Turbulent Combustion: Theory and Modelling
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Lecture – 12
Heat and Mass Transfer

Welcome back. So will continue the discussion on our turbulent combustion and now will move to the topic on the heat and mass transfer. So, these are the things what will discuss and that will make the as I mentioned earlier that will make the building block for the turbulent combustion system.

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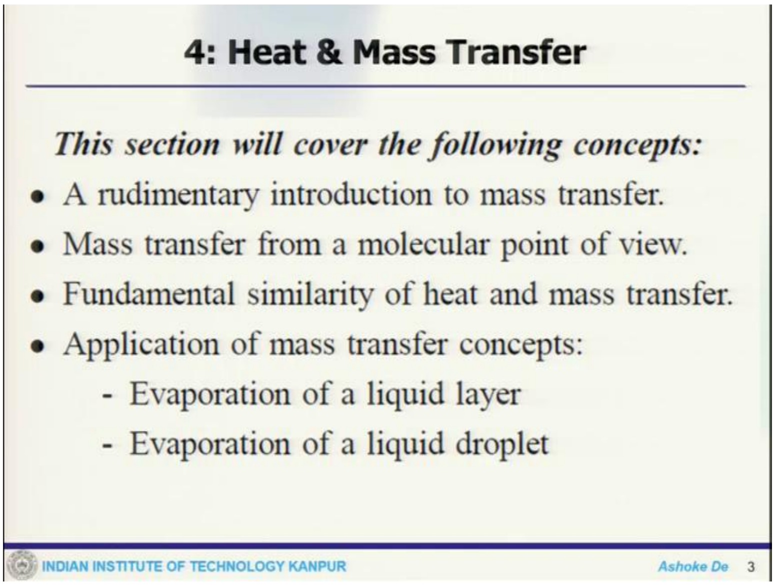

So what will now want to discuss here under this heat and mass transfer this thing is that we will look at the basics of the mass transfer and then will look at from the molecular point of view that means the mixing and diffusion and all this thing. Then we will go to little bit of the multiphase system and look at the evaporation of liquid layer and the droplet. So, this is a part of our two phase system or flow.

So, this will give you an idea how the single phase is different from the two phase system, but the more detailed discussion that will do at the end of this lecture.

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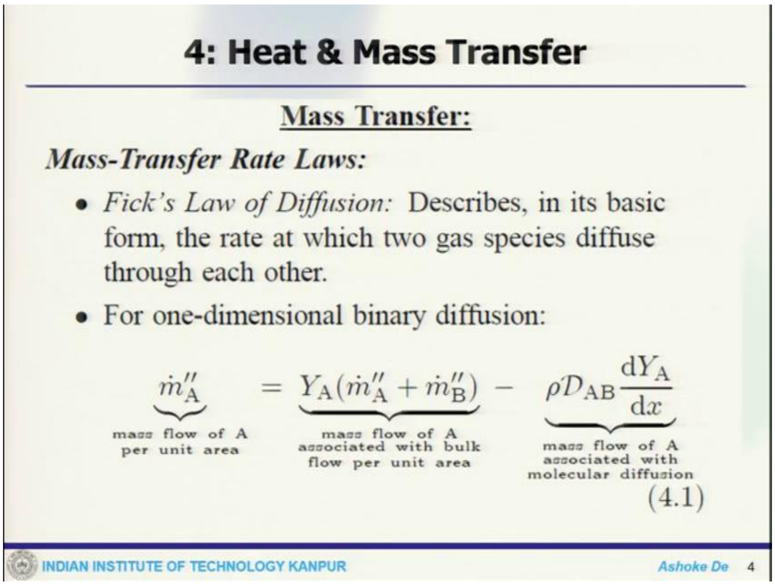

Now what we do in the mass transfer so one, is that I mean in a common sense one can think about that basically whatever mass comes in, it goes out. But when you talk about the transfer that means some mass is transferred. Now there is one important law which comes into the picture is the Fick's law of diffusion. So it describes its basic form so at which two gases diffuse through each other.

So, if I write in one dimensional binary diffusion. So this is a species A the mass flux of the per unit area. So, this is the mass flow of A associated with bulk flow per unit area. This is the mass flow of A within the molecular diffusion. So, this is how one can get it.

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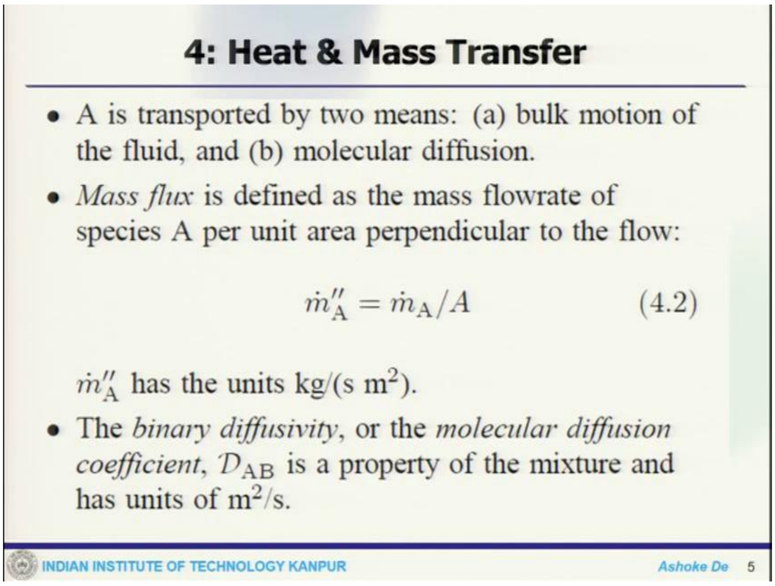

So, here the species A is transported by two means one a bulk motion of the fluid obviously and that is why the flux comes into the picture and in the diffusion that means it just like one can take an example of; if you take a simple room and one corner of the room basically, you want some stick the smell sticks and if you burn those sticks then there would be smoke which is found in one corner of the room. After a long period of time if you keep the room actually locked then the other corner also you get the smell of that nice smelling stick and that happens because of this transport of the species. So that means from one corner of the room, this species is getting transferred to the other corner and that is why the smell is sensed here, the other side. Now we should be slow because this is primarily happening because of the diffusion.

Because you kept the room locked from the outside. So, the internal flow field is also quite calm and laminar so the transfer due to fluid it is not that common due to diffusion so this slow process. So, that the same example, you can do when you burn the stick here and then from the back you actually use a foam. So then within a seconds or minutes probably other corner of the room, you will get to see the smell because that would be transported quickly.

Because they are the bulk motion of the fluid dominates that diffusion. So that is how the species diffusion actually or any scalar diffusion or scalar transport takes place either through the bulk motion or the molecular diffusion. Now you define the mass flux as how much mass is going out per unit area and the binary diffusivity called the molecular diffusion coefficient that is D_{AB} is a property of the mixture and has some units per metre square per second.

