Fundamentals of Transport Processes
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Module No # 05
Lecture No # 25
Mass and Energy Conservation Cartesian Co-ordinates

Welcome to this the twenty fifth lecture in our course on fundamentals of transport processes. Just to recap what we have done so far, we first started of looking at the measurable analysis in order to obtain the relation between average properties such as the average rate of reaction in the reactor as a function of the concentration differences between the fluid in the catalyst surface in the solid catalyzed reaction, the average difference between the shell side and tube side in heat exchanger and so on. And then we looked in some detail at the diffusion process and derived equations for the diffusion of heat, mass and momentum. And then we looked at transport in one directional, unidirectional transport.

First we looked at the transport between two flat plates, both steady and unsteady, and I showed you how to use the method of similarities solution, separation of variables and as well as methods for oscillatory flows. And then we look at the curve linear system, that is coordinate systems where the surfaces of the constant coordinate are no long flat surfaces. These are important in the specialized application, for example if one is interested in trying to describe the flow through a pipe or the transport to a catalyst surface, one would preferred to have a coordinate a system in which the boundary of the volume being considered is a boundary of constant coordinate.

So, because of that it is preferable to work with curve linear coordinate system. The curve linear coordinate system of course, has the advantage that the bounding surfaces are the surfaces of the constant coordinate. So, the boundary conditions get simplified. However, the difficulty is that the equation are slightly more complicated. And we saw that the equations give you are not in the form of just simple second derivatives of the concentration or temperature field, they are slightly more complicated and that is because the surface area varies as the coordinates varies. In this lecture now we are going to start looking at balance equation in all three dimensions.

So, the idea is the following. Rather than writing down a shell individually for each particular configuration that we are considering, we will write down a shell that works for any configuration within the coordinate system being considered and then we will derive equations for the variation of the concentration temperature fields for the coordinate system that is being considered. And once that is done the equation are common. So, when I have a problem in a Cartesian coordinate system, I already know what the equation is. I just need to satisfy the boundary condition, choose a coordinate system for satisfying the boundary condition and then go head and try to solve the problems using some method that some solution procedure.

So, basically I will derived general differential equation which describe the transport of mass and energy within the coordinate system that is being considered. This discussion will be restricted to the transport of mass and energy. Transport of momentum is a little more complicated because momentum itself is a vector. And therefore, there are three components of momentum. Each component can be transported in three directions and therefore, the stress is actually what is called second order tensor. It contains nine component, three directions for the transport and three directions for the momentum itself.

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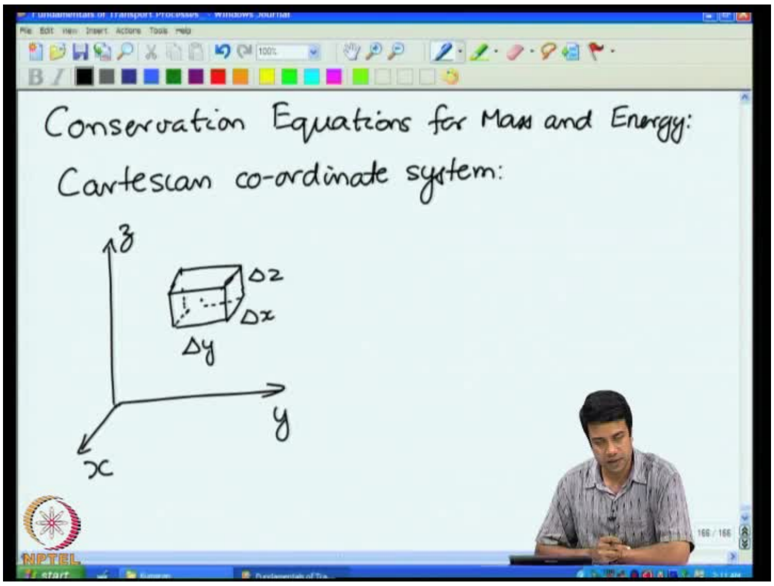

So, we will defer discussions of these two later on. And right now we will just look at conservation equations for mass and energy. So, now we look at the conservation equation for mass and energy and first we will consider a Cartesian coordination system. So, first let us look at a concentration diffusion equation.

So, I have a Cartesian coordination system. And I will not really worry about what problem this conservation equation is being applied to, I will just derive the conservation equation for a differential volume in the Cartesian coordinate system. The differential volume of course, is bounded by surfaces of constant coordinate.

So, in a Cartesian coordinate system this differential volume will be a cubic differential volume. And this has width, delta y, delta x and delta z. The right and left faces are at constant y, the front and back faces are at constant x and the top and bottom surfaces are constant values of z. And I will considered this to be center at the location x, y and z. So, that is bound by surfaces at x plus delta x by 2 and x minus delta x by 2. Similarly y plus delta y by 2 and y minus delta y by 2 and similarly in the z direction.

Now, for this differential volume what is the conservation equation? If I am considering the mass conservation equation, so the equation will be accumulation of mass in time delta t is equal to mass in minus mass out plus a sources or sinks may be present.

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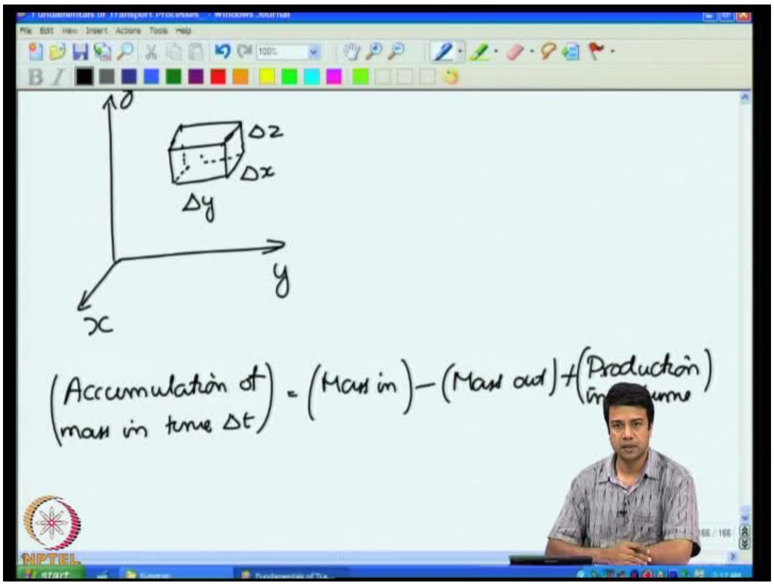

So, I will just put this as a production in the volume. And what I need to do is evaluate this individual terms and put them all together to get a mass conservation equation.

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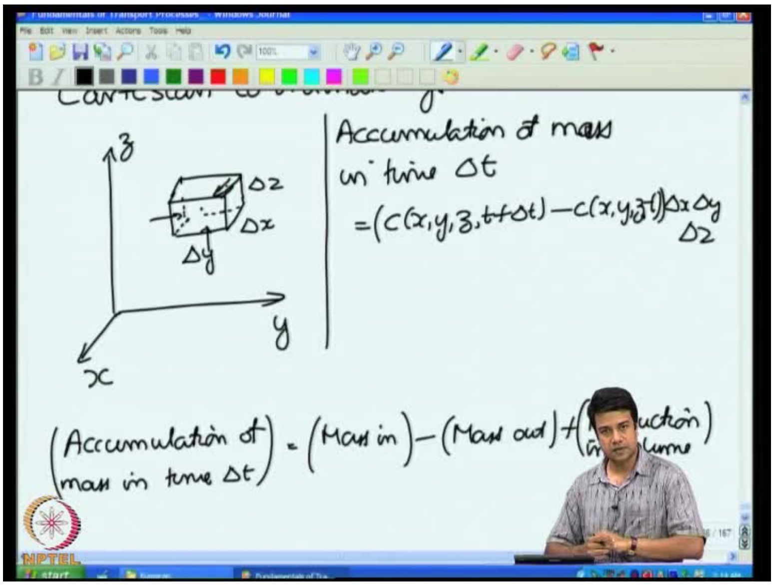

Now, first thing first what is the accumulation? Or is the accumulation of mass in time delta t? This accumulation is going to be equal to the mass at time t plus delta t minus the mass at time t. The mass at time t and t plus delta t are the concentration times the volume. So, this is going to be equal to C at x y z t plus delta t minus C x y z t multiplied by the volume. The volume of this is delta x delta y times delta z. So, that is the accumulation of mass within the time delta t.

