Fundamentals of Combustion

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Lecture - 16

Mass Transfer Basics - Part 01

Fundamentals

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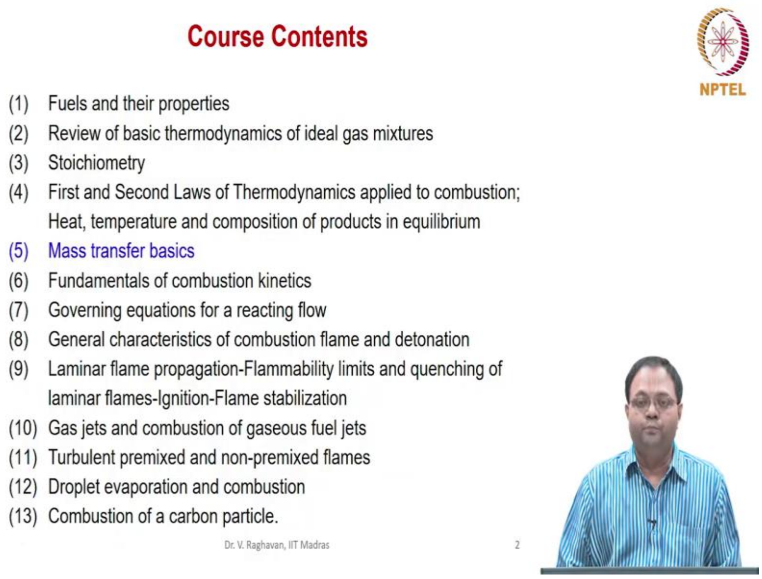

Today, we will cover the topic of Mass Transfer, basic aspects of the mass transfer.

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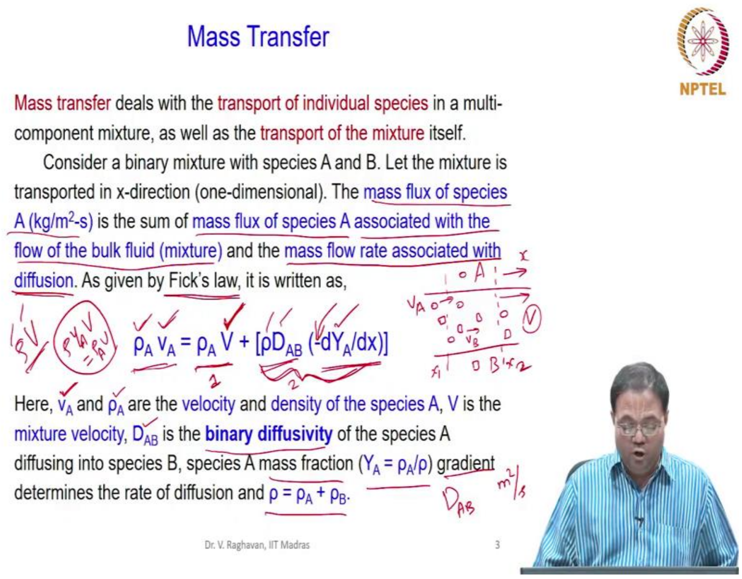

Mass transfer deals with transport of individual species in a multi component mixture. If you have a mixture with several species constituting that, mass transfer deals with the individual transport of all the species as well as the transport of the entire mixture itself.

So, unlike a single component; say for example, a flow of oxygen or nitrogen individually, how it flows as a mixture that needs some additional aspects to be covered.

Let us take a simple case of binary mixture. In a binary mixture two species contribute to that. Here, species A and species B.

Let us also simplify the problem further by taking the transport in only one direction. So, consider x direction only; it is one-dimensional. Later, we can expand it to several other directions.

So, if you take the transport of species A in the mixture, where the species A and B are present and in one-dimension. The mass flow rate of a species per unit area is mass flux of species A.

Let us take species A for example, the unit of the mass flux is kg/m^2-s. So, mass flow rate per second per unit area, this is written as the mass flux of species A.

