

**Fundamentals Of Combustion (Part 1)**  
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**Lecture - 37**  
**Species Transport Equation**

In the last lecture, we basically derived a relationship for mass flux for particular species with respect to stationary coordinate system, right for a methane, right.

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The slide shows the following handwritten derivations:

$$\dot{m}_{CH_4}'' = Y_{CH_4} \dot{m}'' - \rho D_{CH_4-H_2} \frac{dY_{CH_4}}{dx} \quad \text{--- (1)}$$

Diffusional flux for  $CH_4$

$$\dot{m}_{H_2}'' = Y_{H_2} \dot{m}'' - \rho D_{H_2-CH_4} \frac{dY_{H_2}}{dx} \quad \text{--- (2)}$$

Let us consider mixture mass flux,

$$\begin{aligned} \dot{m}'' &= \dot{m}_{CH_4}'' + \dot{m}_{H_2}'' \\ &= Y_{CH_4} \dot{m}'' - \rho D_{CH_4-H_2} \frac{dY_{CH_4}}{dx} + Y_{H_2} \dot{m}'' - \rho D_{H_2-CH_4} \frac{dY_{H_2}}{dx} \end{aligned}$$

note  $Y_{CH_4} + Y_{H_2} = 1$

$$\Rightarrow \dot{m}'' = \dot{m}'' - \rho D_{CH_4-H_2} \frac{dY_{CH_4}}{dx} - \rho D_{H_2-CH_4} \frac{dY_{H_2}}{dx}$$

$$\Rightarrow -\rho D_{CH_4-H_2} \frac{dY_{CH_4}}{dx} - \rho D_{H_2-CH_4} \frac{dY_{H_2}}{dx} = 0 \quad \text{--- (3)}$$

For 'n' th species,

$$\sum_{i=1}^N \dot{m}_i''_{diffus.} = 0 \quad \text{--- (4)}$$

This is mass flux is equal to  $Y_{CH_4}$  into mass flux minus  $\rho D_{CH_4-H_2}$ , and  $Y_{CH_4} dx$ , right. Now I could not really cover in the last lecture, something which need to be discussed now, right. Because this is very important to appreciate the mass transfer process, right. And similarly of course, I can write down for that hydrogen is equal to hydrogen  $\dot{m}$  dot minus  $\rho D_{hydrogen CH_4} D Y_{hydrogen} dx$ .

Let say this is I am considering now as equation one in this today's lecture, right. We let look at what is happening to this bulk flow, right. Let us have a for that let us you know have a better feel of the bulk flow and the diffusional fluxes, right. If you look at these are the basically diffusional fluxes this thing is known as fluxes for methane, right; this for methane and similarly for hydrogen in equation 2, right. Let us consider total mixture mass flux, right mixture mass flux and this mixture is binary in nature, right. What is that? That is basically  $\dot{m}$  dot triple double dash is equal to  $CH_4$  plus  $\dot{m}$  dot hydrogen.

What I will do I will basically use this equation 1 and 2 right. So, what is that?  $Y_{CH_4}$  minus  $\rho D_{CH_4 H_2} \frac{dY_{CH_4}}{dx}$  plus  $Y_{hydrogen}$  minus  $\rho D_{H_2 CH_4} \frac{dY_{hydrogen}}{dx}$ , right.

So, if I will add this together, what it would be? What it would be I can write down this as  $Y_{CH_4}$  plus  $Y_{H_2}$ , yes or no? Can I not write down this portion? And that  $Y_{CH_4}$  plus  $Y_{hydrogen}$ , what is that? One, right? That means, you can note that  $Y_{CH_4}$  plus  $Y_{hydrogen}$  is equal to 1, right. That we know for a binary mixture of methane and methane and hydrogen. And then I can write down this as  $m$  is equal to this portion will be becoming what  $\dot{m}$  is equal minus  $\rho D_{CH_4 hydrogen} \frac{dY_{CH_4}}{dx}$  minus  $\rho D_{H_2 CH_4} \frac{dY_{H_2}}{dx}$ . So, this will cancel it out, right. Yes or no? That means, this term total diffusional term is mass diffusional term is 0, yes or no? Right that means, I can write down this as, right.  $\rho D_{CH_4 hydrogen} \frac{dY_{CH_4}}{dx}$  minus  $\rho D_{CH_4 H_2} \frac{dY_{CH_4}}{dx}$  is equal to 0, right. And this is for the binary mixtures you can also derive that basically for what for the  $i$  species, right. And for what is this thing this is basically? Mass flux due to diffusion.

