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

## Lecture - 46 Mass and energy balance equations in Cartesian co-ordinates. Vector notation

Welcome to our continuing series of lectures on transport phenomena, where we had looked at how to do shell balances for specific problems, which had specific symmetry for example, in a flow past of, I am sorry, the heat transfer and mass transfer in the flat surface where it was infinite therefore, there was only transfer in one direction. Similarly in a cylindrical geometry we looked at transport only in the radial direction. In general problems there is transport in all 3 directions simultaneously, so there is a variation of concentration in all 3 directions and there is a variation of concentration in time as well.

In that case, we can derive general conservation equations in all 3 directions as well as in time which work in which are general so that depend only upon the specific coordinate system that are being used and then for specific problems we can simplify these equations and then use them. So, in that spirit we had started deriving balance equations in the previous lecture.

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Balance equations: Mass ) + Acc. NZ Mass Change in mass ] out C(x, y, z, E)] Dx Dy D2 c(x, y, z, + st) Dx D2 Dt N "x Mass in at surface (y-by) x,y-0%,2 020206 DgDZDE AUDZOE Uz C L AYDZAL Droyot UzClary. Dr Dyst 

We had looked at a Cartesian coordinate system where the surfaces, the planes are surfaces of constant coordinate in this case you have to take a differential volume whose surfaces are surfaces of constant coordinate and then write a balanced equation for that differential volume and I had shown you how we do it in this case. We took a cuboidal volume of volume delta x, delta y, delta z in the 3 directions and wrote a balance which basically stated that change in mass is equal to mass in minus mass out and plus any accumulation the change in mass in time delta t which is equal to the change in concentration times the volume itself now the mass in and the mass out of the surfaces of this differential volume there are six surfaces the left and the right the front and the rear and the top and the bottom. Mass in and mass out could be for 2 reasons, one is due to convection and the other is due to diffusion.

The convective flux is just the normal velocity times the concentration because it is only the normal component of the velocity that is changing the mass within this differential volume. So, the flux is the normal velocity times the concentration for convection and for diffusion it is just the diffusive flux and on the left surface at x minus delta x by 2 when the velocity is positive or the flux is positive mass comes in. So, therefore, the mass in was written as the convective flux times the surface area perpendicular surface area delta y, I am sorry; delta x times delta z times time at that surface plus the diffusive flux times the surface area times the time interval that is was at the left surface where the mass within the volume increases if the flux is positive.

On the right surface, the mass within the volume decreases if the flux is positive therefore, that constitutes a mass leaving the surface that mass convection once again is u y times c that is the flux times the surface area and time and diffusion is j y times surface area times time. And similarly we had calculated fluxes from the front and the rear surfaces which are perpendicular to the x axis. So, they are separated by distance delta x and the top and the bottom surfaces which are perpendicular to the z axis and they are separated by a distance delta z.

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B/ ..... à (uy c+jy) - à (ux c+jx) [ cfx, y, z, t+st)-c(x, y, z, t)] Dr DyD2 · (Uzc+ Jz) ztoxb, yz SOXDYDZOt Drayst (u2c+ j2) 1x, y, 2+025 ((x, y, 2, t+2+) - c(x, y, 2,+) (UyC+jy) =, y-046: +5

Once we had these, we had put all these together to get the balance equation which included the sources in general and then you divide throughout by the volume divide throughout by time to get the difference equation which is the next equation here then take the limit of delta t going to 0 and delta z going to 0 sorry, volume going to 0 and delta t going to 0 to get the differential equation.

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 $\frac{\partial(u_{y}c)}{\partial x} - \frac{\partial(u_{z}c)}{\partial x} - \frac{\partial(u_{z}c)}{\partial x} - \frac{\partial(u_{z}c)}{\partial y} - \frac{\partial($ 3/2+5 d(uxc) \_ 22 38 26 29 dr  $\frac{d}{\partial x}(u_{x}c) + \frac{d}{\partial y}(u_{y}c) + \frac{d}{\partial z}(u_{z}c) =$ 

Had expanded out the differential equation for you and written it in a slightly different form, written in a slightly different form and then I had substituted the constitutive relation in this case Fick's law of diffusion. The flux in the x direction is related to the velocity gradient in the x direction, flux in the y direction related to the velocity gradient in the y direction and similarly for the z direction and you can substitute these in and get an equation of this form which has on the left side the time derivative and the convection terms which are first order derivatives in the spatial locations on the right side is the diffusive term which is a second order derivative.

These equations can be written in a slightly more compact form so that let me go back and draw a coordinate system once again, this is x y and z the velocity is actually a vector it can be written as the sum of the components times the unit vector the unit vectors I will use the symbols e x e y and e z for the unit vectors rather than I j k or some other symbols at your familiar with this notation makes it clear what exactly I am referring to and I will use the underline to represent a vector use the underline rather than using an arrow on top to represent the vector. So, this is the velocity vector, there are 3 components and there are 3 unit vectors. Now the flux that I had here also has 3 components the flux also has 3 components. So, the flux can also be written as a vector, I can write j vector is equal to j x e x plus j y e y plus j z e z and you know what j x j y and j z are. So, is equal to minus d partial c by partial x e x minus d partial c by partial y. So, that is the expression for the flux.