So, A and B constitute the mixture; the mixture itself is flowing with the velocity V and the species A is transported along with the mixture. So, it has a contribution due to the bulk velocity of the mixture. So, that bulk fluid motion that is one component. Second component is the mass flow rate associated with the diffusion. So, what is diffusion? that is what we are going to see now.

So, let us take what is called ordinary diffusion for example. For example, consider a bottle of scent or perfume which is open in a corner of the room. There is no air flow or fans or anything switched on.

So, in a very quiescent atmosphere of air, stagnant air, the perfume bottle is opened on one corner of the room.

So, what happens is slowly you will see that the perfume is propagated to the other end of the room, that is the entire room will now feel the room refresher for example. This is because of what is called diffusion. There is no bulk motion at all.

So, air is still, we are just opening the bottle so that the perfume has a higher concentration near its source, at the top of the bottle; elsewhere the concentration is very low or 0 initially. So, due to the concentration gradient, the perfume is transported equally in all directions.

If you keep it in center of the room, you will see that it will equally propagate through the entire room. The transport of this particular species is due to the gradient in the concentration. So, it has higher concentration at the source, where the perfume bottle is kept and elsewhere, surrounding it the concentrations are initially 0 and slowly the perfume travels equally in all directions.

You know that it is a very slow process, it takes some time before which you will not be able to sense the perfume. Similarly, a leak of our LPG gas in kitchen. It is actually an odourless gas, but for commercial purposes some odours are added. So, that particular LPG you can see that smell coming out slowly as it diffuses.

On the other hand, if you keep the scent in particular corner and also, have a fan just besides that. Then, you can see that the perfume will be transported at a faster rate in the direction of the flow which is imported by the fan. The fan actually causes air flow to go through a particular direction.

The concentration gradient makes the species diffuse slowly in all directions, but if you have a velocity in a particular direction for example, then the bulk flow which is the convective velocity will transport the perfume towards that direction at a faster rate. So, if there is any convection present, that will transport mass.

If there is no convection present, only by diffusion the mass is transported. The perfume is transported like this. After a particular time period, you will see that the concentration gradient seizes or the concentration becomes constant.

So, there is no more transport possible in the diffusional way, if the concentration is constant, then there will be no transport possible.

It becomes 0 or reduces. So, if you take convection additional to the diffusion, you can see that the transport is faster. In general, what we consider is the species A, in this case it is transported due to the convection, if you assume that the mixture which is constituted by species A and B move at the velocity V in the x direction.

So, V is the velocity of the mixture in the x direction, then the species is transported due to the bulk velocity. So, the first term here is the representation for the species which is transported due to convection in the direction of the mixture flow. Then, I told about the concentration gradient. Concentration can be the concentration or mass fraction or mole fraction.

Here, we have written the concentration in terms of mass fraction. So, everything is connected. The mass fraction gradient in the x direction is $-dY_A/dx$ that is the concentration gradient in the x direction.

Negative sign here represents that in the direction of the diffusion gradient, the concentration decreases. So, the gradient is negative; the concentration decreases. It is same as the heat conduction. Heat is conducted from a high temperature point to the low temperature point. So, the gradient in this particular direction is actually $-dT/dx$, if the heat is conducted in the positive x direction.

So, similar to this, you can see that the concentration gradient represented by the mass fraction gradient dY_A/dx is negative. So, here we are only considering only binary mixture. The mixture has only two species A and B like air; which has oxygen and nitrogen.

So, the concentration gradient drives the species A into species B from the point where its concentration is higher to the point where it is lower. The diffusion is proportional to the concentration gradient like the heat conduction is proportional to the temperature gradient. The constant of proportionality is nothing but ρD_{AB}.