So, for  $n$ th species, right summation of  $\dot{m}_i$ , and this is I am saying diffusion.  $i$  is equal to 1 to  $n$  is equal to 0; that means, this is basically is what you call? The total mass flux is equal to 0, for what?

Student: Diffusion.

For the diffusion; that means, total diffusional mass flux will be 0 in a mixture, right. Therefore, the bulk will be coming, you know like, are you getting the very interesting thing you should appreciate; that means, somebody will be moving fast somebody will be moving slow altogether diffusion will be.

Student: 0.

Not affecting the bulk flow that is very important point I am making. And this is due to only molecular diffusion ok, or the due to the you can say, but there will be some thermal diffusion, and this diffusion whatever I am talking about equation 4 is basically for what?

Student: (Refer Time: 07:05).

Concentration due to concentration gradient there will be molecular diffusion. There will be also some molecular diffusion due to temperature that is thermal or the Soret effect.

There will be also the diffuser effect, there will be also pressure diffusion all those things will be that we are not considering, we will be not considering in also later on because it is quite complex in nature.

But, however, when you do actual modeling particularly using the computational tools you will have to consider at least soot effect in the combustion whenever you are taking the hydrogen oxygen system. You cannot afford to say no. Otherwise things would not be good prediction would not be good. So, with armed with these expression particularly keep in mind that equation 3, and also it will be using and for i-th species will be using, and we will be now using this for deriving the species conservation equation, right. Let us do that.

So now, what we will be doing basically looking at the species transport equation we will be deriving this, right.

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Species Transport Equation

Let us carry out mass balance for i-th species

$$\left[ \begin{array}{l} \text{Rate of i-th species} \\ \text{mass accumulation} \end{array} \right] = \left[ \begin{array}{l} \text{Rate of i-th species} \\ \text{mass into CV} \end{array} \right] - \left[ \begin{array}{l} \text{Rate of i-th species mass} \\ \text{out of CV} \end{array} \right] + \left[ \begin{array}{l} \text{Production/Consumption} \\ \text{of i-th species} \\ \text{mass in CV} \end{array} \right]$$

(5)

Rate of i-th species mass accumulation in CV =  $\frac{\partial(\rho Y_i)}{\partial t} (\delta x \times \delta y)$  — (6)

Rate of i-th species mass entering in CV along x-direction =  $m_{i,x}^e \delta y$

" of " " out of CV " " =  $\left[ m_{i,x}^o + \frac{\partial}{\partial x}(m_{i,x}^o) \delta x \right] \delta y$

Net " of " mass along x-direction =  $-\frac{\partial}{\partial x}(m_{i,x}^e) (\delta x \times \delta y)$  — (7)

Net " of " mass along y-direction =  $-\frac{\partial}{\partial y}(m_{i,y}^e) (\delta x \times \delta y)$  — (8)

Mass of production of i-th species in CV =  $m_{i,p}^e (\delta x \times \delta y)$  — (9)

Let us consider that, I mean as usual we will take a infinitesimally control volume in a 2-dimensional situations. This is 0, 0, and this is delta x 0, and you know delta x delta Y this is 0 delta Y. And this is in x direction this is in Y direction, right. We are taking infinite decimally control volume, this is our control volume, it is having face A B and this is face C and this is D, right. This is our control volume basically.

Now, what we will have to consider we will have to consider for  $i$ -th species, right. We are considering  $i$ -th species; that means, the mass flux mass which will be entering mass flux will be what? For due to the  $i$ -th species is this much ok, and what will be coming out of here? And this is in  $x$  direction, right. We will be also considering  $x$  direction plus  $x$  into  $\Delta x$  noise], right. This will be  $\Delta x$ . Now in the similar fashion in the  $Y$  direction, right in the  $Y$  direction, this will be this will be is  $i$   $i$ -th means  $i$ -th species ok,  $y$  mass flux.