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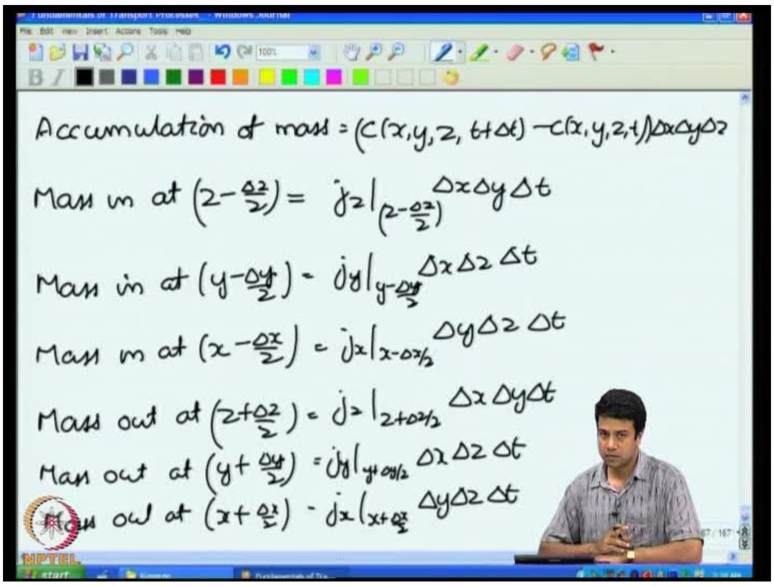

Now, what is the flux in of mass? If I define the flux to be positive, if it is in the plus x, plus y, plus z directions, then there is a input of mass due to the flux at the bottom surface at z minus delta z by 2, at the left surface at y minus delta y by 2 and at the rear surface at x minus delta x by 2. So therefore, there is a flux in at each of these surfaces and at the back surface there is also flux in.

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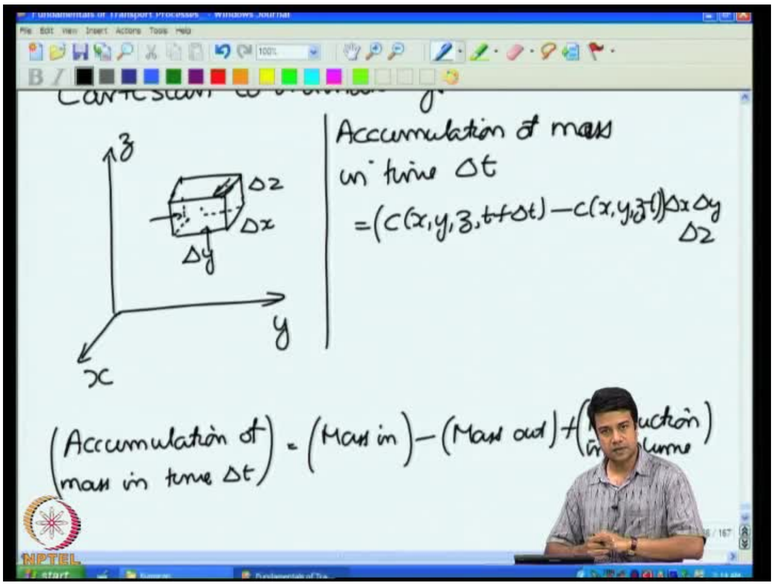

So, what is the mass in at z minus delta z by 2? That is, at the bottom surface of mass in is going to be equal to the flux which is the mass per unit area per unit time times the area times the time interval. The flux in the z direction, the flux we have to considered is the flux that is perpendicular to this surface at the bottom surface. The flux, it is only flux that is perpendicular to the surface that passes through the surface and increases the mass within the differential volume. So, the flux perpendicular to the surface at the bottom surface is the flux in z direction, j z.

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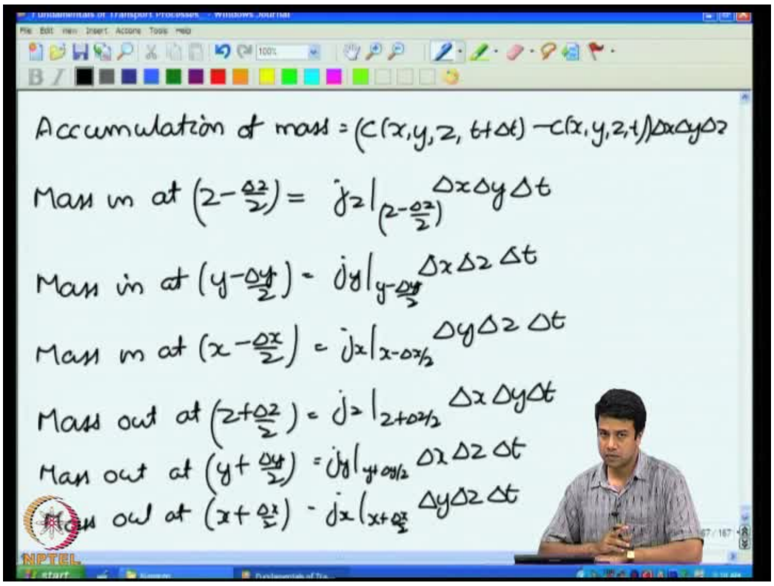

So, therefore, the flux in is equal to j z at z minus delta z by 2 times times the area, delta x times delta y is the area of the bottom surface because the bottom surface has length delta x and delta y times the time, which is delta t the time interval over which we are defining out what is the mass in.

Similarly, there is a mass in at y minus delta y by 2 is equal to j y, j y at y minus delta y by 2. The surface, the left surface at y minus delta y by 2 minus has area delta x times delta z. So, this going to be equal to delta x delta z delta t.

Similarly, there is a mass in at x minus delta x by 2 is equal to j x delta y delta z delta t. So, this is the mass in, I am assuming the flux is positive in the positive x, y and z directions. There is also mass leaving at the top surface, the right surface and the front surface. So, mass out at z plus delta z by 2 is equal to j z at z plus delta z by 2 delta x delta y delta t. Then I have mass out at y plus delta y by 2. Then I have mass out at the front surfaces at x plus delta x by 2. So, these are all diffusion fluxes that are taking place. There is also mass in and mass out because of the convection.

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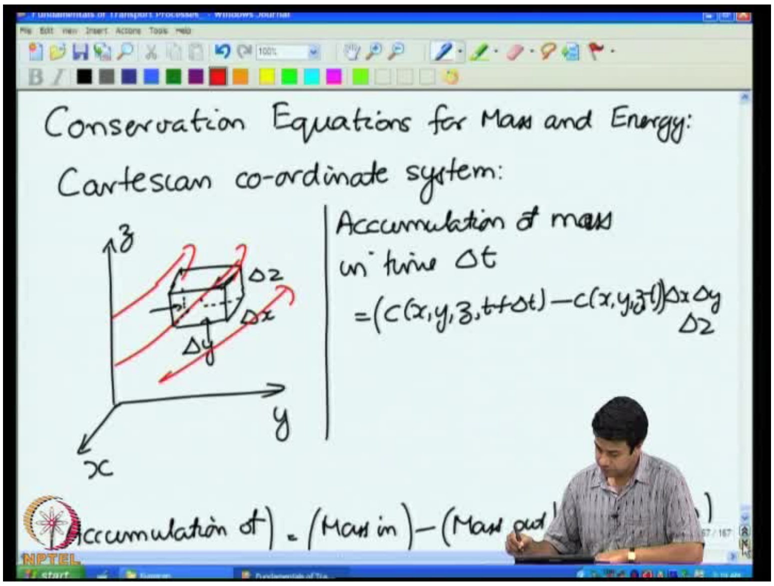

We are considering fluid system and in general, there could be some net fluid velocity going through this. There could be some net fluid flow with a velocity of u x u y and u z. So, there could be mass in and mass out due to convection as well due to the fluid velocity field.

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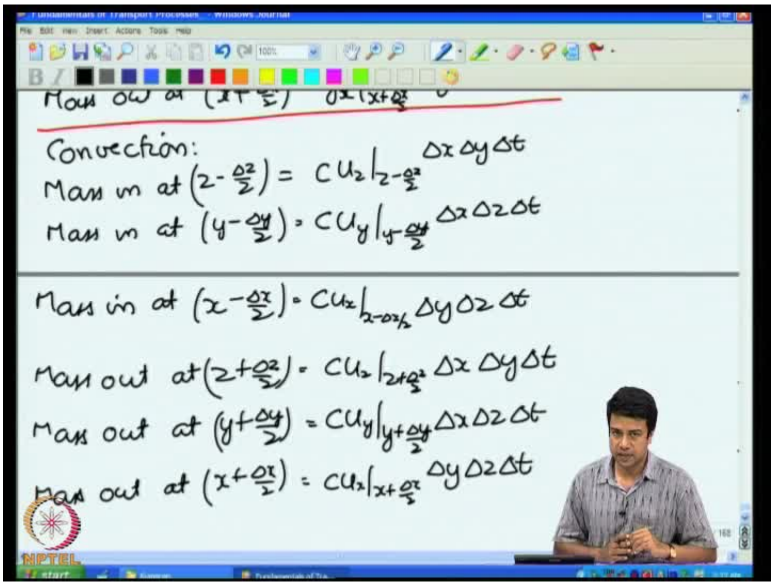

So, what is mass in and mass out due to convection? The mass in due to convection is just equal to the concentration times the velocity, concentration times the velocity is the mass coming in per unit area per unit time. So, concentration is mass per unit volume, velocity is distance traveled by per unit time. So, concentration times velocity is the mass in per unit area per unit time.