ρ is the density of the mixture and D_{AB} is the binary diffusivity; I have given here binary diffusivity of the mixture. It is a very important property. If you take any pair of species say AB, then the binary diffusivity of the mixture, the binary pair D_{AB} is a fundamental property which represents the rate at which the species A diffuses into species B. This is like a thermal conductivity; higher the thermal conductivity, the heat conduction will be higher.

Similar to that, if higher the value of ρD_{AB}, higher will be the diffusion transport of the species A into B. Now, the left hand side represents the mass flux of the species A, that is density of the species A, ρ_A, multiplied by the velocity of species A, v_A. Now, we have to understand that I am introducing one more velocity called species velocity.

So, the v_A is called the species velocity; ρ_A is the density of the species. So, $\rho_A + \rho_B$ will be the total density, ρ. That is what is given, the mixture density ρ in the binary mixture will be the density of the constituent A + density of the constituent B.

But v_A is the velocity of the species A. Let us take a duct for example and let us say the circles are species A. Circles represents species A and squares represents species B. So, this is the binary mixture. So, there are several molecules of A and B which is there and there that is a flow, this is x direction

So, this is x direction and you can see that the velocity of the mixture in this direction. Let it be V, what I have written here. So, this is the velocity of the mixture, capital V, in the positive x direction

So, it is one-dimensional, now just say it is speed. Now, A, the circles will be moving with a velocity of v_A; similarly, B, the squares will be moving with a velocity of v_B.

Individually, species may be moving at the velocity of v_A and v_B and also based upon the concentration. For example, take a particular section here. In this section say x_1, if the concentration of the species A is higher than compared to say a section x_2.

So, at x_1 you have a higher concentration of A; at x_2 you have a lower concentration because there is a decrease in the gradient or the mass fraction.

So, gradient is favorable for the diffusional transport of A in the x direction. So, it has its own velocity. The flux of A is nothing but the product of the density of A (which is nothing but mass fraction into the mixture density) into velocity of species A.

That is on the left hand side, the mass flux of the species A is due to two components. The first component is the bulk velocity, mixture itself is moving with a velocity of V, capital V, and that transports the species A.

What is the total mixture velocity if total density is ρ? So, total flux of the mixture is ρ (the mixture density) × V (the mixture velocity).

So, ρV will be the total mass flux of the mixture. Here, we have the mixture density and mixture velocity. Now, $\rho_A \times V$ will be the convective flux of species A that is the mass flux of species A associated with the flow of the bulk fluid or the mixture.

We can also write this as $\rho Y_A \times V$ will be equal to $\rho_A \times V$. So, that is the first term. Second term as I told you is the diffusional transport, the mass flow rate of A associated with diffusion that is represented here by the concentration gradient.

As I told you in section 1, x_1, the concentration of A may be higher and in section x_2, it may be lower. It may also be otherwise; you can also assume that the concentration of A can be higher at x_2 and lower at x_1.

That means, the species can preferably diffuse in this. Bulk transport may be in positive x direction, but diffusion can be in the other direction also. So, that is also possible. If you take that scenario, second term here represents that.

In the direction of negative gradient of concentration or in this case mass fraction gradient, the species A diffuses in the direction of negative gradient. For example, if x_2 has higher concentration than x_1, then the transport due to diffusion will be in the negative x direction.

This is called ordinary Fick's law; Fick's law incorporating ordinary diffusion. So, this concentration gradient based diffusion is called ordinary diffusion.

Now, this is the important statement, where you have a mass flux of species A represented as the sum of mass flux of species A due to the bulk motion of the mixture +

the mass flow rate of the species A due to diffusion because of the concentration gradient represented here by the mass fraction gradient.

So, the species velocity is v_A density of the species A is ρA and D_{AB} is called binary diffusivity, which is a property of any pair of species A and B and D_{AB} has a unit of m^2/s. It is a diffusion coefficient and is a property. The diffusive transport of species A is dependent on the mass fraction gradient or in general, concentration gradient of the species A. So, this is very important. So, individually you have to have this statement written for all the species A, B.

You need not consider all species, if you have N species, capital N number of species in a mixture, then we have to resolve for at least N - 1 species.