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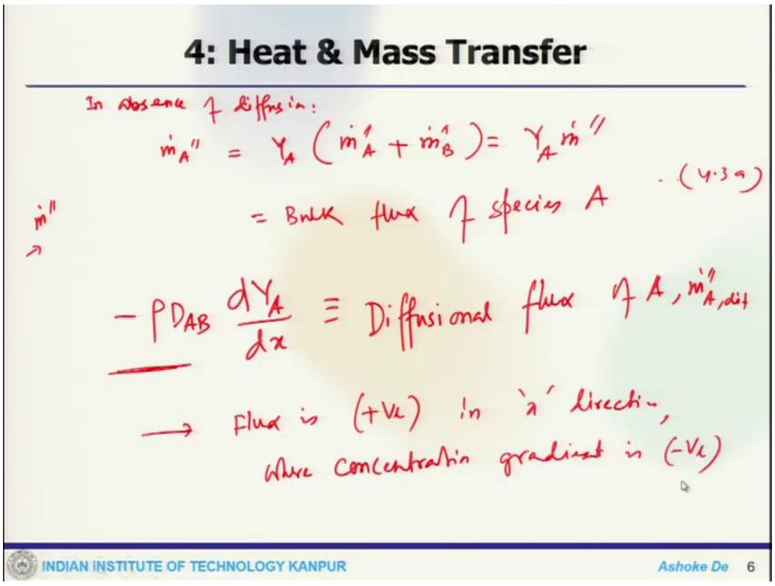

Now in absence of diffusion what you can get is that:

$$\dot{m}_A'' = Y_A(\dot{m}_A'' + \dot{m}_B'') = Y_A\dot{m}''$$

So which is nothing but your bulk flux of species A, ok? And $\dot{m}''$ is the mixture mass flux. Now the diffusional flux as an additional compared to the flux of the A. So, the diffusion flux is:

$$-\rho D_{AB}\frac{dY_A}{dx}$$

Which is the diffusional flux of A. So that is the component of the definition of flux.

So, that would also contribute to that thing. Now the negative signs here in this particular case this negative sign. So, the negative sign causes the flux to be positive in the X direction to this means the flux is positive in x direction where the concentration gradient is negative.

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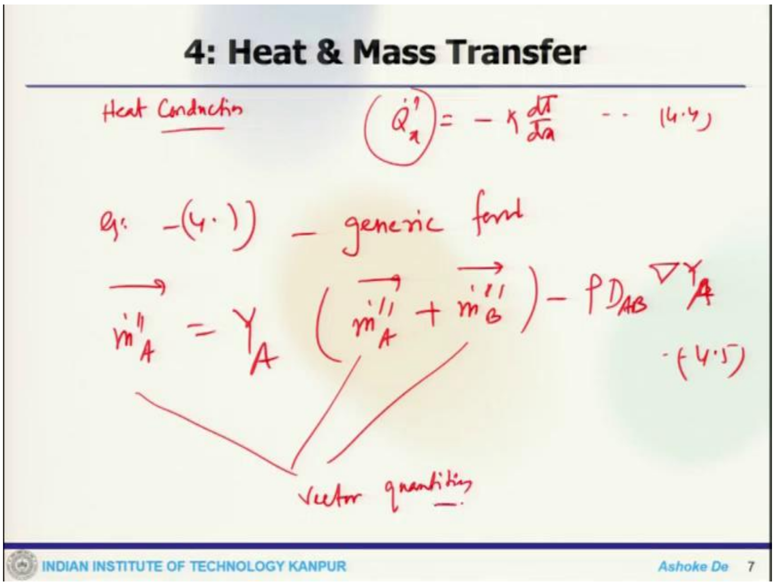

Now if you put analogy between diffusion and the heat conduction then one can look at the heat conduction equation where Fourier law says that:

$$\dot{Q}_x'' = -\kappa\frac{dT}{dx}$$

Ok? Now the expression indicates heat flux whether this case is the heat flux and the other case it is a mass flux. So, both these cases they will and their kind of proportional to the gradient of the either temperature or the scalar quantity the mass.

So, now more generic form would be the equation 4.1 more generic form would be:

$$\dot{m}_A'' = Y_A(\dot{m}_A'' + \dot{m}_B'') - \rho D_{AB} \nabla Y_A$$

Which is 4.5. So, obviously these are all vector quantities.

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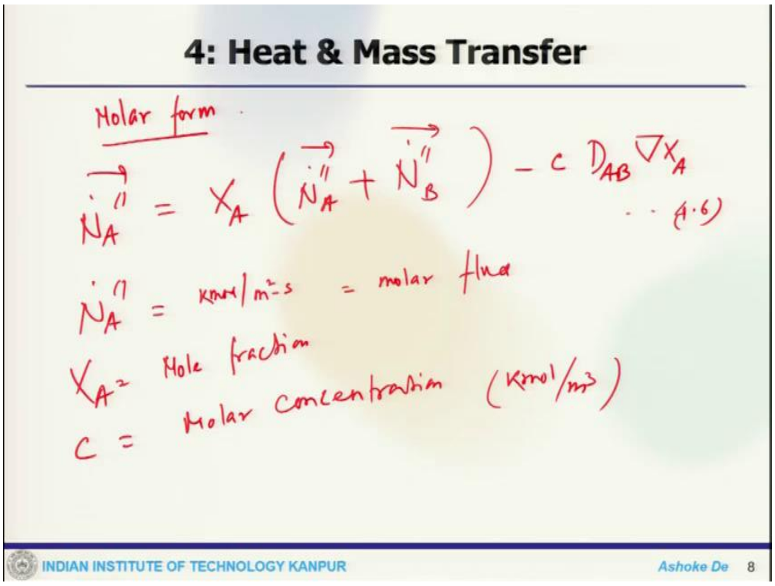

So, molar form of the previous equation so now if we write in the molar form will get:

$$\dot{N}_A'' = X_A\left(\dot{N}_A'' + \dot{N}_B''\right) - cD_{AB} \nabla X_A$$

Where $\dot{N}_A''$ is kmol/m^2-s is the molar flux of the this is the molar flux of species A, X_A is mole fraction and C is molar concentration which is again the unit is this. So, that is how you can write in molar form.

