per unit time, so I have to multiply it by time as well. So, that is a mass that has come in due to convection within a time delta t there is another; so mass input here and that is the second one is due to diffusion; the diffusive mass coming in is going to be equal to plus, the mass flux in the y direction because it is the mass flux in the y direction that is perpendicular to the surface that transports mass from the left side to the right side of this surface. The flux that is along the surface does not transport mass across the surface. So, we have to take the component of the flux that is perpendicular to the surface, this has to be taken at the location x y minus delta y by 2; z times the area delta x, delta z, delta t. So, that is the mass in at the surface y minus delta y by 2.

The first one is due to convection the second one is due to diffusion, what about the mass out on the surface on the right mass out at surface y plus delta y by 2, it is going to be equal to the velocity times concentration at that surface this is the convective mass flux out it is going to be equal to u y times c at x y plus delta y by 2 comma z delta x, delta z, delta t that is due to convection, if the velocity perpendicular to the surface times the concentration at that location is a convective mass and the diffusive mass is just the mass flux; at x y plus delta y by 2 z times delta x delta z delta t.

So, that is at the surfaces on the left and the right, you can do the same thing for the surfaces at the front and the rear. The surface at the rear is the surface at x minus delta x by 2 that is the surface at the rear and for that the convective mass flux will be equal to ux times c because this is the velocity u x that is perpendicular to the surface, the surface at the rear using the y z plane. Therefore, the x direction is perpendicular to that surface, so I have to multiply the velocity in the x direction, times the concentration at the location x minus delta x by 2; y z times the surface area is delta y, delta z, delta t and then I have the flux in the x direction this is the diffusive flux one contribution due to convection the other contribution due to diffusion.

So, the second flux is the diffusive flux; at x minus delta x by 2, y z times delta y delta z delta t. So, if that is the flux coming in at the rear; the flux leaving at the front phase, the flux leaving at the front phase at x plus delta x by 2 will just be equal to the same. In this case if u x is positive the mass is leaving the volume. So, therefore, the flux is equal to plus u x times c at x plus delta x by 2, delta y, delta z, delta t plus j x at x plus delta x by 2, y z, delta y, delta z, delta t.

Now, you can do it for the top and the bottom phases; the bottom phase is at z minus delta z by 2 because the center is at x, y, z therefore, the bottom phase is at z plus delta z, z minus delta z by 2 is equal to u z it that is the perpendicular velocity to the surface times c at x, y, z minus delta z by 2 times the area in this case the surface is along the x y plane. Therefore, the area is going to be equal to delta x, delta y, delta t plus the flux perpendicular to the z direction because that is what is bringing mass into this differential volume at the bottom surface, the flux perpendicular to the z direction at x, y, z minus delta z by 2 delta x, delta y, delta t then you have a mass out; u z times concentration at x, y, z plus delta z by 2 that is the mass leaving at the surface on top is that plus delta l by 2 times the surface area delta x, delta y, delta t plus j z at. So, those are the masses in the masses out, in all cases you can see that you have 2 fluxes one is due to convection, the other is due to diffusion both of these are multiply it by area and pack.

Mass in is the value at x minus delta x by 2, mass out is the value at x plus delta x by 2, the surface area is in both of these cases are the same.

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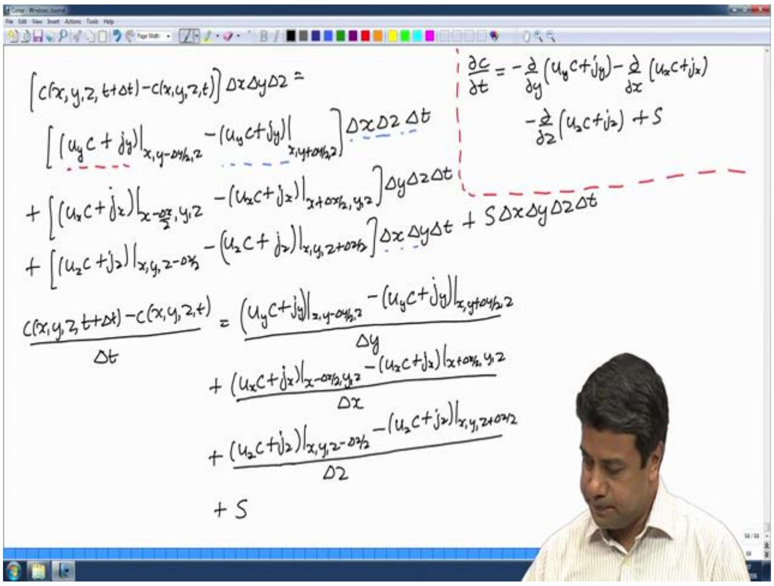