So, these are the things we are doing, but we will have to go back to the main things. What is that? This is the basically species conservation. And species conservation if you look at we know the rate of  $i$ -th species mass accumulation is equal to rate of  $i$ -th species entering into the control volume and rate of  $i$ -th species leaving the control volume, right, plus what it would be there? There will be mass production or congestion of the species, isn't it? There will be something which we did not considered in the last lecture. So now, then only we can you know look at this conservation.

So, let us consider, let us carry out mass balance for  $i$  th species.  $i$ -th species means it can be methane it can be hydrogen it can be anything you know, like, if it is a binary mixture it will be methane and hydrogen. So, that what is that that is basically rate of  $i$ -th species mass accumulation is equal to rate of  $I$  th species entering into species mass, right. Into CV minus rate of  $i$ -th species mass out of CV plus production and destruction, ok, I am just production and ok, should I write destruction also of  $i$ -th species mass in control volume. Keep in mind that this equation is what we call 4 or 5 just check.

Student: 5 (Refer Time: 14:01).

5.

Student: (Refer Time: 14:02).

5 makes sense.

Now, what is this rate of species of mass accumulation? Rate of  $i$ -th species mass accumulation in CV will be  $\rho_i$  into  $\Delta x$  into  $\Delta Y$ . Into of course, one therefore, volume is taken care, right; and rate of  $i$ -th species mass entering into CV along what?  $X$  direction, what it would be? It will be  $x$  into  $\Delta Y$ , is this along with this space  $A$ . And

rate of i-th species mass out of control volume along x direction will be  $\rho_i \mathbf{m} \cdot \mathbf{i} \times \Delta x \Delta y$ .

So, if you look at net rate of i-th species mass, you know, along x direction what it would be? It will be nothing but you I have done earlier same thing. So, it will be minus  $\rho_i \mathbf{m} \cdot \mathbf{x} \Delta x \Delta y$ , yes or no? Is it ok? And similarly, net flux net rate of i-th species mass along Y direction, what it would be? It will be minus.

Student: (Refer Time: 17:04).

$\rho_i \mathbf{m} \cdot \mathbf{y} \Delta x \Delta y$ , right mass of production of i-th species is basically in CV, what it would be into  $\rho_i \Delta x \Delta y$ , right into one basically, right. Now in equation 5, all the terms we have derived. If we will just include that in the equation 5, right. If I say this is maybe I can say this is your 6 this is 7 8 and 9. So, using equation 6 7 8 9 in equation 5, right.

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By using Eq (6), 7, 8, 9 in Eq (5), we can have

$$\frac{\partial(\rho Y_i)}{\partial t} + \frac{\partial \dot{m}_{i,x}}{\partial x} + \frac{\partial \dot{m}_{i,y}}{\partial y} = \dot{m}_i''' \quad (10)$$

The mass flux of i-th species along x-direction

$$\dot{m}_{i,x} = \rho_i \sum_{j=1}^N \dot{m}_{i,x} - \rho D_{ij} \left( \frac{\partial Y_i}{\partial x} \right) = \rho_i \dot{V}_x - \rho D_{ij} \left( \frac{\partial Y_i}{\partial x} \right) \quad (11)$$

Similarly the mass flux of i-th species along y-direction:

$$\dot{m}_{i,y} = \rho_i \sum_{j=1}^N \dot{m}_{i,y} - \rho D_{ij} \left( \frac{\partial Y_i}{\partial y} \right) = \rho_i \dot{V}_y - \rho D_{ij} \left( \frac{\partial Y_i}{\partial y} \right) \quad (12)$$

By using Eq (11) and (12) in Eq (10), we can have

$$\frac{\partial(\rho Y_i)}{\partial t} + \frac{\partial(\rho \dot{V}_x Y_i)}{\partial x} + \frac{\partial(\rho \dot{V}_y Y_i)}{\partial y} = \frac{\partial}{\partial x} \left( \rho D_{ij} \frac{\partial Y_i}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho D_{ij} \frac{\partial Y_i}{\partial y} \right) + \dot{m}_i''' \quad (13)$$