So therefore, the mass in at z minus delta z by 2 due to convection is equal to the concentration times the velocity, velocity perpendicular to the surface. Because it is only the velocity perpendicular to the surface that is increase the mass within this volume, the velocity perpendicular to the surface times the area, area in this case is delta x delta y delta t. Similarly, one will have mass in at y minus delta y by 2. In this case, one has to take the velocity component perpendicular to the surface at y minus delta y by 2 which is the velocity in the y direction. So, this is equal to C u y. The mass in at the rear surface at x minus delta x by 2.

One can similarly write down expressions for the mass that is leaving. Mass out at z plus delta z by 2 is equal to C u z and z plus delta z by 2 is equal to C u z and z plus delta z by 2 delta x delta y delta t. Then mass out at y plus delta y by 2 is equal to C u y at x plus…

Note that there are two contributions to the mask coming in to the differential volume and leaving the differential volume. One is due to the diffusion flux j x j y and j z, the other is due to the convection due to the mean velocity that is C u x C u y and C u z.

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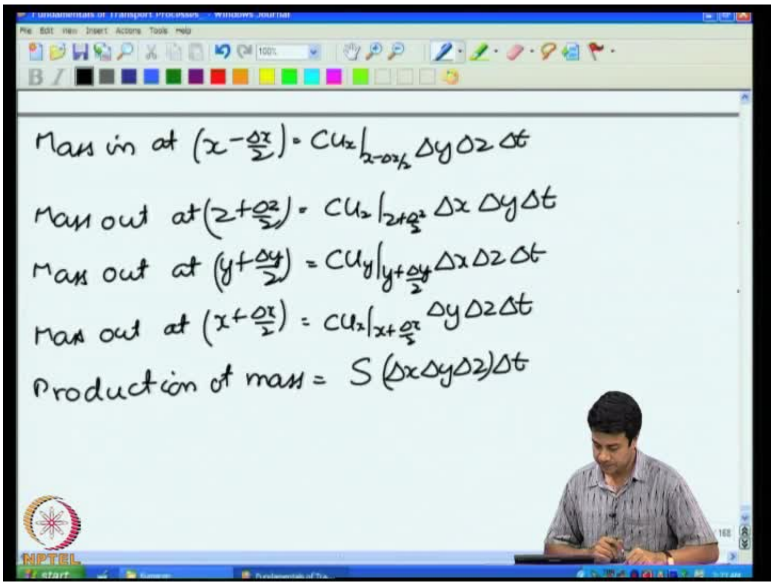

So, these are the three contribution. In addition, there could be a source, a production of mass. This is going to be out the form some production, this is per unit volume per unit time times the volume delta x delta y delta z into the time delta t, because the time delta t is the time period over which that production has taken place. So, these individual terms have to be put into the mass conservation equation. And we have to obtain a differential equation for the concentration field. Mass in minus mass out plus production into volume.

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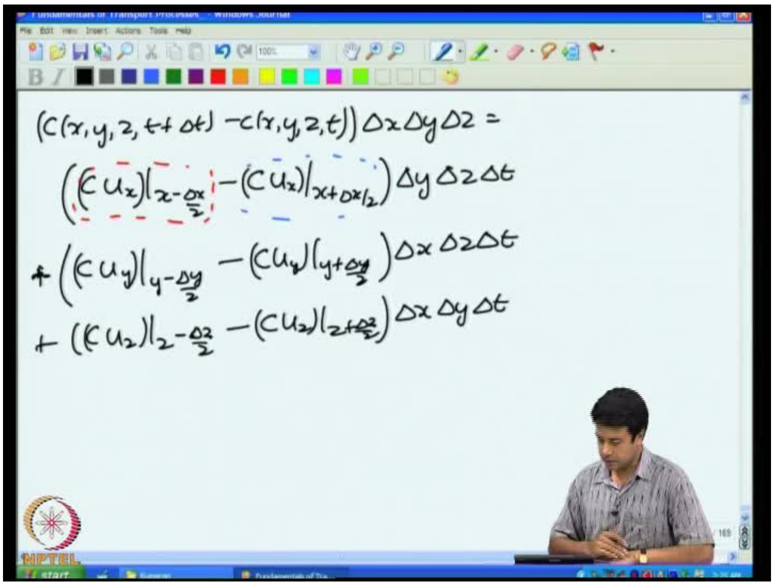

So, in this differential equation on the left hand side I am going to have C at x y z t plus delta t minus C at x y z t times delta x delta y delta z. On the right hand side there is mass in on three faces, mass out on three faces due to two reasons- first is convection, second is diffusion. Let us write down those two individually.

First due to convection. The mass in at the front and back faces is going to be C u x at x minus delta x by 2 minus C u x at x plus delta x by 2 into area into time. For the front and back faces the area is delta y delta z delta t. Note that, the first term here was the mass that came in, this was the mass in and the second term here is the mass that is leaving, this differential volume. Then, the y direction, so you get C u y at y minus delta y by 2 minus C u y into delta x delta z delta t plus C u z at z minus delta z by 2 minus C u z delta x delta y delta t. So, this is the convective part of the fluxes coming into and out of the differential volume.

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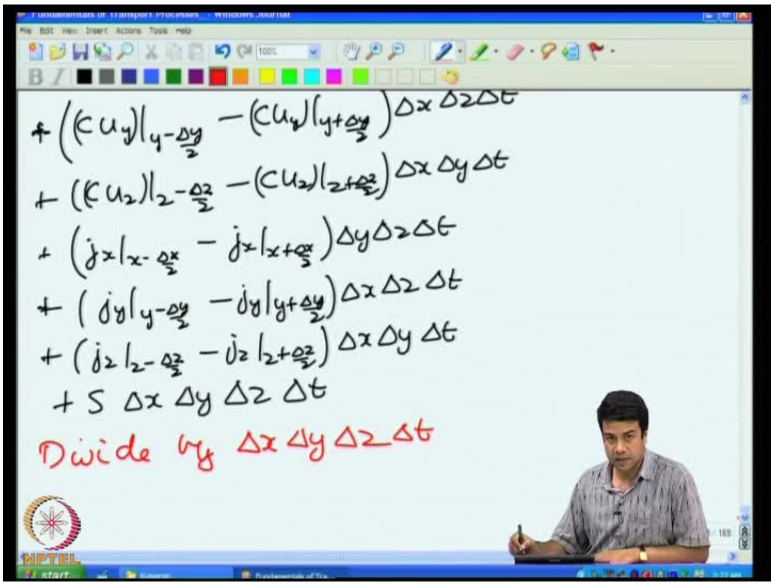

And then there is the diffusive part, so that diffusive contribution is j x at x minus delta x by 2 minus j x at x plus delta x by 2 delta y delta z delta t plus j y at... So, this is the final expression for all of the masses coming in and going out. In addition, I have the source term which is s delta x delta y delta z delta t.

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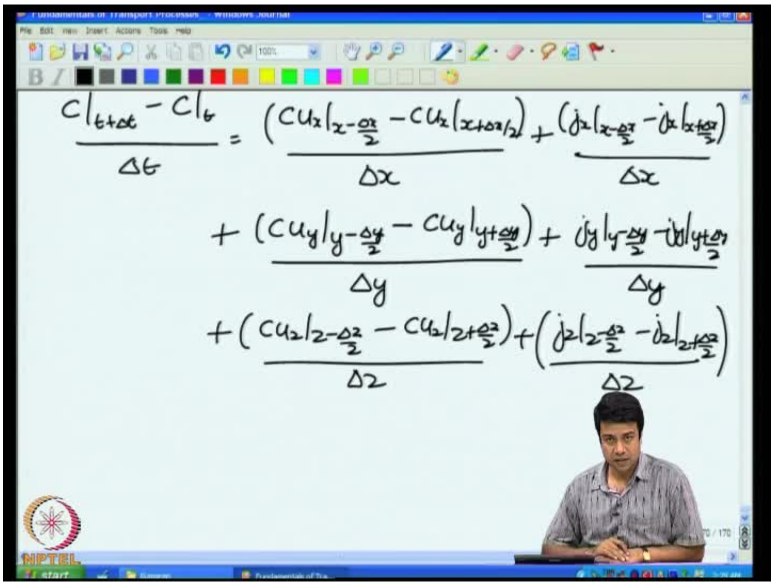

So, this is the final long expression. And now I can divide throughout by the volume and time. And the equation that I get will be C at t plus delta t minus C at t divide by delta t is equal to… plus C u y… Now, this is the final expression and now if I take the limit delta x delta y delta z and delta t going to 0, you can see that the left hand side is just dc by dt. On the right hand side the first term is C u x at x minus delta x by 2 minus C u x at x plus delta x by 2 divided by delta x.