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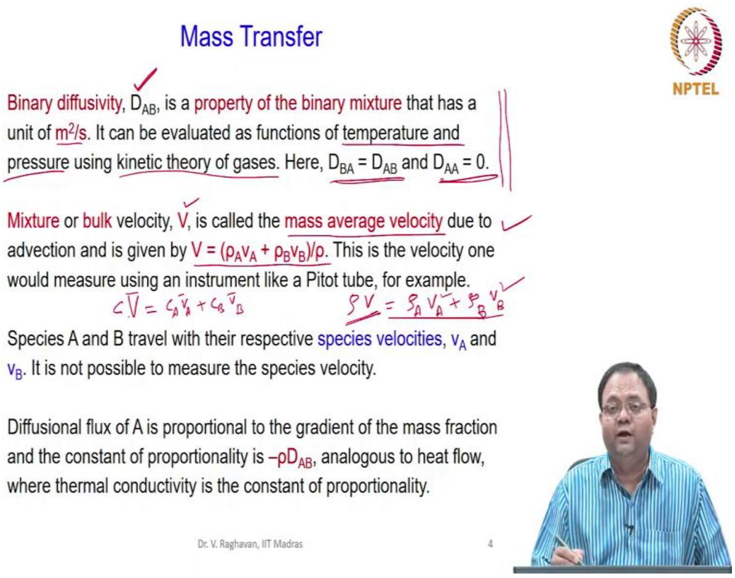

Now, binary diffusivity, D_{AB} is the property of the binary mixture constituted by any two species A and B. It has a unit of m^2/s and this is evaluated by using fundamental principles of kinetic theory of a gases like thermal conductivity etcetera, we can also have a theoretical basis to evaluate this, it can also be measured and validated and it is a function of temperature and pressure. It is function of molecular weight also. For example, if you have a pair of species, say hydrogen and oxygen. Hydrogen is very light species so, the molecular weight of this mixture is actually very low because of the hydrogen's presence.

So, what happens? You can see that diffusivity will be very high. On the other hand, if you take say for example, LPG or one of the constituent of LPG say butane, the molecular weight is higher.

So, butane, carbon dioxide, where the molecular weight is 44 etcetera, you can see that the diffusivity will be lower; the heavier be the species, the diffusivity will be lesser and this is a fundamental property; D_{AB} is the fundamental property which says the rate at which a particular species A will diffuse into B.

This is same otherwise. For example, when B diffuses into A, the rate at which B diffuses into A will be same as the rate at which A diffuses into B. So, we can prove that D_{BA} (you write B in this effect first) that means, the rate at which B is diffusing into A will be same as the rate at which A is diffusing into B; here, species cannot diffuse into itself.

That means, that $D_{AA} = D_{BB} = 0$. For single component, only one species is there; oxygen, carbon dioxide etcetera, in that case there is no diffusion at all. A single component species does not have any diffusion, it can flow only by convection.

So, this is very important. The additional component which is coming in a multi component mixture is the diffusion of the species due to the concentration gradient. So, we have to at least resolve this for our problems and this binary diffusivity is a fundamental property. Like any other property say, k, μ etcetera this is also a property and this is a transport coefficient, diffusion coefficient. So, D_{AB} is a mass diffusion coefficient. Then, mixture velocity or bulk velocity V is also called mass averaged velocity. Please understand that we are writing the concentration gradient in terms of mass fraction here. In the previous slide, we have written it in terms of mass fraction. So, what you end up in getting is the mass average velocity, the mixture velocity, this is the velocity which we can measure.

For example, if the mixture is flowing, The mixture of oxygen, nitrogen and carbon dioxide, some proportions of these species involved in the mixture are flowing in a duct in one-dimensional x direction.

Now you put a probe like pitot tube and measure the velocity. The velocity what it will measure is only the mixture velocity. At any point, if you measure the velocity, it will be only the mixture velocity. This velocity is actually contributed by all the species velocities. For example, in the binary mixture we can write $\rho V = \rho_A v_A + \rho_B v_B$.