For axis-symmetric geometry (r-z), the species equation becomes

$$\frac{\partial(\rho Y_i)}{\partial t} + \frac{1}{r} \frac{\partial(r \dot{V}_x Y_i)}{\partial r} + \frac{\partial(\rho \dot{V}_z Y_i)}{\partial z} = \frac{\partial}{\partial r} \left( \rho D_{ij} \frac{\partial Y_i}{\partial r} \right) + \frac{\partial}{\partial z} \left( \rho D_{ij} \frac{\partial Y_i}{\partial z} \right) + \dot{m}_i''' \quad (14)$$

I can write down that as equation 6, 7, 8, 9 in equation 5, we can have  $\rho_i \mathbf{Y} \cdot \mathbf{i} \Delta x \Delta y$  plus  $\rho_i \mathbf{Y} \cdot \mathbf{j} \Delta x \Delta y$  is equal to this is equation 10. Am I right?

So, if you look at what is this term? This is known as source term, right. And how will get this thing? You know, we have already derived that from the chemical kinetics, right. We can find out what it would be using Arrhenius laws and other things we have derived, you remember that? So, now this is the non-linear in nature, this will be non-linear in

nature, because you it will be dependent on the temperature. Dependent on the other factors concentration because you do not know that. Now coming back to these, right we have already derived a relationship for mass flux of  $i$ -th species along the  $x$  direction, right., right. That is mass flux of  $i$ -th species along  $x$  direction, what it would be?  $\rho v_x$  minus  $D_{ij}$ , right. This we have already derived.

And similarly, mass flux of  $i$ -th species, similarly, the mass flux of  $i$ -th species along  $Y$  direction would be, and keep in mind that, these theme if I consider, what is this one? Any idea? This will be nothing but your  $m_x$ , which is nothing but your  $\rho v_x$ , yes or no? Similarly, if I sum sum means this is  $i$  is equal to  $n$ , all the species, it will be binary 2 if it is you know whatever the number 10 plus species you are considering ten. So, this also will be equal to  $m$  dot  $i$   $Y$  is equal to  $\rho v_Y$ , yes or no? Right?

So, what I will write down, I can write down here itself as  $\rho v_x$  minus  $D_{ij}$ . Similarly, I can write down  $\rho v_Y$  minus  $D_{ij}$ . Let us say this is 11, and this is 12 by using equation 11 and 12, in equation 10, we can have plus  $\frac{d}{dt}$  is a  $\frac{d}{dt}$  by  $dy$ . Plus, this is some (Refer Time: 14:55) might these 3 dash means, per unit volume that you should keep in mind.

Now this is your expression for  $i$ -th species. Are you getting? And what is saying? This is basically the unsteady term, this term is unsteady, and this is mass flux of  $i$ -th species along  $x$  direction, this portion, right. Right this is mass flux of  $i$ -th species along  $x$  direction. Of course, the similar thing is here, this portion, right. And this is due to diffusion, right this mass diffusion term along  $x$  direction, right. Gradient diffusion gradient basically and this is a source term, and this is the mass diffusion along the.

Student:  $Y$  direction.

$Y$  direction, this is basically mass diffusion in  $Y$  direction.

So, for axis symmetric, you know, the species conservation equation would be, geometry will be using basically what we call  $r$   $z$   $\theta$  coordinate system, but; however, we will be considering  $rz$ , ok, the species equation becomes  $\frac{d}{dt}$ , plus  $\frac{1}{r} \frac{d}{dr}$  by  $r$   $\rho v_r$   $Y$   $I$ , right. plus are is equal to  $D_{z\rho} D_{ij} Y$   $i$  by  $D_z$  by  $r$   $\rho r D_{ij} Y$   $i$  by  $D_r$  plus  $m$  dot, thus  $i$ . Keep in mind that this is a thing, and generally this what you call axial diffusion; that means,  $z$  is your axial, right.  $Z$  is your axial direction that is very, very

small, right. Is neglected as compared to what? Radial diffusion, this approximation will be making in whenever we are dealing with what you call z diffusion flame because z diffusion flame will be using this axisymmetric equations. So, therefore, it is very important to look at it and similarly you can write down for spherical coordinate system also, yes.

Student: (Refer Time: 29:18) triple dash (Refer Time: 29:18) triple dash, you know.

Tripled dash yes is, right. This will be thank you very much. We will stop over here. And in the next class we will be discussing about energy equation. And also, a little bit about term terminology, about turbulent flow, and then that will be the end of your thing ok.

Thank you very much.