I can write the flux also as a vector the flux has a direction there is a particular direction in which that mass transport is taking place just as the velocity is a vector at some point in the flow it could have some particular position. The flux is also a vector at any location it could be in one particular direction, I can resolve that vector into the fluxes along the x y and the z direction - the component of that is j x j y in j z and if I add up j x times that unit vector plus j y times that unit vector plus j z times the unit vector e z I get a vector flux, there is a resultant of these 3 fluxes is the resultant of these 3 fluxes the vector addition of these 3 fluxes. So, I can also represent the flux as a vector.

Now you can see that in this I have d c by d x times e x d c by d y times e y and d c by d z times e z that is acting on the concentration field. This I can write it as minus d times e x d s d by d x plus e y times c where this thing is now a vector in itself, it is a differential operator, but it is the vector differential operator. So, if I take d c by d x at a given location at a given location the concentration field will vary in all 3 directions I can take the variation the x direction d c by d x variation of the y direction d c by d y variation the

z direction d c by d z and then I can add these 3 after multiplying them with the unit vectors to get a resultant vector. So, this thing is a resultant vector of the concentration variations in the 3 direction this is a resultant vector of the concentration variation in the 3 directions you can define this vector it is usually written by the gradient symbol grad is equal to e x times partial by partial x plus e y times partial by partial y and if I define it this way I can simply write the flux as minus d gradient of the concentration so that is how I would write the flux in terms of a vector derivative of the concentration field so, let us go back and look.

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We have defined the velocity field as e x u x plus e y u y plus e z u z, define the flux as e x j x plus e y and I have defined a vector derivative a vector spatial derivative as Del is equal to e x partial by partial x plus. So, these are the 3 operators have defined now this will help me write the equation much more compactly. So, the first thing give the flux j vector is equal to minus d into e x partial c by partial x plus e y partial c by partial y plus e z partial c by partial z.

This I had written as minus d times the gradient of the concentration, concentration is the scalar that gradient operator is a vector. So, I get a flux that is a vector. Now let us go back to the conservation equation, the conservation equation that I had was d c by d t is equal to I am sorry; now these terms here I can write them as a e x d by d x plus e y d by d y plus e z d by d z dotted with u x look at this expression when you take the dot

product of 2 vectors you have to multiply their components and dot the unit vectors you have to multiply the component and dot the unit vectors.

So, if you take for example, the first term in this expansion which consists of taking the dot product of these 2, what you get is e x d by d x of u x, I am sorry, u x e x and there is a dot product you have to multiply the components and dot the vectors in this particular case the unit vector e x is independent of position if you recall in a Cartesian coordinate system x y and z, the unit vectors do not change with position e x, e y, e z that the same regardless of what the position as that is not true in curvilinear coordinate systems as we shall see a little later in the Cartesian coordinate system the unit vectors are independent position. So, I can take the unit vector out of the differentiation. So, I will get e x dot e x d by d x of c u x is equal to d by d x of c u x because a unit vector dotted with itself gives you 1.

Let us take the second term in the series is when this operator acts from the second term here. I get e x times d by d x of c u y e y once again unit vectors independent of position. So, I get x dot e y d by d x of c u y and e x dot e y is equal to 0 because they are perpendicular to each other. So, this term becomes 0, similarly this first term acting on the third term here will also give you 0. So, only the components that are acting on the same in the same direction for example, the gradient of the u x velocity times concentration the derivative with respect to y of u y times the concentration. So on those are the only terms that will remain and therefore, this equation will reduce to this equation that I heard here if I take the dot product of this dot product is just dot product of Del dot u c. So, the first term is the gradient operator dotted with the concentration times the velocity.

Therefore this second term in the equation can effectively be written as partial c by partial t plus del dot u c this is called the divergence the dot product of the gradient operator with the vectors called the divergence of that vector similarly the term on the right can be written as e x d by d x dotted worth j x same argument when you take the dot product e x dot e x is one e x dot e y and e x dot e z are both 0. So, therefore, this will just give you del dot j vector and of course, there is a negative sign here, it was a negative sign here therefore, on the right side I will have minus del dot j and as you can see this is an extremely compact form of writing the same equation provided they define

the del dot operator as e x d by d x plus e y d by d y plus e z d by d z, and then I have j is minus b grad c. So, if I substitute this, I will get minus del dot minus d grad c.

Note that the dot product is now between these 2 gradient operators not focus between these 2 grains operators if d is independence position this just becomes equal to d del square c where this del square is del dot del is equal to e x dotted with itself and once again you can see that e x dot e x is 1, e x dot e y is 0 therefore, only the terms which involve derivatives of the same coordinate will be multiplied by 1, derivatives of 2 coordinates will be multiplied by 0 and therefore, this just gives me d square by d x square make this someone else. So, this will be equal to d square by d x square plus d square by d y square plus t square by t z square.

