

Fundamentals Of Combustion (Part 1)

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Lecture - 30

Transport Equations and Molecular Model for Transport Process

Let us start this lecture with a thought process chronic consumerism is consuming the cultural heritage of Mother India, at this moment at an alarming rate. Why I am saying, you people to take care of it. Let us now recall what we learnt in the last lecture; we basically looked at how to handle, you know the diffusivity you know particularly for momentum, and the heat transfer. So, we have derived constitutive equation for momentum transfer right, and also the heat transfer right.

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MASS TRANSFER

- > Two parallel plates-separated by 'Y'.
- > Upper plate is maintained wet.
- > Lower plate is kept dry (dehydrating agent)
- > Water vapor evaporates at upper plate
- > Partial pressure of water vapor is maintained at saturated vapor pressure of water
- > Thus concentration gradient exists between the two plates
- > **Mass flux**-proportional to concentration, C_A inversely proportional to distance Y_D

Handwritten notes:

Molecular weight
 $n_A'' \propto \frac{C_A}{Y_0} \propto \frac{C_A - 0}{0 - Y} \propto \frac{dC_A}{dy}$

$n_A'' = -D_{AB} \frac{dC_A}{dy}$ — (1)

$\Rightarrow n_A'' = -D_{AB} MW_A \frac{dC_A}{dy} = -D_{AB} \left(\frac{MW_A}{R_u T} \right) \frac{dP_A}{dy}$

$\Rightarrow n_A'' = -D_{AB} \frac{dP_A}{dy}$ — (2)

molecular diffusivity (m^2/s)
 $n_A'' = -D_{AB} \frac{dY_A}{dy}$ — (3)

For an ideal gas:
 $C_A = \frac{n_A}{V} = \frac{P_A}{R_u T}$; $P_A = f_A \frac{P}{f}$
 $\Rightarrow f_A = \frac{P_A MW_A}{R_u T}$
 $Y_A = \frac{f_A}{f}$

And today we will be looking at the mass transfer, if you look at mass transfer you know like it is due to the molecular motions. And you know the very example of that suppose some of you might be using perfume suppose you are having perfume, but I could smell that you are having perfume provided I am having a good nose, or sensor in is good enough. And there will be transfer of mass, and that mass transfer takes place because of what, because of what you call the concentration gradient.

Let us consider the in the similar way we have deal to it considering the kind of you know space, where there is a gradient. For example: if I consider you know some region

Y D and let us say that is a some water in this we are having porous which is at you know kind of a gaseous state; that means, steam right saturated steam, and this is having here and this is of course, 0 at t is equal to 0 there is nothing you know like lake kind of things there is no water as such, but air may be there right, you cannot avoid air such (Refer Time: 02:29) make it vacuum.

And let us say in these plates you know in some reason here, which I will be using such that 0 you know water vapour will be there. How can you conduct experiment, I can have something which can observe the water moisture that is basically silicone gel I can use, and then some kind of a this thing which will keep it, and suddenly at t is equal to 0, I will start then what will happen; that there will be what you call this concentration gradient will be existing here between these upper plate that is y directions here, right and between these 2 plates, and there will be the mass will be transferring, because the concentration gradient is there therefore this concentration will be changing due to the molecular motion. And the mass flux if you look at it is you know goes on changing with respect to time it may be different profiles right, it may be different profiles kind of things as the time increases right.

So, what will happen that if a lot of time is a laps then it will be attending a steady state values right. And the final distribution of concentration in a steady state the profile will be looking like that, if I consider this as a x and this is your y direction, the mass flux you know is proportional to the concentration C_A which is here right and of course, this will be at a 0 concentration kind of things.

So therefore, this will be let us considered as a mole fraction right, because number of moles per unit volume is basically what do you call the concentration. So therefore, the mole fractions of what do you call A if I say this is space is a is proportional to C_A by Y I can say this is D I am using D diffusivity the distance right, and that is proportional to C_A divide by 0 minus y is proportional to $d C_A$ by $d y$ right, if I put this thing as a mass flux what I have to do, basically allowed to say that I will multiply you know this things, and I can write down let me first write down this A is equal to diffusivity D A B minus sign will be there, and $d C_A$ by $d y$, right. So, I can say this is equation 1, and if I say I want to have a mass flux what I will get, I will basically multiplied by w_A , here and this side I will multiplied by w molecular weight of A, right.

This is molecular so then I can write down as this is mass flux of A is equal to minus $D_{AB} \frac{dC_A}{dy}$ right, and now I will be more interested to express this in terms of the density rate, for that I will use an ideal gas right for an ideal gas, we know that C_A right is nothing, but your n_A by V is equal to P_A by $R U T$ P_A is partial pressure of species a right.