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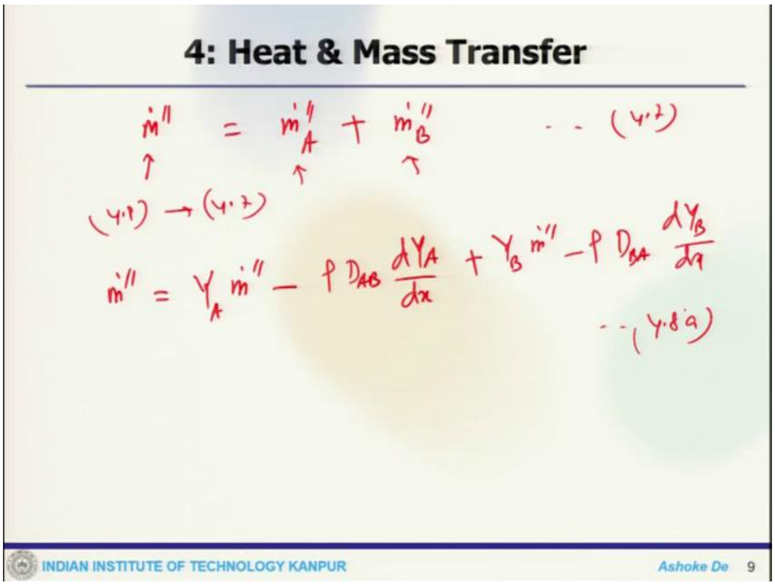

So, meanings of bulk flow and the diffusion flux can be better explain if we consider that:

$$\dot{m}'' = (\dot{m}_A'' + \dot{m}_B'')$$

This is the mixture flux. This is the flux of A and this is flux of B. And if you substitute this species fluxes form so, 4.1 to 4.7, you get:

$$\dot{m}'' = Y_A\dot{m}'' - \rho D_{AB}\frac{dY_A}{dx} + Y_B\dot{m}'' - \rho D_{AB}\frac{dY_B}{dx}$$

So that is what you get.

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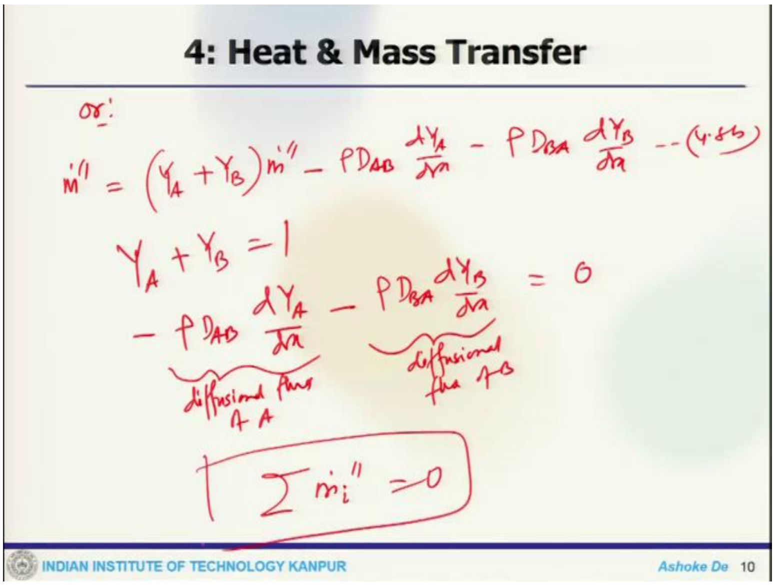

Or one may write:

$$\dot{m}'' = (Y_A + Y_B)\dot{m}'' - \rho D_{AB}\frac{dY_A}{dx} - \rho D_{AB}\frac{dY_B}{dx}$$

Now if you have a binary mixture which means:

$$Y_A + Y_B = 1$$

Then you get:

$$-\rho D_{AB}\frac{dY_A}{dx} - \rho D_{AB}\frac{dY_B}{dx} = 0$$

So this is your diffusional flux of A and this is your diffusional flux of B. In general one can write that:

$$\sum \dot{m}_i'' = 0$$

So, that is what one can write in generic form?

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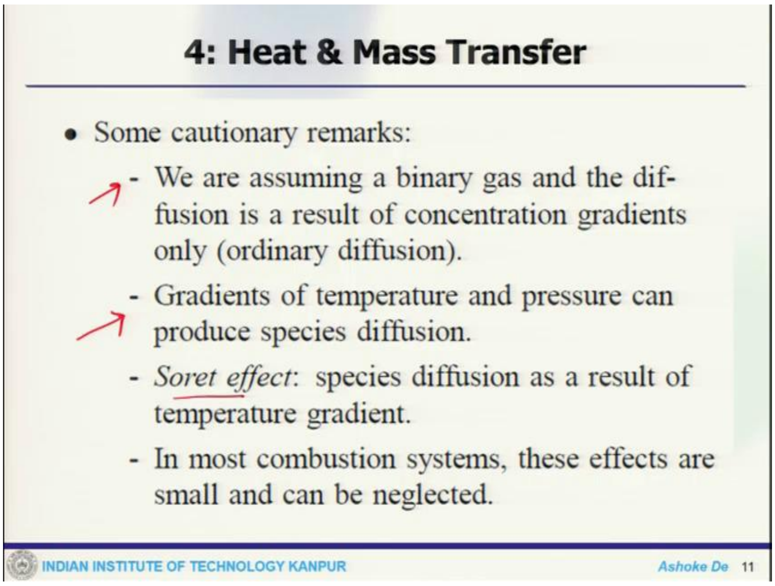

Ok some cautionary remarks. So we are assuming it is a binary gas and the diffusion is a result of concentration gradient only that is a first one. So that means ordinary diffusion. Now gradient of temperature and pressure can produce also diffusion species, so that what happens in any realistic system? Also there is known as Soret effect which is the species diffusion as a result of temperature gradient. So but this is quite small in combustion system so can be neglected.

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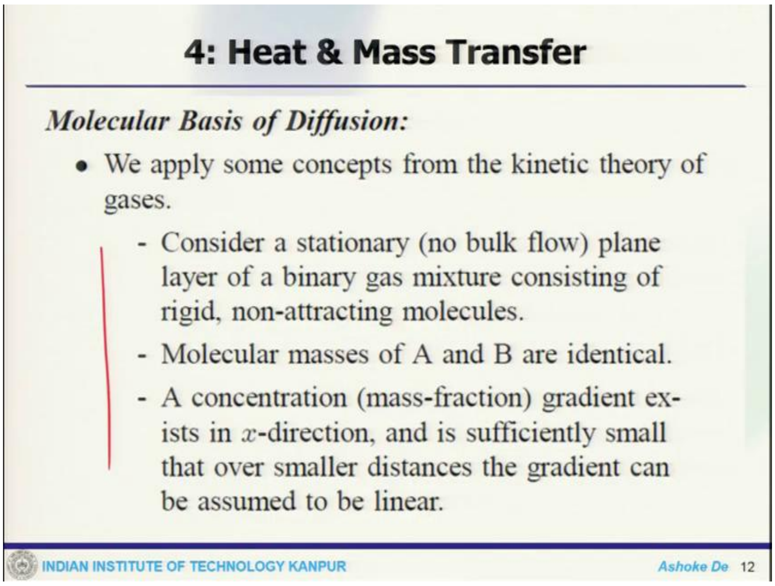

Now if you look at the molecular basis of this diffusion now what you are applying is the concept from the Kinetic Theory. So, you consider a stationary plane layer of binary gas mixture consisting rigid non attacking molecules. So, the molecular masses of A and B are identical. So, these are sum of this and the concentration gradient exist in a direction and sufficiently small over small distances gradient to be linear.