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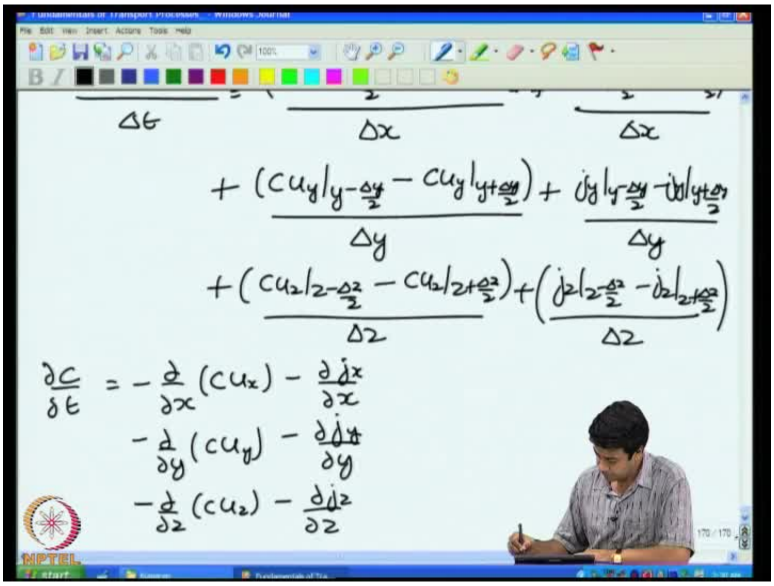

So, therefore, this term is partial is negative of d by dx of C u x, because the derivative is the values at x plus delta x by 2 minus the value at x minus delta x by 2 divided by delta x. So, this is the negative of that derivative. Minus partial j x by partial x minus d by dy of C u y minus partial j y by partial y minus d by d z of C u z minus partial j z by partial z. I can put this equation in a more compact form.

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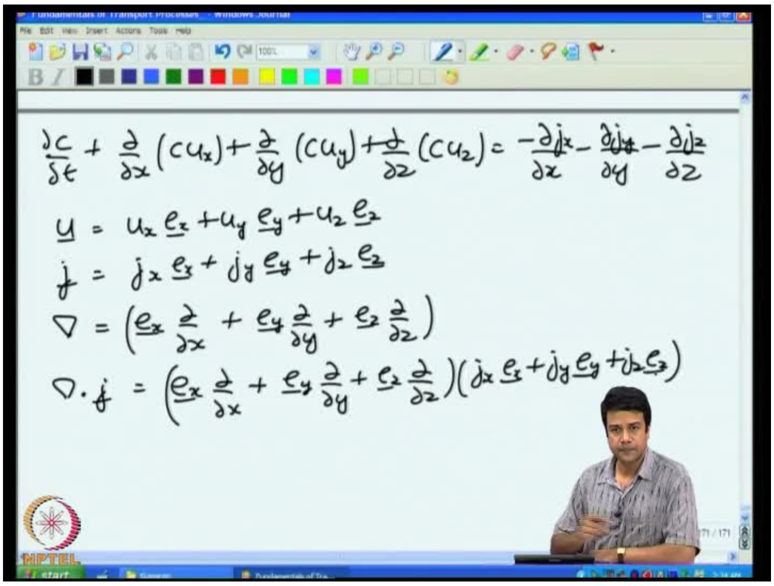

dC by d t plus d by dx of C u x plus d by dy of C u y plus d by dz is equal to minus dj x by dx minus dj y by dy minus partial j z by partial z. Now, these equation can be put into a more compact form if I define the vector, u vector is equal to u x e x plus u y e y plus u z e z.

Note that when we are taking the partial derivatives we are keeping all the other coordinates a constant. When we take the partial derivative with respect to x for example, y z and t are all maintained a constant. When we take the partial derivative with respect to y then x z and t are constants.

So therefore, we take the partial derivative with respect to one variable, all the others are kept a constant. So, I can define a velocity vector which is basically the component times the unit vector. e x is the unit vector in the x direction, e y is the unit vector in the y direction and e z in the unit vector in z direction. Similarly, one can also define a vector flux, j vector is equal to j x e x plus j y e y plus j z e z. So, this is the vector flux.

And I know the derivatives here, I can also define a vector derivative, a vector derivative operator. This is called the gradient operator, which is e x d by dx plus e y d by dy plus e z d by dz. We have defined these vector and gradient operator in terms of an underline coordinate system, the Cartesian coordinate system. However, this vector they have properties which are independent of the coordinates system that are being analyzed, that is true for the velocity vector, it is also true for the gradient. We would not be able to cover that right now, but we will see it later.

For the present, we will define all of these in terms of the unit vectors with reference to an underline coordinate system. So, you can see that if I take del dot j, the dot product of this operator and j, this is equal to e x d by dx plus e y d by dy plus e z d by dz of j x e x plus j y e y plus j z e z. When we take the derivatives the unit vectors are independent of position.

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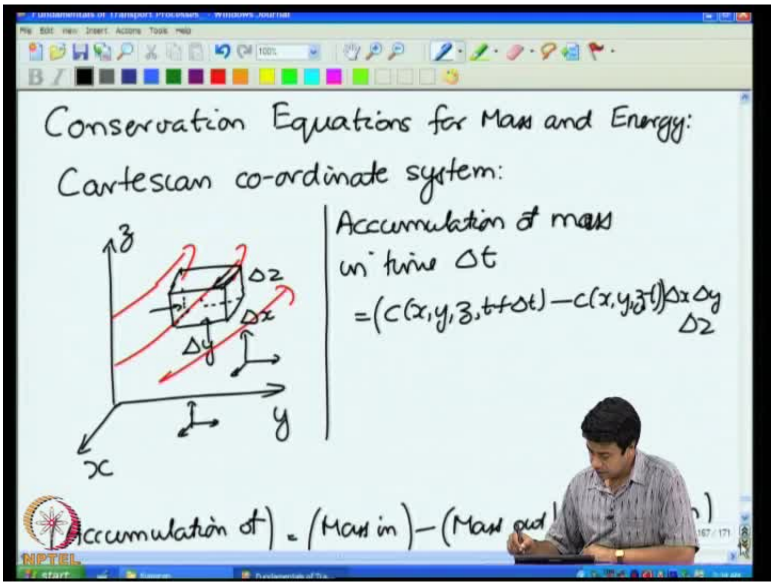

In this Cartesian coordinate system, the unit vectors are exactly the same at each location. The three unit vectors, they are exactly the same at each and every location. So, they are independent of coordinate system. So therefore, when I am taking the derivative here the unit vector come out of the differentiations sign because they are independent. And I have a dot product here between the gradient operator and the unit vector, therefore I will just get this is equal to d j x by dx plus partial of j y with respect to y plus partial j z by partial z.

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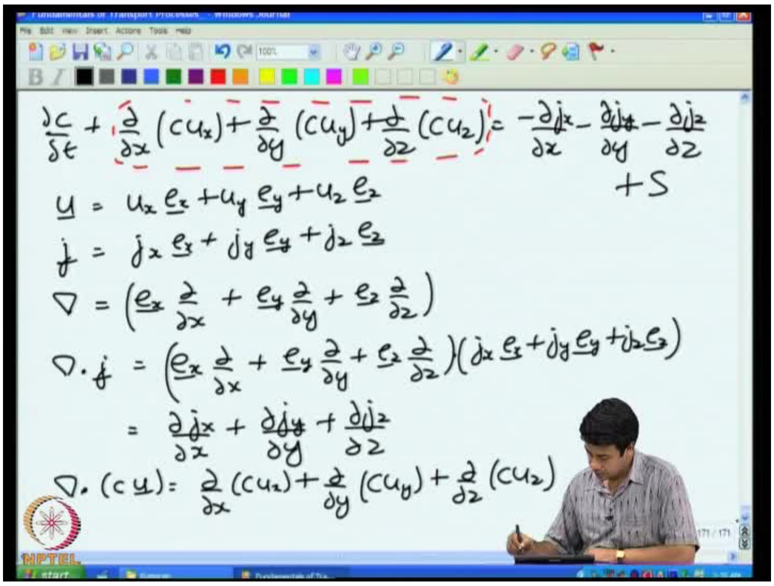

I should have the source term S over here. So therefore, I can write the right hand side as minus del dot j, where del is a vector, j is a vector. Similarly, this three terms on the left hand side I can write as del dot C u vector, which will be equal to d by dx of C u x plus d by dy.