And similarly, I can write down P_A is $\rho_A R U T$ by molecular weight of a right M_A , and if you look at this in place of C_A , I will be putting this like a P_A by $R U$, I can right down minus $D_{AB} \frac{M_A}{R U T} \frac{dP_A}{dy}$ this nothing, but your D_{AB} by $d y$ right. So, M_A by $R U T$ if you look at so, if I will take this inside right, what it will be it will be we know that basically ρ_A will be P_A , M_A by $R U T$ is it. So, therefore, I can write down here this if I will take inside of these you know differential, because I will say it is not really changing with respect to that, why because this is the isothermal we are not considering there is a change in temperature, and then however then I can write down $\dot{M}_A$ is nothing, but D_{AB} into ρ_A by $d y$ right. Let us say this is 2 keep in mind that this ρ_A is nothing, but you mass you know transfer per unit volume density right mass per unit volume.

And D_{AB} is the molecular diffusivity, and whose unit is metre square per second right and of course, we know that ρ_A , I can express this in the terms of Y_A also Y_A what is that ρ_A by ρ yes or no. So, I can express this express you know mass flux, A minus $D_{AB} \rho \frac{dY_A}{dy}$.

Now, thus again also we will have to find out you know how we can get the values for diffusivity that is a very important point we need to look at it, but let us know basically summarise what we have learnt ok. And also look at in a very you know compact forms, and find out whether it is similar, you know if you look at Newton's law of viscosity.

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General Transport Equation: $\Theta = -D \frac{d\psi}{dy}$ $\Theta = \text{Flux related to mass, momentum, Energy}$

Law	Θ	D (m ² /s)	Main Quantity, ψ
Newton's Law of Viscosity	τ	ν	ρV (momentum/volume)
Fourier's Law of Conduction	$\dot{q}''$	α	$\rho C_v T$ (Internal energy/volume)
Fick's Law of Diffusion	$\dot{m}_i''$	D_{ij}	ρ_i (mass/volume of i th species)

$\nu = \text{Mass / Momentum / Energy}$
 $Pr = \text{Prandtl Number} = \frac{\text{Momentum Diffusivity}}{\text{Thermal Diffusivity}} = \frac{\nu}{\alpha}$
 $Sc = \text{Schmidt Number} = \frac{\nu}{D}$ Thermal diffusivity $\Delta = D$
 $Le = \text{Lewis Number} = \frac{D}{\alpha}$ Mass diffusivity
 $Le = \frac{\nu/D}{\alpha} = \frac{Sc}{Pr} ; \Rightarrow Le Pr = Sc$

This what you call is a tau that is your shear stress, and this is momentum diffusivity, and rho V is the momentum per volume right, and this alpha for the you know Fourier law of conduction is a heat flux right, and alpha is thermal diffusivity.

And of course, this I have given the C V at T, I will be using internal energy per unit volume, you can say enthalpy per unit volume also write, but this is we are considering both are same. And so far this Fick's law of diffusion is concerned, and this is m dot triple dash i d i j, and this is rho I basically mass per unit volume of I species right.

Now, I can write down that as you know single you know equations in similar format, I cannot say single equations either a compact format, then theta is equal to minus D you know d psi by d y, and theta if you look at what is the theta theta is basically the flux you know flux.

Because the shear stress is nothing, but you force per unit area right, and heat flux right Q, Q dot double dash is a flux. So, I can say the flux related to what it can be mass momentum right, not together all mass or momentum or energy any one of them right, and psi if you look at is basically the properties it can be mass, momentum, or energy right. So, you can write down in a very compact you know what we call format right.

You can just substitute these values, you can keep in mind that these you know we will be finding out we will be using this relationship, and it is very easy to remember this you

know because of this very simplified form of that; however, these all these units are what it is metre square per second all this diffusivity, one is momentum diffusivity, thermal diffusivity, and then molecular diffusivity. And we will see later on that we do you some non dimensional number parameters right, and to so, that it will be easier to handle right, one will be using Prandtl number right that is nothing, but your momentum transfer right, divided by the heat transfer, and μ by α right.

There is also another number which will be using is Schmidt number is nothing, but your momentum diffusivity I can put that way actually is not instead of transfer, I would like to put it as a diffusivity that is better, thermal diffusivity not heat diffusivity. This is again the momentum diffusivity by the mass diffusivity right D .

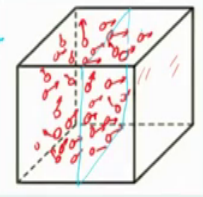
And there is a of course, Lewis number is α by D right, this is thermal diffusivity right, and mass diffusivity keep mind that this is both d are same like saying D is equal to D , I am using that ok. So, we can get a relationship right, basically if you look at Lewis number I can write down as Schmidt number right.