So, when I add all of these up, I will have a term on the left hand side which is the concentration at x, y, z, t plus delta t; minus the concentration at x, y, z t into the volume delta x, delta y, delta z that is the net rate of change of mass within this differential volume I am sorry there is the change in mass in this differential volume in a time delta t.

On the right side you have multiple terms the first term is along the y direction that we had done earlier, that is mass coming in at x minus y minus delta y by 2 and leaving at y plus delta y by 2. So, therefore, I will have the u x times c at y u x times c plus I am sorry this should be the y direction for plus t y at x y minus delta y by 2; z that is the flux coming in due to convection and diffusion. The flux leaving is u I c plus j y; at x y plus delta y by 2 comma z. The whole thing has to be multiplied by the perpendicular area delta x delta, z times time. So, this first term here is the mass that is entering, if you recall in the previous section this is the mass that is entering these first 2 times.

The next two terms are the masses that are leaving, so, these 2 terms are the masses that are leaving this differential volume. In both cases the surface area is the same and the time interval is the same, then I will get terms in the y in the z direction which looks very similar. So, this will be plus u x c plus j x at x minus delta x by 2; y z minus u x c plus j x at x y I am sorry x plus delta x by 2 y z and the surface area perpendicular to the x direction is delta y, delta z, delta t and the next one will be the top and the bottom phases, the bottom phase first u z c plus j z; at x, y, z minus delta z by 2 minus u z c plus j z at x, y, z plus delta z by 2.

In this case, the surface area is going to be delta x, delta y, delta t the bottom and top phases are along the x y plane. So, the surface area is delta x times delta y and then I had another source here that is the source per unit volume per unit time is some reaction within the volume, the rate of change of concentration is what is specified by the reaction rate. Therefore, the change in mass is going to be equal to the reaction rate, times the volume times time delta x, delta y, delta z that is the volume times delta t. So this is the balance equation and now I divide throughout by volume, divide throughout by time. So, if I divide throughout by volume and time I will get on the left side and get c of x, y, z, t plus delta t minus c at x, y, z, t by delta t. On the right side and get u y c plus j y at x y minus delta y by 2 z minus, the whole thing now will be divide it by delta y.

Because I had a delta x, delta z here and delta t and they divide it throughout by a volume and time, so this is what I will get for the y direction. Similarly you will get for the x and z directions, so the x direction you will get u x c plus j x at x minus delta x by 2 y z minus u x c plus j x at x plus delta x by 2; y z divided by delta x and then in the z direction you will get u z c plus j z at x, y, z minus delta z by 2 minus u z c plus j z and x, y, z plus delta z by 2, the whole thing divided by delta z that is because here my area was delta x delta y and I was dividing throughout by volume plus the source time. So, that is the difference equation now I take the limit delta x, delta y, delta z going to 0.

So, on the left side I will just get, so let me just write it here on the left side I just get partial c by partial t in the limit as delta t goes to 0. On the right side the first term is u y c plus j y at y minus delta y by 2 minus y plus delta y by 2. The derivative is the value at y plus delta y by 2 minus the value at y minus delta y by 2, so that is the derivative. So, this is actually the negative of the derivative minus d by d y of u y c plus j y; that is in the y direction, you will get a similar expression in the x and the z directions minus d by d x of u x c plus j x minus b by d z for u z c plus j z plus any source.