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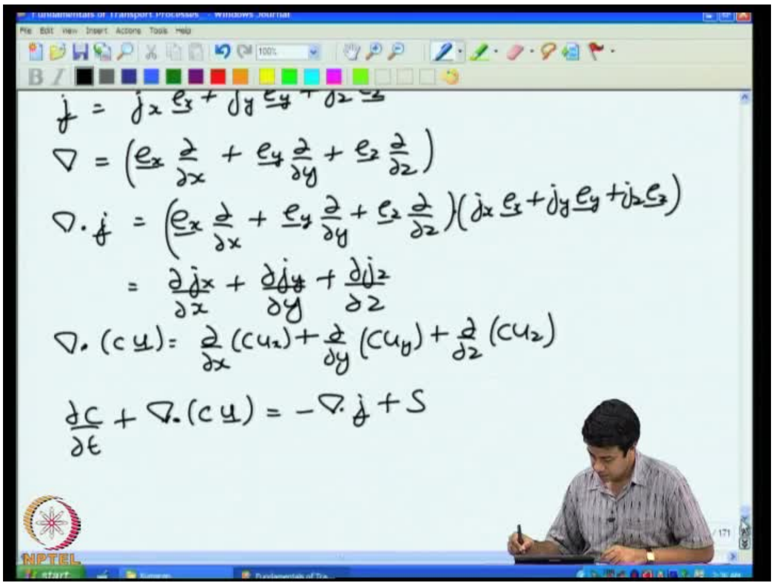

So, if I use these then the equation gets considerably simplified. The equation is just dc by d t plus del dot C times u. Note that this operator is acting on both C and u is equal to minus del dot j plus any sources that are present. So, for a three-dimensional system this is the equation for the concentration field. Of course, we still have to find out what is the flux in terms of concentration in order to get a closed equation. That is of course, given by fix law of diffusion.

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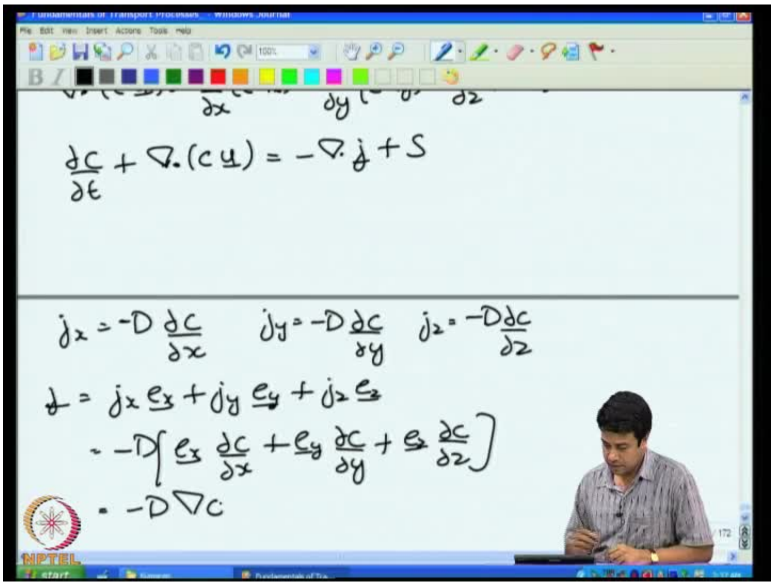

Fix law of diffusion basically states that j x is equal to d times partial C by partial x j y is equal to, there is a minus sign here, of course, the concentration the flux goes in the direction of decreasing concentration. Therefore, j vector which is equal to j x e x plus j y e y plus j z e z is equal to minus d into e x dc by dx plus e y dc by dy. It is basically equal to minus d times the gradient of C, where the gradient operator is what I had defined for you earlier. This is the gradient operator e x d by dx plus e y d by dy plus e z d by dz.

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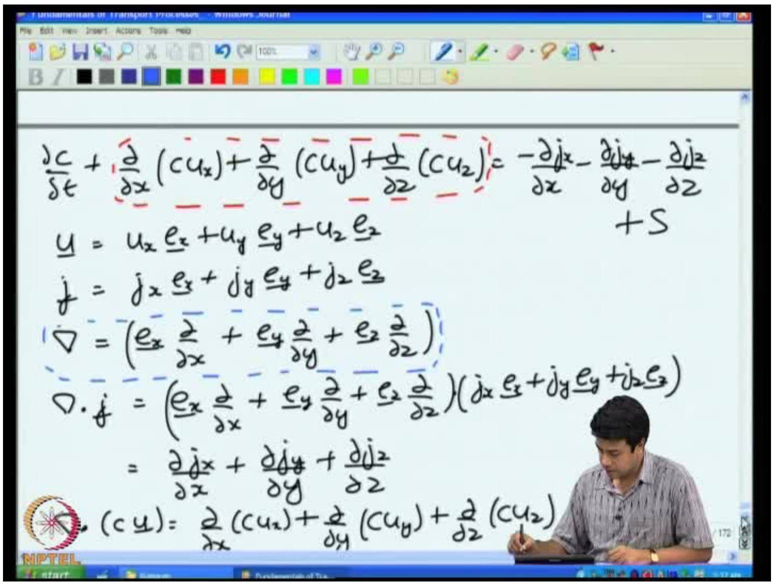

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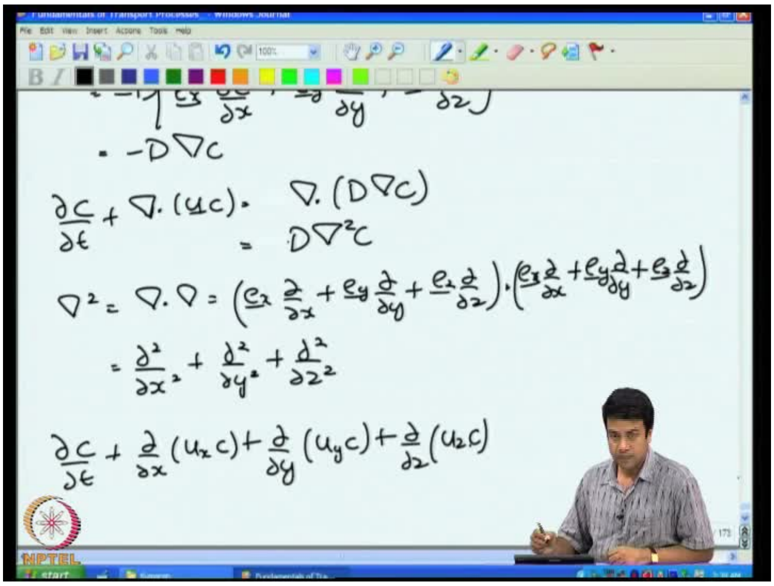

Therefore, if we put this n to the mass conservation equation, we get dc by dt plus del dot u c is equal to minus del dot d grad C. And if the diffusion coefficient is independent of position, I can take that out of the differential because the gradient consist of derivatives due to x y and z. So, if I take that out I will get minus d del square c, where del square is equal to del dot del, which is equal to e x d by dx dotted with itself. This just becomes equal to d square by dx square plus d square by dy square. So, this is the second, this is called the Laplacian operator. So therefore, my final mass conservation equation can be written as dc by dt plus d by dx of u x C plus d by dy of u y c plus… This will be equal to d into d square c by dx square plus d square c by dy square, that is in a Cartesian coordinate system.

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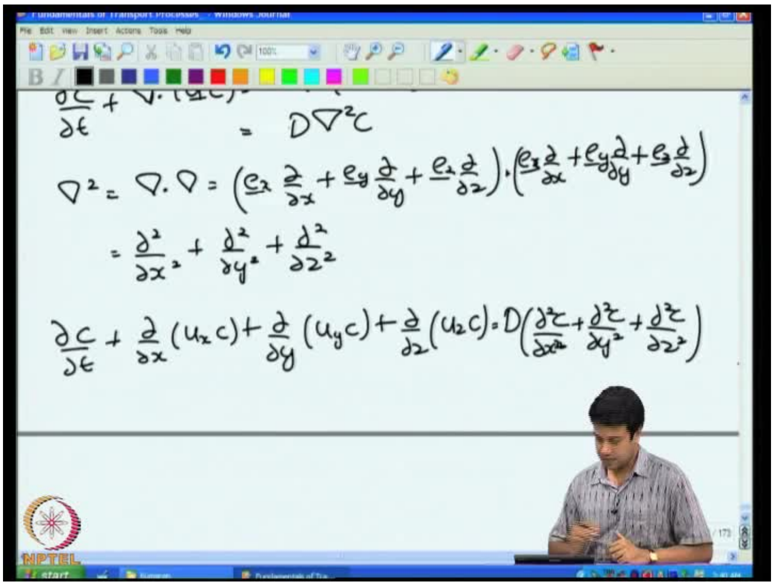