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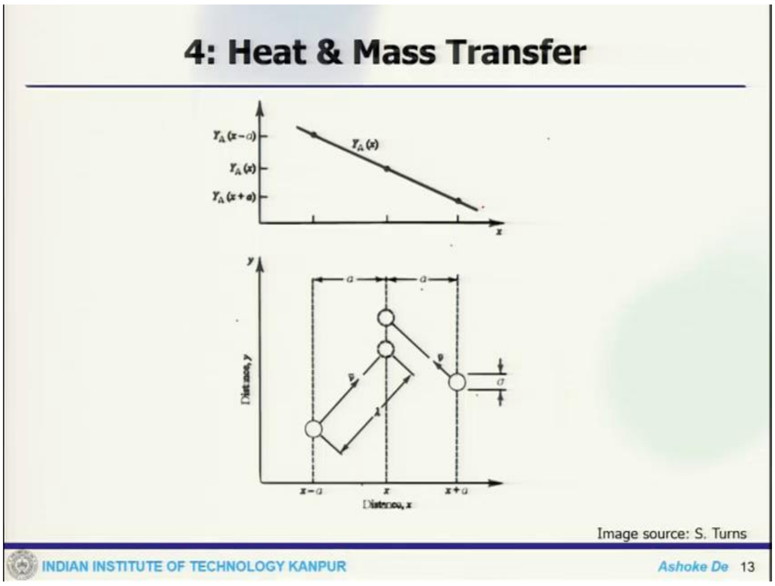

So, that if you want to just mention here, if you put that back in a plot, this is how they look like. This is distances. This is Y_A (x) and all this.

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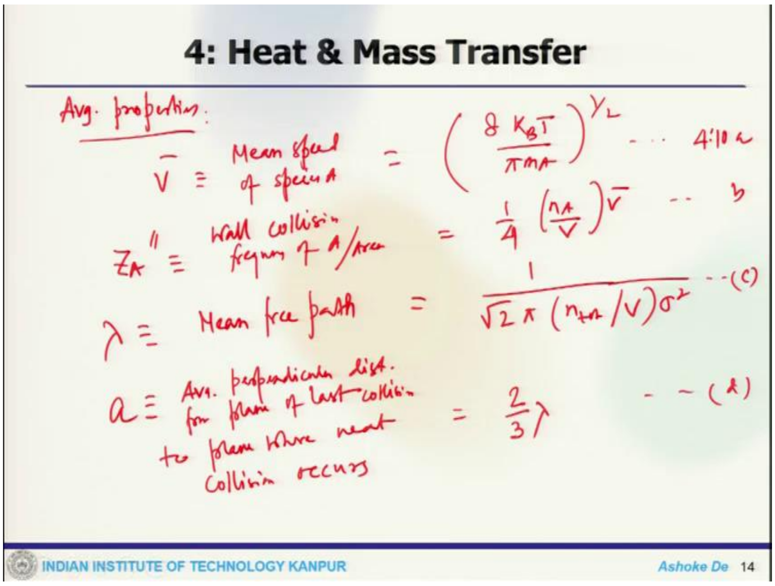

So, from kinetic theory average molecular properties one can calculate. So, these are all average properties so one may calculate that that is mean speed of species so that is:

$$Mean\ speed\ of\ species\ A = \left(\frac{8K_BT}{\pi m_A}\right)^{1/2}$$

This is your wall collision frequency of A per unit area which is:

$$Wall\ collision\ frequency\ of\ \frac{A}{Area} = \frac{1}{4}\left(\frac{nA}{V}\right)\bar{V}$$

Which is nothing but mean free path. So, that will give you:

$$Mean\ free\ path = \frac{1}{\sqrt{2}\pi(n_{tot}/V)\sigma^2}$$

And finally this is average perpendicular distance from plane of last collusion to plane where next collusion occurs which is:

$$a = \frac{2}{3}\lambda$$

So this is your 4.10a, b, c, d these are all 4.

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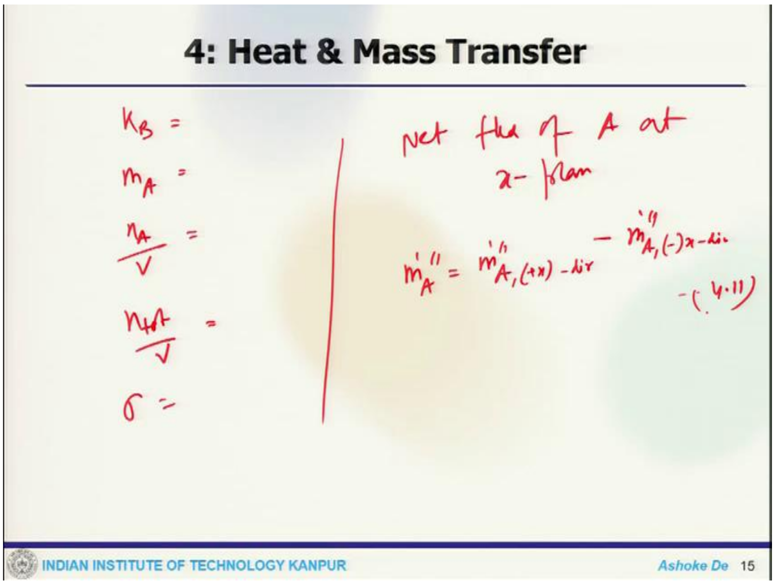

Now all this what you have got is that here K_B is Boltzmann constant, m_A is your mass of a single a molecule, (n_A/V) is your number of molecules per unit volume, (n_{tot}/V) is the total number of molecules per unit volume, $\sigma$is the diameter of both A and B molecules then one can write:

$$\dot{m}_A'' = \dot{m}_{A(+x)dir}'' - \dot{m}_{A(+x)dir}''$$

So that is what one can write.