Now, the total mass flux of the mixture (by mass conservation), $\rho V = \rho_A v_A + \rho_B v_B$.

So, from this definition, we can write the mixture velocity capital $V = (\rho_A v_A + \rho_B v_B)/\rho$, and this is the velocity which you will measure, or if you want to solve the flow using CFD, this is what you will solve using the continuity and momentum equations.

This is called mixture velocity or mass averaged velocity. This is very important. This you can measure or you can calculate using any equation. Now, if you want to write this in terms of mole fractions etcetera; then instead of mass averaged velocity, it will be mole averaged velocities.

So, instead of density, concentrations will appear there. If you write in terms of concentration, then you can write the concentration of the mixture $c \times \overline{V}$, I will say V overhead bar. So, this concentration of mixture into the velocity of the mixture, now I am putting V overhead bar to represent that this is a molar based calculation.

So, $c \times \overline{V} = c_A \times \overline{v}_A + c_B \times \overline{v}_B$. So, this is the concentration-based conservation. It is a general practice to write the conservation in terms of mass. So, we need not consider this.

As I told you each species is moving with its own velocity v_A and v_B. So, A moves with the velocity of v_A and the B moves with the velocity of v_B, it may be in multi direction also; it need not be in one direction, that may be vector also.

We can extend this one-dimensional to multi-dimensional later. Apart from this, it is also diffused from the high concentration zone to the lower concentration zone and this can oppose, the diffusion can oppose the convection and vice versa.

Now, species A and B travel with their respective species velocities v_A and v_B and it is not possible to measure this. Then how will you resolve this equation? That is what we are going to do; we can measure the first term. That is density can be measured or it can be calculated.

Similarly, you can calculate the mass fraction. You can actually take out the mixture at a particular point and see what is the concentrations of each species in the mixture at that point. So, velocity of the point can be measured.

Now, if you have a binary mixture, then D_{AB} can be evaluated using theoretical approach. You have some values based upon some correlations giving you the value of D_{AB}. Now, concentration at two points if you can measure, then you can also know the concentration gradient.

So, what we actually measure is the right hand side, you can measure or calculate the quantities in the right hand side and evaluate the mass flux of species A. So, that is what is going to be used in the species conservation equations later. So, we cannot measure this species velocity or calculate this directly.

You have to calculate this using the expression shown before or you can measure only the mixture velocity capital V, calculate the diffusion part and calculate the species velocity.

Now, coming to the second term in the right hand side of the previous equation, diffusional flux of A is proportional to the gradient of the mass fraction.

Here, I am writing in terms of gradient of mass fraction, as I told you concentration gradient can also be used and the constant of proportionality is nothing but $\rho D_{AB,}$ I will not take the minus here.

So, ρD_{AB}, this product is the key proportionality constant here and this is analogous to the heat flow, where thermal conductivity will be the constant of proportionality and the gradient is as such negative representing that the flow of the species A takes place from the higher concentration to the lower concentration, exactly same as the heat flow occurring from a higher temperature point to the lower temperature point.

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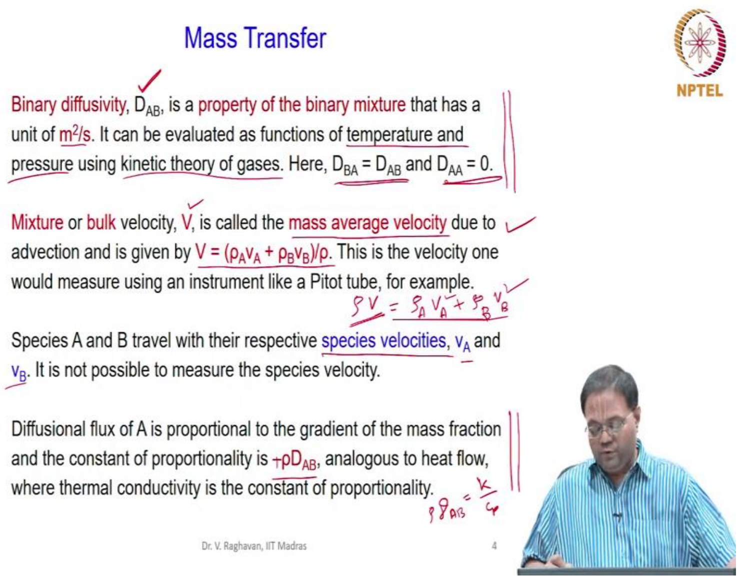