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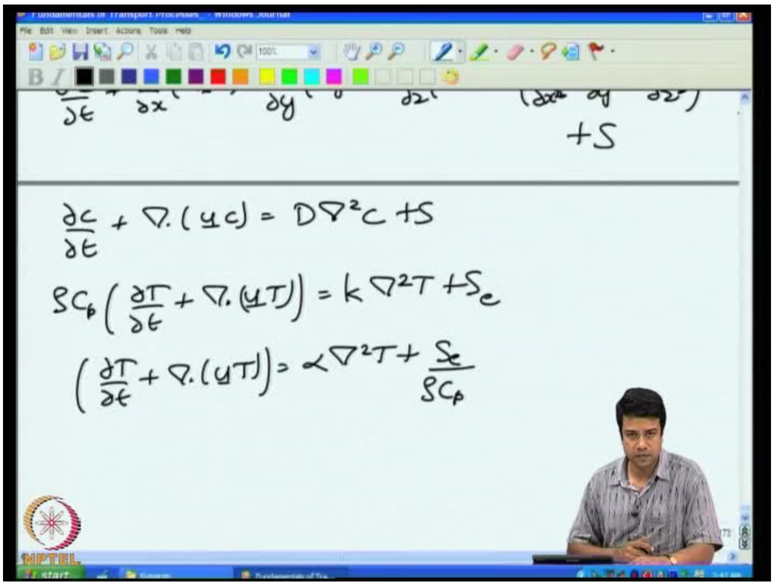

Alternatively, I can also express this as dc by dt plus divergence of u c is equal to D del square C. So, this is the mass conservation equation, a general mass conservation equation for a three-dimensional Cartesian coordinate system.

Let me state at this point that this will also be the mass conservation equation for cylindrical and spherical coordination system, only thing is that the divergence operator and the Laplacian del square have to be differently defined in that case, this equation is general. And in general, you will of course have a source here. Equivalent equation for energy transfer, row C p into dT by d t plus del dot uT is equal to alpha del square T, this is k thermal conductivity plus the source of energy. Alternatively, dT by dt plus del dot uT is equal to alpha del square T plus the source divided by row C p.

So, these are alternate forms of the energy conservation equation and you can see that both the mass and energy conservation equation have exactly the analytical form. Both of them are first order differential equations in time, so you need one initial condition. A second order differential equation in space, so you need at least two boundary conditions in each coordinate that you consider. So, this is the mass conservation equation, how do you solve this?

The solution procedure as I said is identical to what we had in when we did unidirectional transport there is not much difference between the solution procedures for this problem and the solution procedure for the unidirectional transport problem. So, I will briefly go through a simple problem to illustrate how everything that we had learnt for unidirectional transport can be transferred easily to the present problem.

In unidirectional transport, whenever we had a problem we first did a shell balance to get the differential equation and then tried to solve it. In this particular case, we already known what the differential equation is, so there is no need do a shell balance. So, we will just define the problem and straight away go to find the solution.

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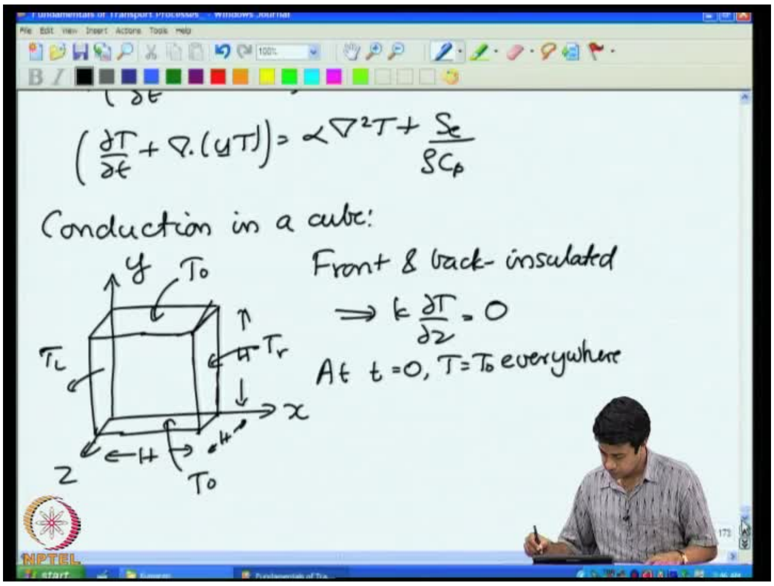

So, the first problem I will take is the conduction in a cube. We have a cubic volume, let us assume that the mean velocities are all 0. We are looking at the unsteady conduction within this cube. So, I have a cubic volume of side H in all directions. So, it leaves the coordinate system here, x y and z. Now, the front and back phases of this cube we will assume are insulated. So, there is no net flux condition. Front and back insulated, which implies that k times dT by dz is equal to 0 at the surfaces, the variation of temperature with respect to the z coordinate times the thermal conductivity gives you the flux at the front and back surfaces. Since the front and back surfaces are insulated there is no net flux at these two phases. And the top and bottom surface are at temperature T naught, the left surface is at some temperature T l, and the right surface is at some temperature T r.

So, I have a cube in which the front and back are insulated, the top and bottom are itself at temperature T naught and the left and right are at some temperature T l and T r, and what about the time dependence? At time T is equal to 0, T is equal to T naught everywhere. That is I have a cube which is insulated in front and back surfaces so that there is no heat transferred across. Initially, the entire cube was at temperature T naught, at time T equal to 0 instantaneously it is raised the left and right faces to temperatures T l and T r. And I need to find out what is the temperature within the cube due to diffusion. This is an unsteady state problem. There is no velocity though, there is no mean velocity therefore, ux uy and uz are all 0.

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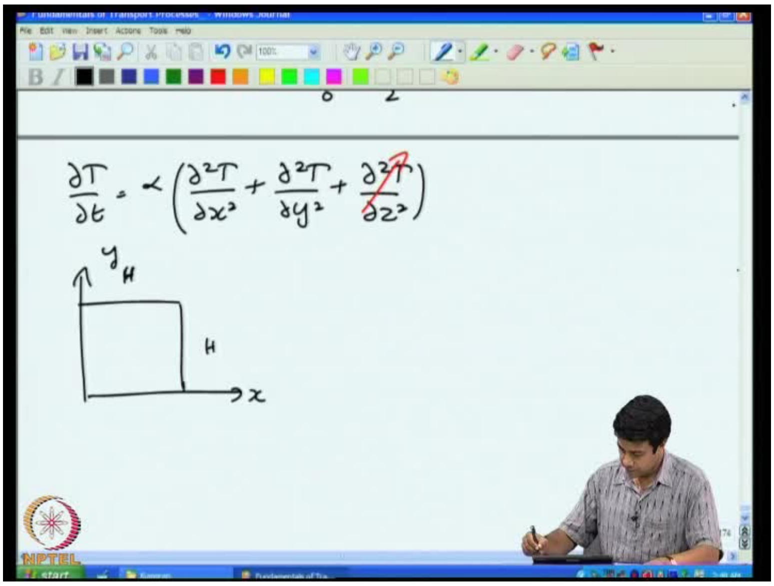

So, this is an unsteady state diffusion problem. So, let us start, no velocity therefore the equations are dT by dt is equal to alpha times d square T by dx squares plus… There are no sources or sinks within this volume.

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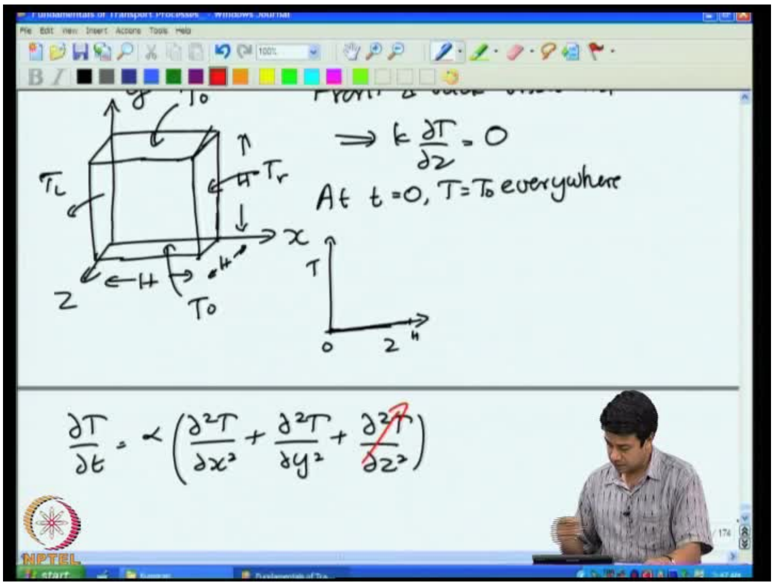

Note that the front and back faces are insulated; that means, that k times dT dz is equal to 0 on the front and back faces. That means, if I plot the temperature as a function of Z along the cube from 0 to H, the slope is 0 here, the slop is 0 here.