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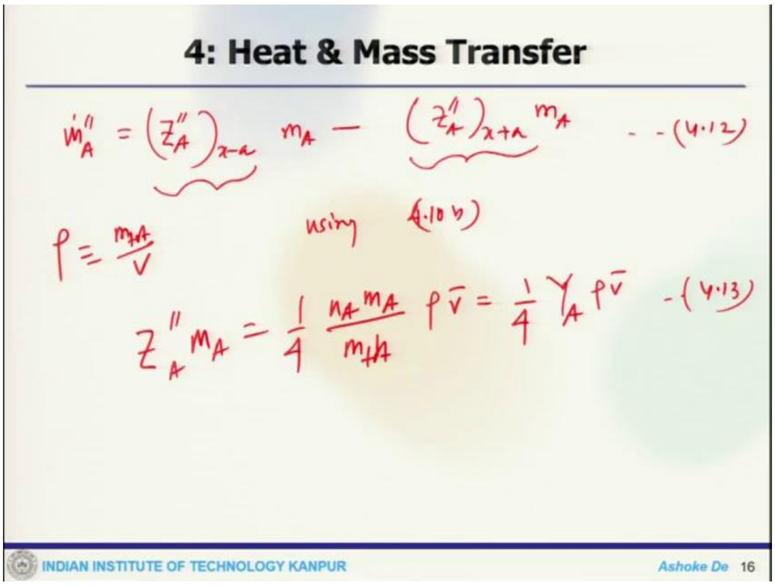

Now if you bring in the collision frequency in terms of collision frequency. This is:

$$\dot{m}_A'' = (Z_A'')_{x-a} m_A - (Z_A'')_{x+a} m_A$$

This is your number of A crossing plane X originating from x-a and this is number of A crossing plane X originating from the plane x+a. So, these are components since now:

$$\rho = \frac{mA}{V}$$

Then we you can relate this collision frequency to the mass fraction. Using 4.10b, so one can write this and this is how one can correlate things with each other:

$$Z_A'' m_A = \frac{1}{4}\frac{n_A m_A}{m_{tot}}\rho\bar{V} = \frac{1}{4}Y_A\rho\bar{V}$$

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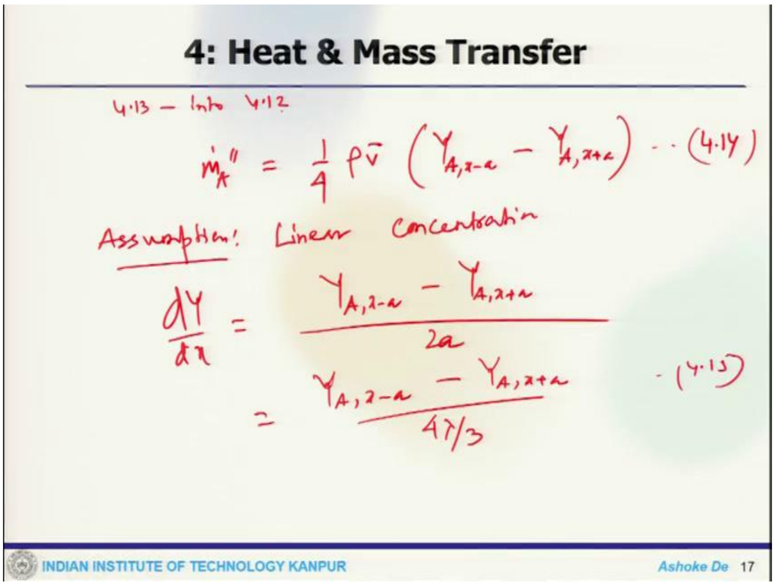

Now you substitute 4.13 into 4.12 so we get:

$$\dot{m}''_A = \frac{1}{4}\rho\bar{V}\left(Y_{A,x-a} - Y_{A,x+a}\right)$$

So that is 4.14, now you may assume linear concentration. So one of the assumptions is the linear concentration, so, concentration assumption and then you can find:

$$\frac{dY}{dx} = \frac{Y_{A,x-a} - Y_{A,x+a}}{2a} = \frac{Y_{A,x-a} - Y_{A,x+a}}{4\lambda/3}$$

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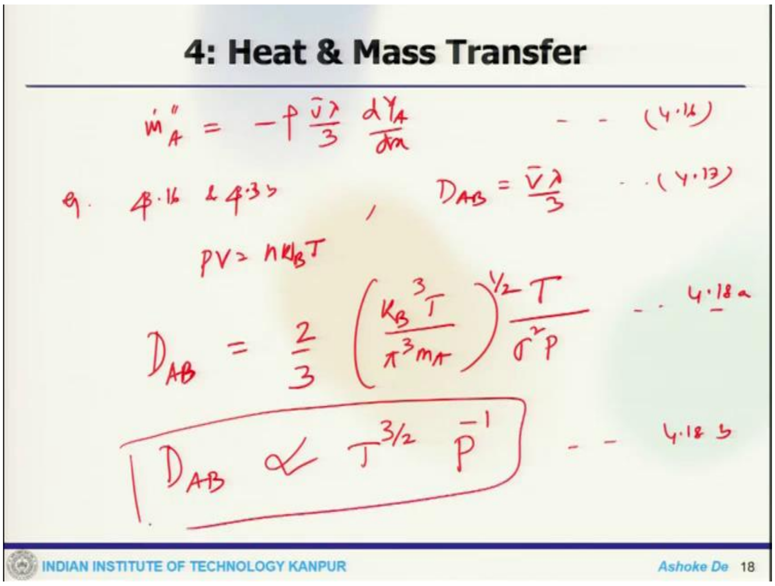

Now from this 4.14 and 4.15 one can write that:

$$\dot{m}''_A = -\rho\frac{\bar{V}\lambda}{3}\frac{dA}{dx}$$

Now if you compare equation 3.16 with 3.3b our D_{AB} is nothing but:

$$D_{AB} = \frac{\bar{V}\lambda}{3}$$

So, this should be 4.16 with 4.3b. Now substituting this $\bar{V}$ along the ideal equation of state which is equals to:

$$PV = nK_BT$$

We get:

$$D_{AB} = \frac{2}{3}\left(\frac{K_B^3T}{\pi^3 m_A}\right)^{1/2}\frac{T}{\sigma^2 P}$$

So, that is your binary diffusion coefficient or one can write:

$$D_{AB} \propto T^{3/2}P^{-1}$$

Which is important correlation and from which clearly says that the diffusivity depends on temperature and pressure.