I can write down μ by divide μ by α this will be so, this is nothing, but your Schmidt number like, I can say this is as a Prandtl number this is as a α and this I am calling as a Lewis number. So, μ by D is nothing, but your Schmidt number, and then μ by α is nothing but your Prandtl number. So, I can write down as Lewis number Prandtl number is equal to Schmidt number. Now question arises how we can determine this properties from the molecular theory of point of view right that is the very important point what we need to look at it.

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Molecular Model of Transport Process

Molecule Motion : Chaotic in nature



Maxwell Boltzmann Distribution

$$F(v) = 4\pi \left[\frac{M}{2\pi R_u T} \right]^{3/2} e^{-\frac{M v^2}{2 R_u T}} v^2$$

v : molecule speed.

$$\bar{v} = \sqrt{\frac{8 R_u T}{\pi M}} = \sqrt{\frac{8 k_B T}{\pi m}}$$

So, because these are the properties what we you know the thermal diffusivity, mass diffusivity, and then what you call a momentum diffusivity, but however we will be more interested in what are the properties, like your viscosity conductivity and the what you call the mass diffusivity right. So, far that what will have to do will have to basically invoke the molecular model of the transport process; that means, what we have looked at kinetic theory of gases will have to look at that. Let us consider take a cube and where this molecules will be moving in or like this will be moving this direction right and right kind of thing it will be moving at a very different velocities.

It will be in random order right all will be moving at different velocity in different direction that it will be in chaotic in nature right, and there will be basically complete this order, the way you know we operate you know particularly our traffic in Kanpur will be in chaotic sense. Similarly molecules will be moving in a very chaotic way. But however, there will be some order right because it will be going and colliding with the surfaces for example, there is a surface here right there is surface you know total 6 walls are there, if I consider a you know surface like that, let us say surface in between right. This surface what will be happening the molecule will be going and act in a like atom body, then imaginary surface you say.

And then there will be change in the momentum rate of change of momentum will be there will be some pressure, which will be acting, there will be also you know some

molecules as moving so, that they will be changed in the energy level right. Similarly this will be transport of the what you call molecules right, because and that depends on what that depends upon the velocity, and when it is you know moving we know that it will be moving with the various velocities like RMS velocity we of considerate, it will be consider can also I can think of something average velocity is not it.

And we can think of something what we call probability of the velocity right most probable velocities. So, if you look at generally, because these molecular motions will be in chaotic in nature right, molecular motions will in chaotic in nature right. So therefore, what will happening we cannot really deal with the molecules. So, for that will have to look at some properties right, will have to use the statistical tools right, you can handle the statistical, and when you handle this statistical. So, we have looked at Maxwell Boltzmann you know distribution Maxwell right distribution.

That we have already seen I am just again rewriting the distribution right, $M W$ by $2 \pi R U T$ upon V square keep in mind that V is the molecular speed, and if you take this average values you will get basically V average, you know what will be dealing with average values which will be nothing, but what you call root over $8 R U T$ by $R M W$.

I can write down also $8 k B$ $k B$ is your Boltzmann constant into π by mass right, mass is the M is the mass of molecule right, and keep in mind that in this whenever it is moving, and there will be some kind of a average properties which will be coming in any plane regions, and this will be dependent on what this properties you know the rate of change of momentum or you know there will be molecular changes, taking place between multiple layer to layer. Let us see this is one layer to another layer, there will be some continuous properties which will be there it will be continuous, but in the molecular sense it will be random are you getting. For example each individual we are in a random fashion, but we look at a nation or some state you know it will be getting.

So, this kind of things which will be in the macroscopic level, but in the microscopic level, but when you talk about in the microscopic level, there will be some kind of properties right, and then that will be dependent on what a transport of this moment of mass and energy will be dependent on what on the average molecular speed of the right average molecular speed. And also it will be dependent on the collegian distance, or what we call mean free path, if the what you call molecular speed is higher; that means, there

will be net flux will be higher, if molecular free path will be higher average molecular free length or free you know path if it is higher what will happen the flux also will be higher.

Now we need to basically now consider this thing, and find out a relationship between what you call you know this properties with this molecular speed, and the mean free path for that will derive a relationship between further mean free path is not it. Because we have not derived relationship, for that purposes what will do will consider that you know like a simple case in which single molecule all molecule will be identical with the same diameter right of V travelling with molecular speed average molecular speed V average right V average kind of thing, and then will consider that. So, that then will derive relationship between the molecular diameter, and the number density, and then what you call and relate that thing to your mean free path.

So, that will do in the next lecture, and electron after that will be looking at basically how to relate these things to your properties right that will be doing.