So, that is going to be the differential equation, the balance equation for the concentration field that includes both convection and diffusion convective transport across surfaces due to the mean fluid flow as well as diffusion across surfaces due to the concentration variations.

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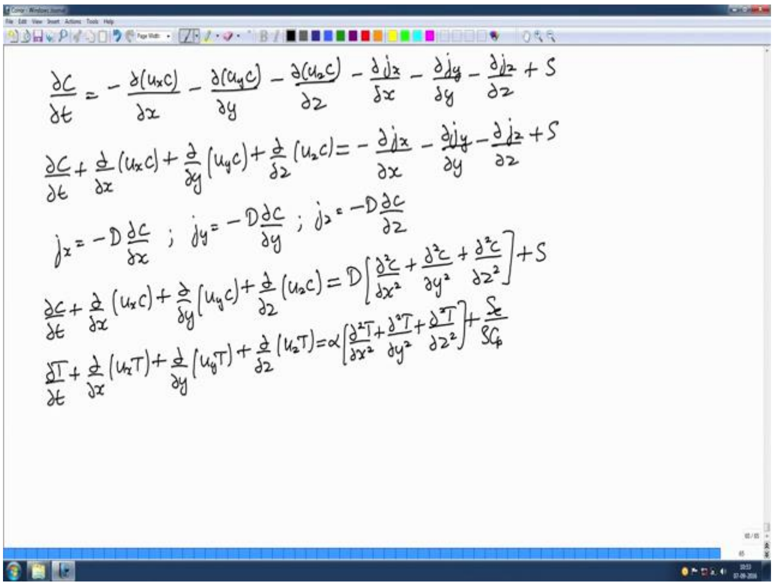

So, this equation can be written as partial c by partial t; just expanding it is minus partial of u x c by partial x minus partial of u y c by partial y, minus partial of u z c by partial z, minus partial j x by partial x, minus partial j y by partial y by partial z plus source and it is conventional to write the convective terms on the left side of the equation and the diffusive terms on the right side of the equation; it is conventional to write this as d c by d t plus d by d x of u x c plus d by d y of u y c plus d by d z of u z c equal to minus partial j x by partial x, minus partial j; y by partial y plus the source, so that is the conservation equation.

Now, I have to use the constitutive relation for these fluxes; in general if the material is isotropic; the flux j x will be equal to minus d partial c by partial x, j y is equal to minus d, partial c by partial y; j z is equal to minus d partial c by partial z; this is the generalization of Fick’s law for diffusion in three dimensions. The flux in the x direction is equal to the diffusion coefficient times the variation the gradient in that direction, similarly in the y direction the flux is equal to the diffusion coefficient times the gradient in the y direction and similarly in the z direction negative sign because there is transport of mass from regions of high concentration to low concentration and so if I substitute this into the conservation equation and consider that the diffusion coefficient does not depend upon position, the equation that I get will be of the form partial c by partial t plus d by d x of u x c plus d by d y of u y c is equal to d square c by d x square.

So, that is the mass balance equation for this particular case; for the concentration field. So, the temperature field I will just substitute temperature instead of concentration and the thermal diffusion coefficient instead of the mass diffusion coefficient; that works provided the thermal conductivity and the specific heat and density or rather the thermal diffusion coefficient it is independent of position. So, in that case you will get an exact analogy is equal to alpha if I should put a source here my apologies plus the source of energy by rho C p. So, there is a thermal energy conservation equation for a Cartesian coordinate system.

I will look at these equations once again and try to write them in a slightly different form that is easier to manipulate, try to give you some physical understanding of what each of these terms means before we go on to looking at conservation equations in a curvilinear coordinate system in a spherical coordinate system. So, that discussion of how to write these equations more compactly we will look at in the next lecture and then we look at conservation equations in a spherical coordinate system. The form of the equations when written in vector form which I will show you a little later turn out to be the same regardless of which coordinate system it is written in. If the forms of the differential operators will change, but the form of the equations themselves when written in vector form will end up being the same independent of coordinate system, I will show you that as we proceed in the next lecture; we will see you then.