So therefore, there is no forcing on the front and back faces. There is nothing to keep the temperature different from the initial temperature in the front and back faces. Since there is no heat flux in that direction, one would not expect any variation of temperature in that direction. There will be variation of temperature only on the flux is non-zero, so that the temperature gradients are non-zero. So, straight away from the fact that there is no flux on the front and back faces, one can straight away say that there is no dependence of temperature on the Z coordinate.

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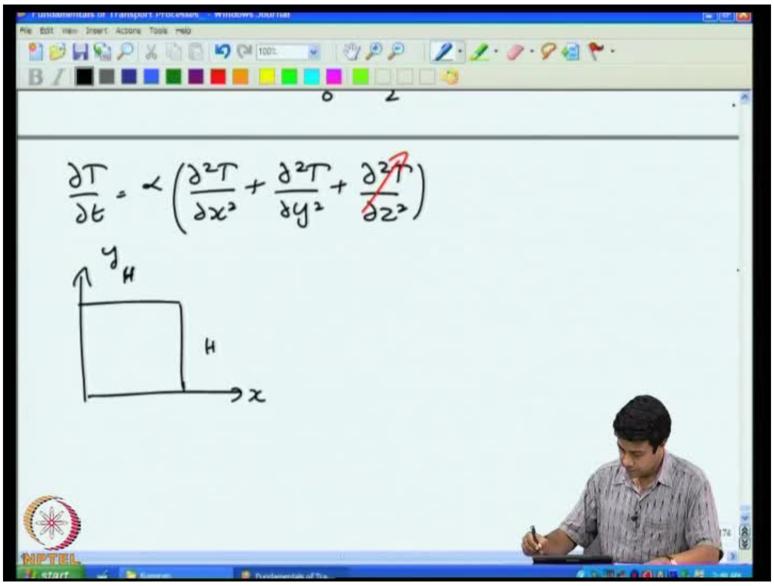

So, therefore, the variation of temperature with z becomes identically equal to 0 and one can neglect variations in the z direction. So, in that case it becomes a two-dimensional problem. Two-dimensional problem, x y on a square of side H, where I have on the top and bottom faces, I have T is equal to T naught and T is equal to T naught, T is equal to T l on the left phase and on the right phase T is equal to T r, the temperature on the right face.

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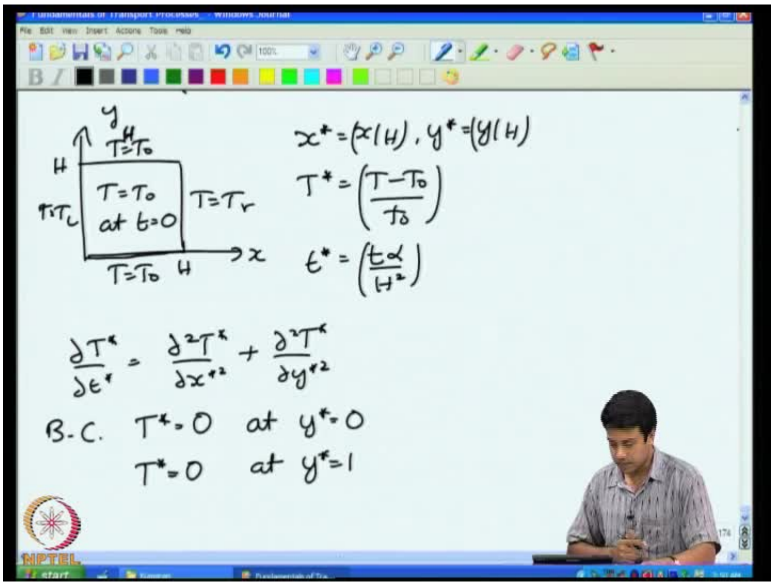

And I have to solve this problem. Initially at time T is equal to 0, T is equal to T naught at T is equal to 0. So, first things first, we scale our coordinates. The simplest scaling to use for the length of course, since both the height and width of this cube are H, I can use x star is equal to x by H and y star is equal to y by H. So, that is scaling for x and z. The temperature, I can define a scale temperature as T minus T naught by T naught. Why I am doing this? Previously when we discussed separation of variables problems, I said that we have to get homogeneous boundary conditions on at least two faces. If I define T star is equal to T minus T naught by T naught, then T star becomes 0 at the bottom and the top and therefore, I get homogenous boundary conditions. We will see the importance of this a little later. In addition, this is a transient problem, so therefore I can define the scale time as t times alpha by H square. Once I do that my equation becomes partial T by partial t star is equal to partial square T by partial x star square plus T square T by dy star square.

What are the boundary conditions? The boundary conditions are T star is equal to 0 at y star is equal to 0, that is this bottom phase. So, at the bottom phase T is equal to T naught and therefore, T star is equal to 0. T star is also equal to 0 at y star is equal to 1. y is equal to H is the top face, therefore y star is equal to y by H is equal to 1. So therefore, T star is equal to 0 at y star is equal to 1. T star is equal to T r minus T naught by T naught at T l minus T naught by T naught at x star is equal to 0.

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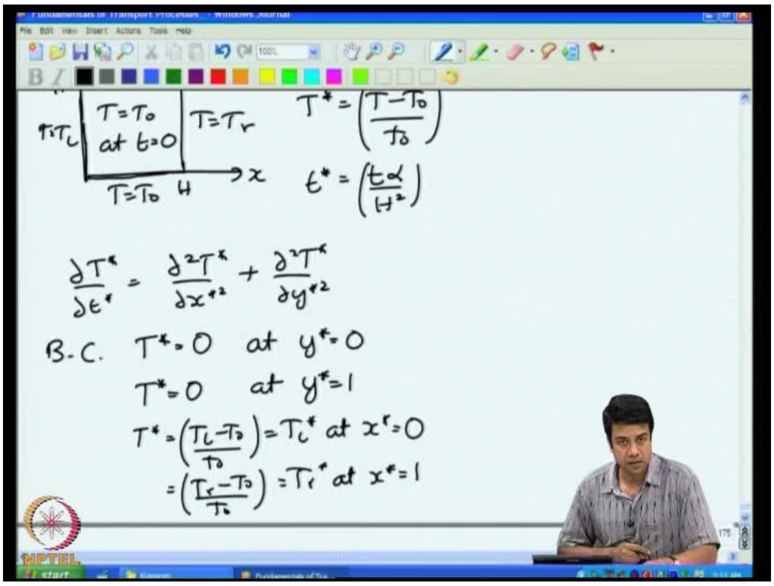

On the left face T is equal to T l therefore, T star is equal to T l minus T naught divided by T naught. And I will call this as T l star at x star is equal to 0 and is equal to T r minus T naught by T naught is equal to T r star at x star is equal to 1. So, those are the boundary conditions on the bottom, top, left and right.

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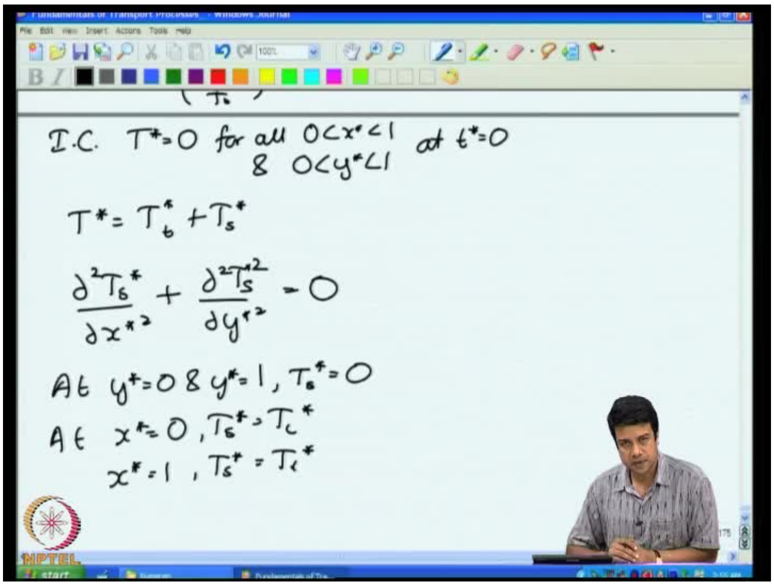

I also have initial conditions. T star is equal to 0 for all 0 less than x star less than 1 and 0 less than y star less than 1. If we were within the domain, T star is equal to 0 because T is equal to T naught at the initial time, T star is equal to 0. So, at the initial time the temperature is equal to 0 everywhere. And at that particular time you have put in two source on the right and the left, there is constant temperature condition on the top and the bottom and you want to find out what is the temperature profile as a function of time.