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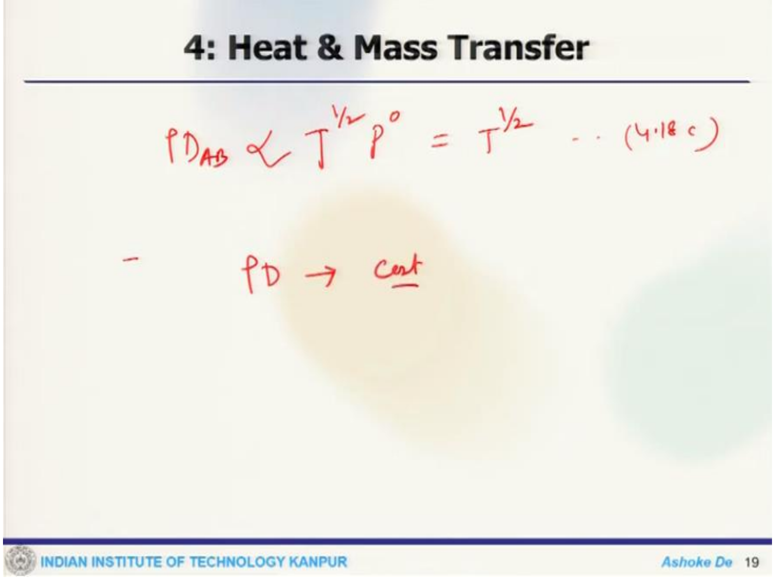

So, mass flux is ρD_{AB} which is proportional to $T^{1/2}P^0$ which is essentially $T^{1/2}$ 4.18. In some practical of simple combustion calculation actually the temperature dependence is essentially neglected and ρD_{AB} can be treated as constant. Now if we compare the heat condition, we apply the same kinetic theory concept the transport of energy. Same, assumption in the molecular diffusion and V and Lambda have same definition.

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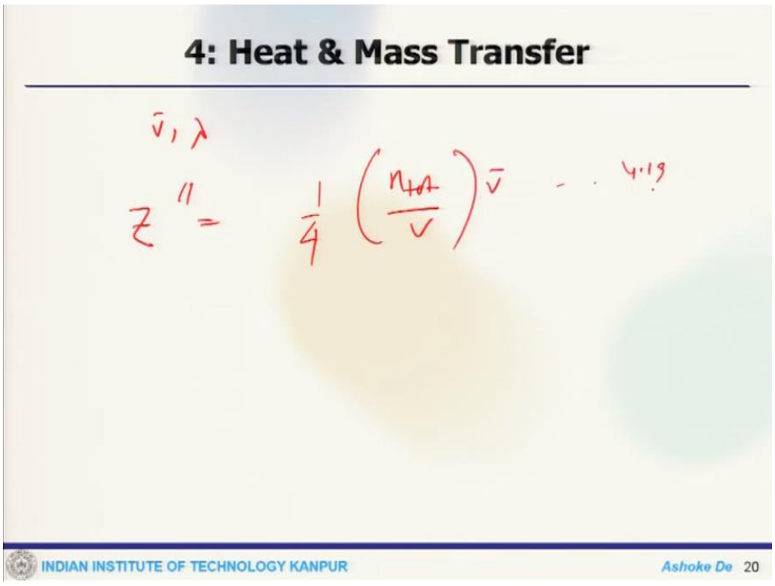

So, the molecular collision frequency one can get:

$$Z'' = \frac{1}{4}\left(\frac{n_{tot}}{V}\right)\bar{V}$$

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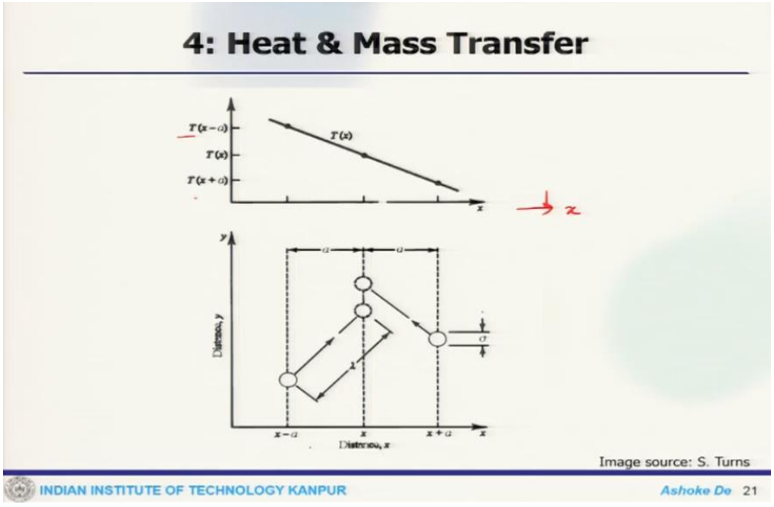

So, that is what you get and if you put that thing in a plot, this is how the temperature along the X direction with the temperature profile is the plane x-a and this is x+a, and if you look at that distance in the y and this is the plane with the diffusion properties changes. Now in the no interactions at a distance or hot sphere model of the gas the only energy storage mode is molecular translation energy, kinetic energy.

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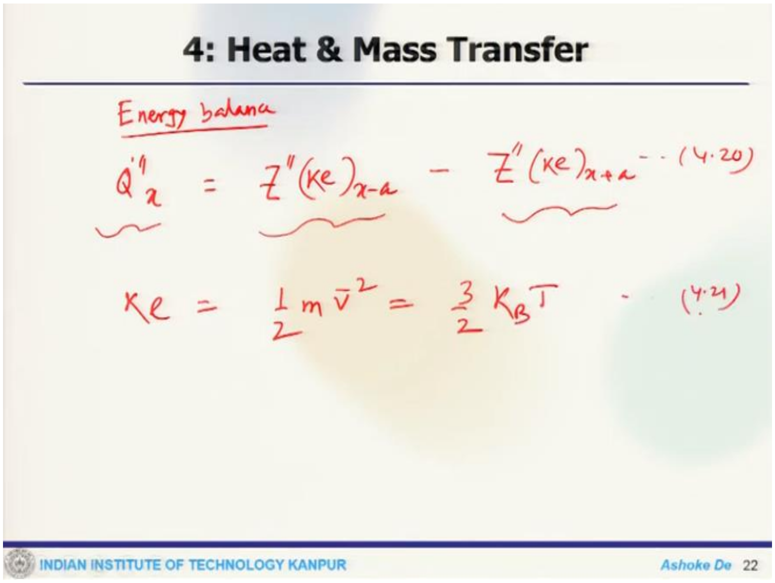

If you write energy balance so you will have $\dot{Q}_x''$ that is net energy flux in the X direction. Now kinetic energy flux with molecules from x-a to x would be collision frequency $(Ke)_{x-a} – Ke_{x+a}$. So this is your heat flux in the X direction. This is kinetic energy flux with molecules from x-a to x, this kinetic energy flux with molecules from x+a to x. Now Ke is given by:

$$Ke = \frac{1}{2} m \bar{V}^2 = \frac{3}{2} K_B T$$

So, that is the correlation that you have for kinetic energy.