So, that is called heat diffusion here it is called mass diffusion. It is very important to understand this. You can see that ρD_{AB} will be equal to k/c_p, we can show this.

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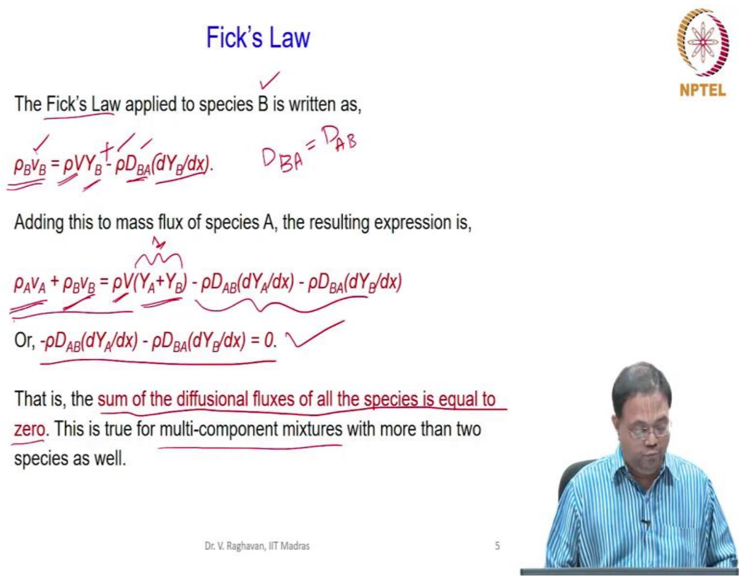

Now, let us write the Fick's law. As we wrote for the species A, let us write that for the species B. So, the net flux of species B, $\rho_B v_B = \rho V Y_B + \rho D_{BA}(dY_B/dx)$

Now, I am writing the diffusion coefficient or the binary diffusivity in the other way, the rate at which the species B diffuses into A that is D_{BA}; but we know that D_{BA} will be equal to D_{AB} in a binary scenario so that into the gradient of B in the x direction.

So, again it represents that if the concentration gradient decreases or the Y_B is higher at x_1 and lower at x_2, then the flow will take place from x_1 to x_2.

Now, you can have a similar equation for A and this is the equation for B; add these two So, $\rho V = \rho_A v_A + \rho_B v_B = \rho V(Y_A + Y_B) - \rho D_{AB}(dY_A/dx) + \rho D_{BA}(dY_A/dx)$. $Y_A + Y_B = 1$. Because in a binary mixture, the sum of mass fractions of each species will be equal to 1 so, that is unity.

Now by definition, $\rho_A v_A + \rho_B v_B = \rho V$. So that means, these terms here will cancel each other. So, this term here will go to 0 that means, the diffusion flux of A plus the diffusion flux of B.

In a binary mixture, there are two species A and B, diffusion flux of A plus diffusion flux of B is equal to 0 or you can say that the sum of diffusional fluxes of all the species is equal to zero. In a mixture, if there are N species, add the diffusion flux of all species, that should be equal to zero.

So, this is for a multi-component mixture, you can extend this binary to any multi component mixture, where there are more than two species. This is one of the important thing; this is actually used as constraint to derive some important aspects of the flow. So, this is very important.