So, how do we solve this problem? First things first, we need to find out what is the steady state temperature profile. What does the temperature go to in the limit as T goes to infinite. In that case, you need to know what is the final steady state temperature profile. As the time goes to infinity the system should attain the steady state, where the temperature is independent of time. So therefore, first thing is we will separate out T star into transient part plus a steady part. The steady part of the temperature is the temperature in the limit as time goes to infinity. In that limit, you have a cube with T l on the left face, T r on the right face, top and bottom are at 0 temperature and you want to know what is the temperature, within the cube.

So, in this steady state for the steady problem, the equation becomes d square T s by dx square plus… by dy square is equal to 0 because there is no variation time. And the boundary conditions for this are at y is equal to 0 and y star is equal to 1, T steady is equal to 0. And at x star is equal to 0, that is the left face, the steady temperature is equal T l star. And at x star is equal to 1 the right face, the steady temperature is equal T r star. So, this is the steady state problem for a two-dimensional heat conduction.

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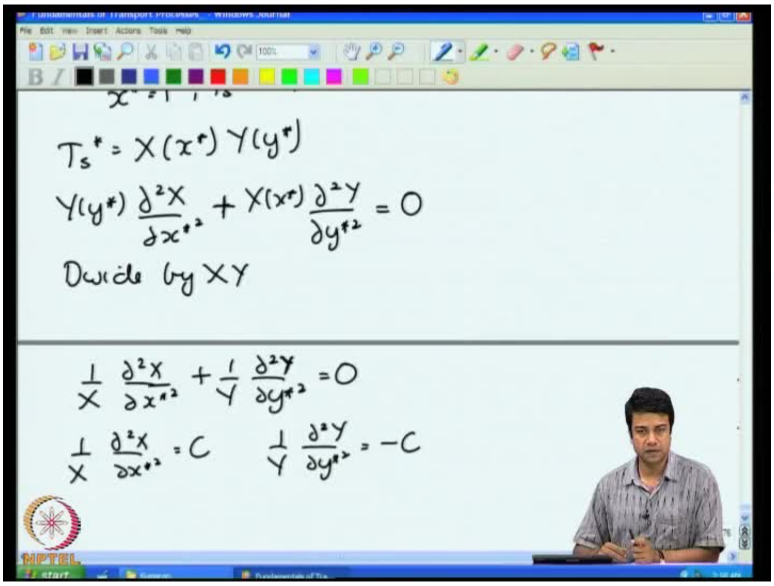

How do we solve this? We use the method of separation of variables. I say that T s star is equal to sum function of x times some function of y. So, I separate the variables into two parts, one of which is only a function of x, the other is only a function of y. I put that into the differential equation and divide throughout by x times y. So, I put this into differential equation and I will get y of y d square X by dx star square plus X d square y by dy is equal to 0 and I divide by x times y.

And that is going to give me 1 by X d square X by dx square plus 1 by Y d square Y by dy square is equal to 0. So, I have the sum of two function, one is only a function of X, the other is only a function of Y, the sum of the these two function has to be equal to 0, means that each of these individually has to be a constant.

Because if one of those function was not a constant, if X was a function of X for example, I could change X and keep X a constant and only one term would change, the other term would remain the same and that would no long satisfy the equality. Therefore, each of this individually has to be equal to a constant. Therefore if that constant is C, then I will have 1 over X d square X by dx star square is equal to C and 1 by Y d square Y by dy star square is equal to minus C, so that the sum of these two terms is identically equal to 0. Should this constant be positive or negative? If you recall when we did steady state problems, since we solved the separation of variables for the transient part of the equation and the sign of the constant was fixed by the fact that at long times the transient part of the temperature had to come back to 0. At long times the transient part of the temperature had to decrease to 0, which means that the transient part had to exponentially decreasing and that effectively fix the cost in that case. In this case, how do we determine whether this constant has to be positive or negative? Give it some thought and we will continue the separation of variables in this steady state problem in the next lecture.

So, I will continue with this and will tell you how to decide whether this constant has to be positive or negative. So, briefly in this lecture we started of determining a general differential equation for transport and Cartesian coordinations. The fundamental principle, the rate of change, the amount of concentration increase or decrease within the differential volume has got to be equal to sum of what comes in, what goes out as well as any production within that volume.

The change within that volume is equal to the change in concentration times the volume. And what comes in is due to two reason, one is due to diffusion the flux and the other is due to convection. The conductive transport is just equal to the velocity times the concentration itself, because the flux due to convection is equal to the concentration mass by unit volume times of velocity, which is length per time, velocity perpendicular to the surface length per time, multiply those two it gives you mass in per unit area per unit time, which similar to a flux. And therefore, we can add up the two contribution, one due to convection and the other due to diffusion, and divide thought out by volume and delta T and we get an equation, for a general equation for conservation in three-dimensional.

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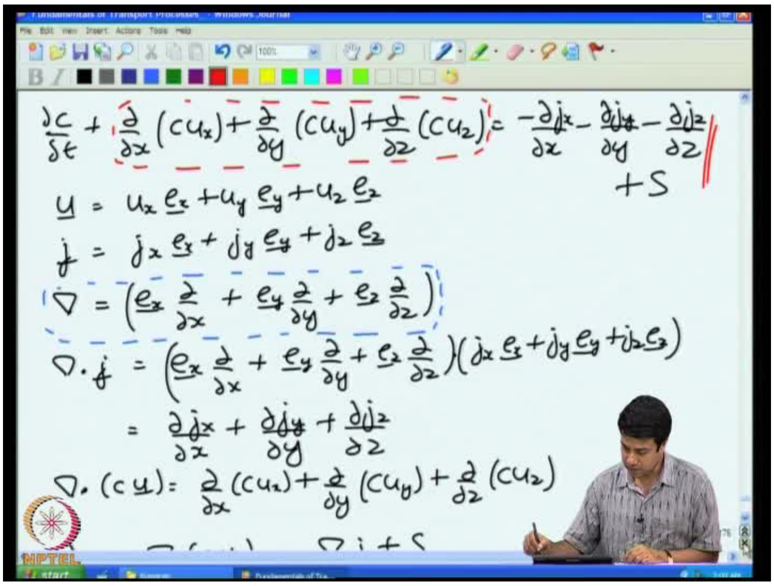

So, we saw this general equation for conservation in three-dimensions here. And I showed you how to write that in a more compact form. We defined the vector velocity, velocity is of course a vector, it has three components. The vector flux, once again this has three components. Flux gives you a rate of transport in one particular direction perpendicular to a surface, so it has a direction associated with it.

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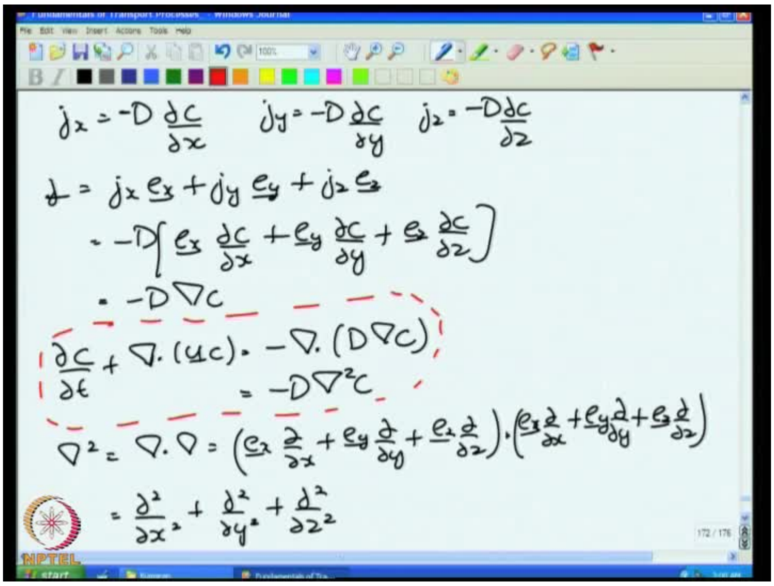

And in terms of that you can get a fairly simple form for the conservation equation and this was the form that we ended up with for the conservation equation of mass. Similar form for the conservation equation of energy, except that we substitute temperature instead of concentration and we substitute the thermal diffusivity instead of the mass diffusivity.

When we started solving a simple problem the heat conduction in a cube, note that this is now a 2 two-dimensional problem, it is not unidirectional. There is transport both in the x and the y directions. Because it was insulated in the z direction, there was no transport in that direction, but the procedure that we will formulate here will apply equally well even when there is transport in the z direction. So, procedure will be exactly the same. We will continue solving this problem in the next lecture. We will see you then. Thank you.