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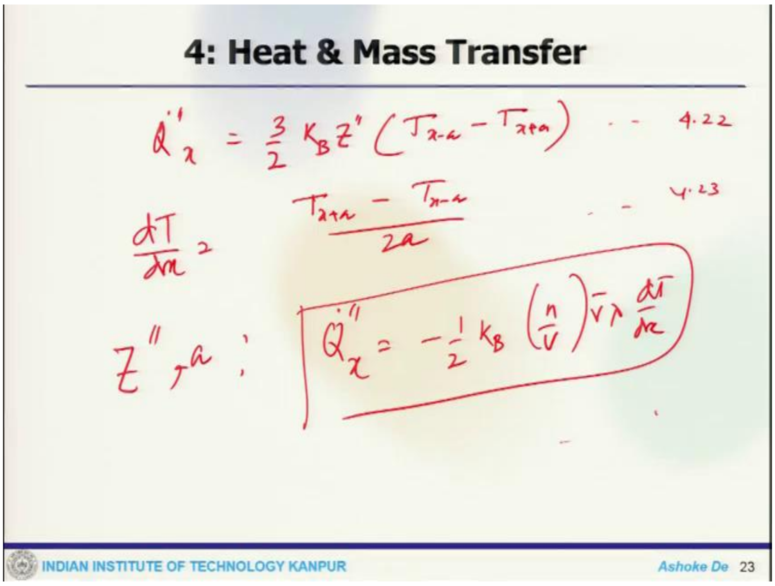

Now, one can write the heat flux and can be correlated with temperature and the heat flux one can write like:

$$\dot{Q}_x'' = \frac{3}{2} K_B Z'' (T_{x-a} - T_{x+a})$$

So and the temperature gradient is:

$$\frac{dT}{dx} = \frac{T_{x+a} - T_{x-a}}{2a}$$

That is the simple interpolation one can write. Now if you put this 4.23 into 4.22 then you get the definition of heat flux and one can get:

$$\dot{Q}_x'' = -\frac{1}{2} K_B \left(\frac{n}{V}\right) \bar{V} \lambda \frac{dT}{dx}$$

So, this is a relation that you get for heat flux.

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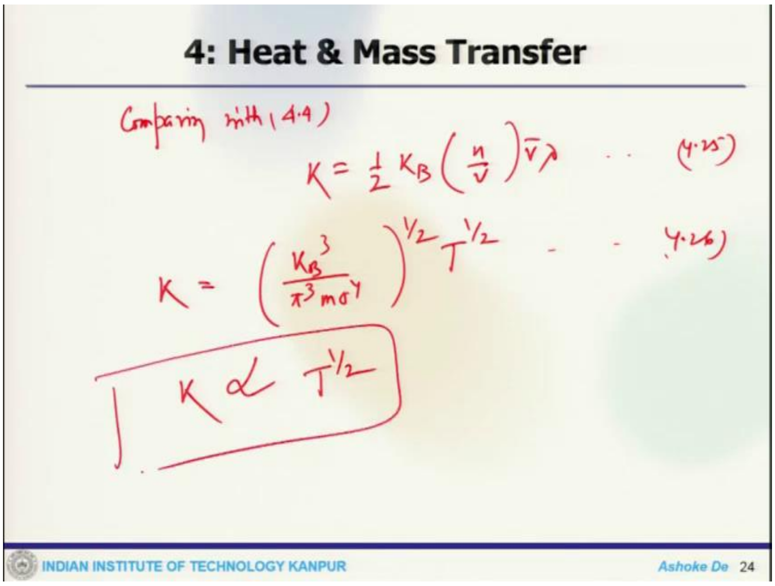

Now you compare with 4.4, now comparing with 4.4 you get:

$$K = \frac{1}{2} K_B \left(\frac{n}{V}\right) \bar{V} \lambda$$

Which is now in terms of T and molecular size. You can also represent K as:

$$K = \left(\frac{K_B^3}{\pi^3 m \sigma^4}\right)^{1/2} T^{1/2}$$

Now which says the dependence of K on temperature similar to ρ_D. So, one can write K is proportional to $T^{1/2}$. So that means there is a proportionality with temperature dependency for real gas dependency of T is quite large.

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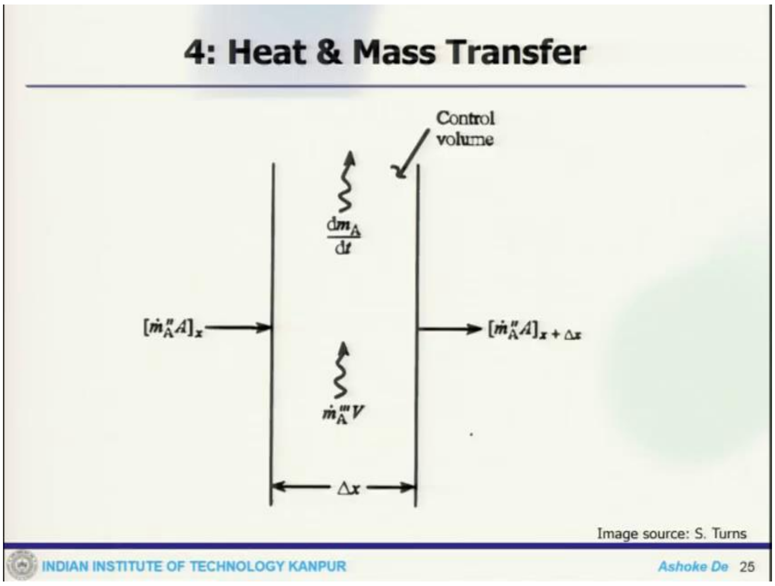

So now if you take this where the species A coming out from this plane which is x and x+Δx is going out this much and along this direction this is your control volume.

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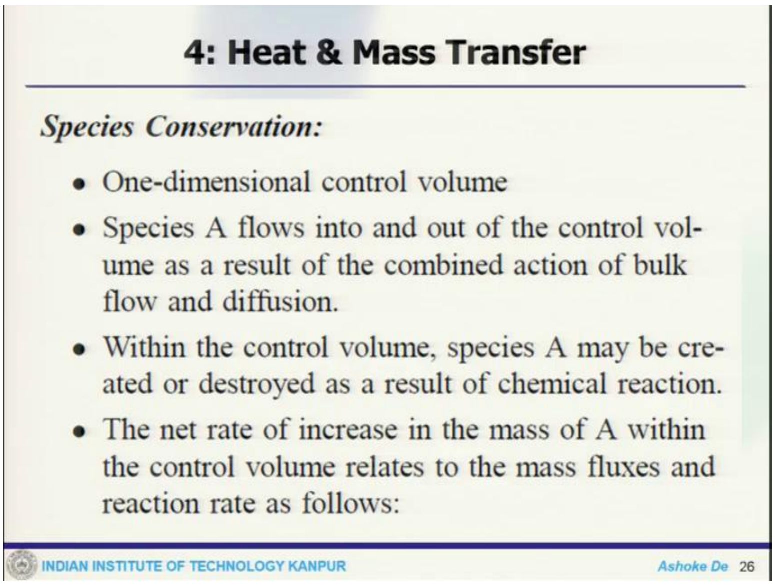

Now species conservation one can write it in one dimensional control volume. So this is 1-D control volume species A flows into and out of the control volume due to the effect of bulk flow and diffusion. Putting the control volume, we may be created or destroyed result of chemical reaction. And now the net rate increase of mass in the control volume is the mass flux of the reaction.