It contains the second derivative with respect to x y and z. So, in this vector notation my differential equation has taken the form partial c by partial t plus del dot u c is equal to b del square c.

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Where, this del dot u c on the left side is partial by partial x of u x c plus partial by partial y of u y c plus partial z by u z c and on the right side, I have d into d square c by d x square, this is called the Laplacian, this operator is called the Laplacian and this thing here the del dot of a vector is called the divergence of that vector. So, this is the general form of the conservation equation this form.

This is general, the interpretation of the divergence the explicit expressions for the divergence the laplacian will depend upon the coordinate system. In this particular case when I took del dot del there was a derivative acting on the unit vectors, but that was 0 because in the Cartesian coordinate system the unit vectors are independent of position that is not in general true in other coordinate systems.

Therefore, the forms of the laplacian and the divergence that is del dot equal to e x sorry these forms will change when you go to another coordinate system; however, this equation does not change the general equation that you have d c by d t plus the divergence of u times c on the left side and a diffusion coefficient times the laplacian of c on the right side that does not change, that is the same for all coordinate system when written in this vector form; however, these things will change. So, the next lecture I will derive for you the conservation equations in a spherical coordinate system.

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X y z was the Cartesian coordinate that we were using, when you have a spherical geometry you would expect the a coordinate in which this surface is a surface of constant coordinate that is a spherical coordinate system in which one of the coordinates is just the distance from the center r, one of the coordinate is just the distance r from the center from the origin.

However you need 2 other coordinates to completely specify a location in the Cartesian coordinate system, we had x y and z to completely specify in this case r is just a distance

from the center; you need 2 other coordinates to completely specify a point in this spherical coordinate system and those 2 coordinates are actually the angles made by this radius vector with the coordinate axis one of these is what is called the azimuthal angle theta which is the angle made by the radius vector with the plus z axis and the second one is what is called the meridional angle phi, if I take a projection of r onto the x y plane if I take a projection of r onto the x y plane and I calculate what is the angle that this makes with the x axis that is what is called the meridional angle phi.

You can easily see that this z is basically equal to r times cos theta, this height is r times cos theta because theta is the angle made with this z axis, this projection is equal to r sin theta. So, therefore, I have z is equal to r cos theta the projection along the x y plane, the projection along the x y plane is basically root of x square plus y square that is the projection that is length of this line of the projection along the x y plane that is equal to r sin theta and this makes an angle phi with the x axis therefore, x will be equal to r sin theta cos phi y will be equal to r sin theta sin phi. So, there is a conversion from the spherical coordinate system to the Cartesian coordinate system the radius is just equal to square root of x square plus y square plus z square distance from the origin is the radius.

Now, theta is the angle from the plus z axis therefore, theta can vary only from 0 to pi, is it is theta is angle from the plus z axis when theta is equal to pi you reach the minus z axis when theta is equal to pi you reach the minus z axis and you cannot go any further therefore, theta has to be between 0 and pi because theta is equal to pi is the minor z axis once you reach the minus z axis that is the maximum you can go you cannot go any further. Phi on the other hand is the angle around the z axis, phi is the angle around the z axis the angle made with the x plane around the z axis.

Therefore, phi can go from 0 to 2 pi this spherical coordinate system is something that most of you would have seen in the past that is what is used for example, for defining the latitudes and the longitudes on the globe on the earth. The z axis is the north south axis from the 2 poles so that is the z axis. The equator, we write it as 0 latitude that is because we take the latitudes to be 0 at the equator and it goes to plus 90 at the north pole and minus 90 at the south pole the northern latitude and the southern latitude. In the spherical coordinate system this north pole will correspond to theta equal to 0, I take theta from the plus z axis therefore, the north pole would correspond to theta equals 0; it would increase theta will be ninety at the equator and then one eighty at the south pole and you cannot

go any further because the south pole is on the minus z axis so that is theta. Whereas, conventionally on the globe theta the latitude is 0 at the equator when expressed in terms of theta it is equal to 0 at the north pole it goes to 180, it rather than going from 0 plus 90 and 0 to minus 90 and phi is the meridinal direction. And phi goes from 0 to 360 all the way around the globe that is the angle phi here.

In the globe this is measured from the 0 meridian is z that at grange in England, it passes through there you can choose any arbitrary reference for the meridian it goes from 0 to 360. So, these are the angles - theta and phi in this spherical coordinate system.

In the next lecture, I will construct a differential volume in this spherical coordinate system and write a balanced for this differential volume. As I said below before in the differential volume, the coordinate, the surfaces have to be surfaces of constant coordinate; that means that in this case the surfaces have to be surfaces of constant theta, constant r and constant phi rather than constant x y and z as we had in a Cartesian coordinate system. So, we will construct those surfaces and then write the flux balance for those surfaces in the next lecture and then we will derive the conservation equation in a spherical coordinate system, but when written in vector form the equations are exactly the same. So, we will continue this derivation of a spherical coordinate system in the next lecture, we will see you then.