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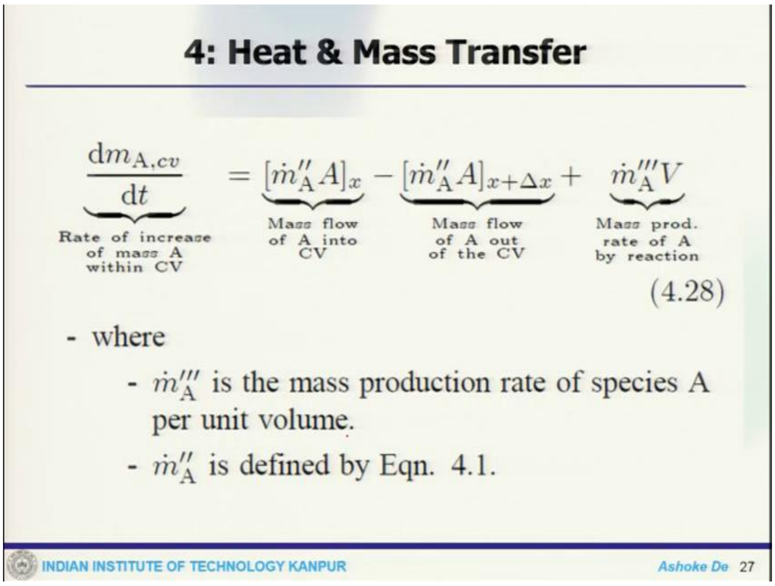

So, what we can write as that this is the rate of increase of mass A within the control volume so $\left(\frac{dm_{A,cv}}{dt}\right)$ for control volume with respect to time. This is the mass flow A into CV that we have already seen from the control volume. This is the influx this is the out flux. This is the mass flow out of the control volume. This is at plane x and this is a plane x+Δx and mass production to the control volume.

So if mass production of species per unit volume if there is no mass production this term will not contribute to anything else.

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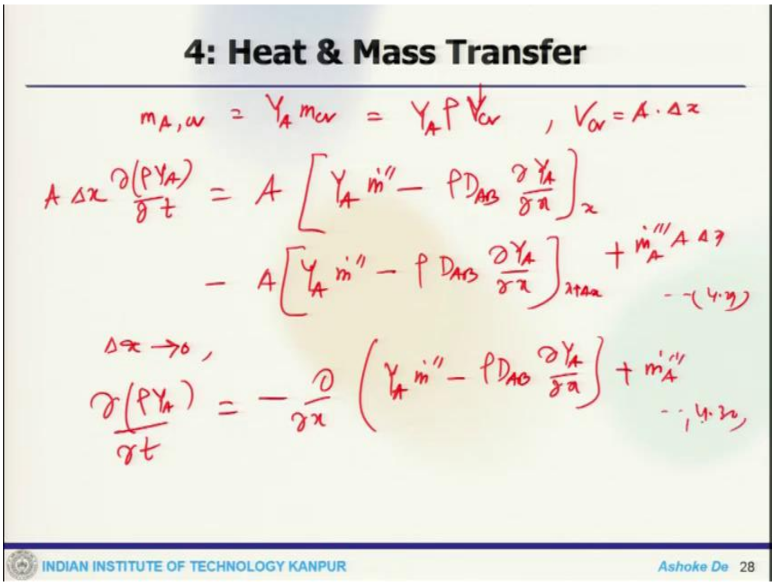

Now it in the control volume:

$$m_{A,cv} = Y_A m_{cv} = Y_A \rho V_{cv}$$

And volume of control volume is:

$$V_{cv} = A.\Delta\text{x}$$

Then what we can write the previous equation show 4.28 one can write as:

$$A.\Delta\text{x}\frac{\partial(\rho Y_A)}{\partial\text{t}} = A\left[Y_A\dot{m}'' - \rho D_{AB}\frac{\partial Y_A}{\partial x}\right]_x - A\left[Y_A\dot{m}'' - \rho D_{AB}\frac{\partial Y_A}{\partial x}\right]_{x+\Delta\text{x}} + \dot{m}_A'''A\Delta\text{x}$$

This is rewriting the previous equation 4.28 into this. Now dividing this both side by $A\Delta$x and taking the limit that Δx tends to zero then what we get:

$$\frac{\partial(\rho Y_A)}{\partial\text{t}} = -\frac{\partial}{\partial x}\left[Y_A\dot{m}'' - \rho D_{AB}\frac{\partial Y_A}{\partial x}\right] + \dot{m}_A'''$$

So, this what you get.

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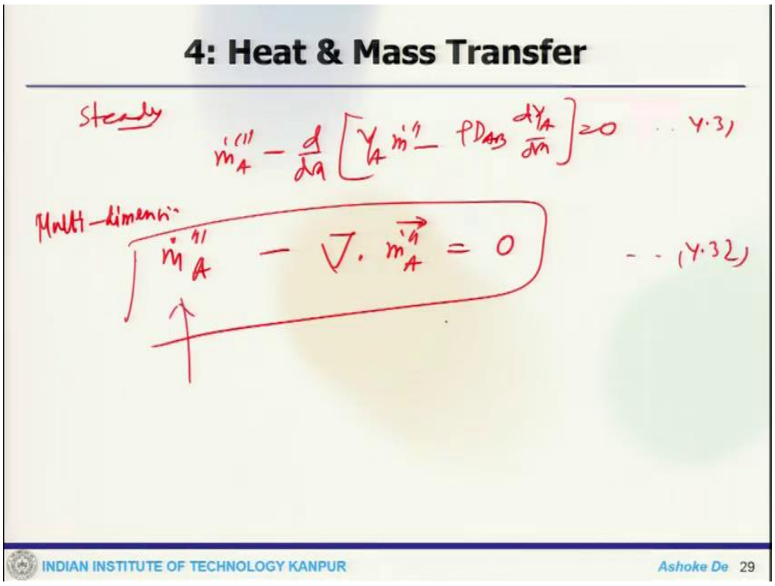

Now for steady flow one can simplify this as:

$$\dot{m}_A''' - \frac{d}{dx}\left[Y_A \dot{m}'' - \rho D_{AB} \frac{\partial Y_A}{\partial x}\right] = 0$$

So this is 4.31 is a steady flow one-dimensional form of species conservation for binary mixture for multidimensional case this can be written as for multidimensional one can write as:

$$\dot{m}_A''' - \nabla \overrightarrow{\dot{m}_A'''} = 0$$

So this for multidimensional phase where this is the net rate of species A production by chemical reaction. And this is the net flux species A out of the control volume. So this is how you can get from 1D and multidimensional case. We will stop here and continue the discussion in the next lecture.