Turbulent Combustion: Theory and Modeling Prof. Ashok De Department of Aerospace Engineering Indian Institute of Technology-Kanpur

Lecture-4 Thermo-Chemistry

Okay, welcome back. So let us continue the discussion on this turbulent combustion. So where we are into the business is that different combustion system.

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The most efficient		examples	
he cleanes	st -		*
The most dangerous			Spark-ignited gasoline engine
1	PREMIXED		Low-NO, stationary gas turbine
Always stoichiometric,			Flat flame
			Bunsen flame
ess efficie	nt -		Aircraft turbine
Less clean.			Hydrogen-oxygen rocket motor
Less dangerous			Diesel engine
1	NON-PREMIXED (DIFFUSION)		Pulverized coal combustion
			Candle flame
	1	LAMINAR	Radiant burners for heating
	1	Ť	Wood fire
	FUEL/OXIDIZER	FLUID	EXAMPLES

So, you can see how we broadly classify the system which we have discussed that one of the thing is that either premixed system or non-premixed system or partially premixed system. So here we now concentrate more on the two of these and see premixed flame or the system which could be either turbulent and you see some of the examples here. So is a spark ignition engine gasoline engine, which is turbulent low NO_x stationary gas turbine.

If you look at the laminar, there are flat flames, Bunsen flame, which is the simple claims which are the laminar flame. Now when you come down to differences, so one of the important things of pre-mixed flame is they are quite efficient and also not only that they are the cleanest, combustion that one can have but at the same time, these things nothing comes as free, of course, this is also quite dangerous.

And why it can be dangerous because we have already seen some example where instability actually triggers. Now another side of it non-premixed flame where this kind of problem may not be there and this could be also laminar or turbulent in nature where you have candle flame, Bunsen flame, wood fire and these are aircraft engine, rocket, motor diesel engine these are the things. So, this classification based on your fuel oxidizer mixing and the fluid motion.

But at the same time, when you look at the non-premixed or diffusion system, they are always asymmetric that means the reaction zone of the combustion takes place at the stoichiometric situation they are obviously less clean. So the problem of your emission becomes quite dominant here and that is why one has to control or the same time they are less efficient, but obviously you get some benefit that also it is not that dangerous.

So, that means controlling a pre-mixed flame is quite challenging compared to a non premix flame. Non premixed flame or the control of a non-premixed flame is not that straightforward as one can see.



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Now this is again an image which clearly shows a simple diffusion flame and this is a methane which is burning in here. And from this side, you have a diffusion flame completely and this side

you go to premixed system. That means from the diffusion slowly you go. So that means in between there would be something partially pre-mixed. And then you go to premixed system and the important observation one can have there is in flame structure. Flame structure then same colour so these are the differences or visible differences one can have as soon as you and this yellow line and all these things which represent that there are unburned situation. So here premixed system shows that you can have a clearly nice blue flame that means everything is getting burnt here. There is a lot of unburned hydrocarbons or something is there that is why you get this kind of yellowish nature.

Now usual practice you need to store your reactant separately for safety, but you may burn them in premixed mode for performance and pollution because as I said, your premixed flames are quite efficient, so that means you have better performance and also emission is not that high in premixed flame. But at the same time, your device need fast mixing system.



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So there are which are the issues which can lead to your problems which usually happens in LP system that means lean premixed system one the biggest problems is that it has a instability problem or flashback problem. So if you see this kind of a; but there is a question may come why one would like to have a lean premixed system. So, the lean premix system advantage is that it reduces the NO_x rapidly with the flame temperature.

And this is one of the schematic of that kind of a premixed system where air fuel is mixed and say injected to the chamber under swirling condition and then secondary air comes through, tertiary comes through for so but the Lean system has a problem of this and this is another example where methane is actually added with different percentage of hydrogen and you can see the upstream portion of the injector how the flame actually moves so there is a movement of flame this is called flashback.

Or in this particular example, you can see there are some waves which are generated and that will lead to some sort of instability problem that is called the combustion instability. So one can expect to have a lean premixed system to have better performance, less pollution, but at the same time it will become more susceptible to flash back or instability.



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And if that kind of situation happens, this is one of the picture one can see what happens to the burner assembly. So this is a one which is actually damaged. This is a new one, one can see so it is a nice-looking burner setup. But because of this instability or flashback kind of things, this has been completely damaged. So that is why control of premixed flame or the handling of premixed flame is not that easy. It has certain issues, it is quite dangerous also.

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Now, one can classify these things in a different way is also so far. We are making the classification based on the flow and how the mixing takes place that means either premixed or non-premixed mode. Now apart from that, one can have a classification like unconfined flames. That means the flame is not confined within a chamber or something or rather it is not kept within a confinement so you can have pre-mixed flame, laminar flame and the other is the confined planes. But in regular practice most of the practical systems, they are confined or either or recover heat or mechanical power so engine, so they are in that way nature.

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Now, some example of your confined and unconfined flame. This is the same example where you have a diffusion flame and you go to premixed flame. So this is unconfined flame that means the burner is exposed to the open air and this is the image of a confined flame where combustion is taking place within the combustor wall. So there are some differences. What are those? One of the biggest difference is the velocity field which are quite different because density changes due to dilatation.

So that is one of the important differences between now in a confined system, you have walls. So heat transfer becomes quite important because once you have wall then heat transfer and then the cooling of the wall, these issues will come into the picture. So it is not that straightforward that if you have a confinement so one and unconfined flames have some list of challenges, but at the same time confined flame has certain other challenges.

Another important aspect is that acoustics can become important and also induce combustion instabilities. Which are dominating multiple present programs? So that means people are now looking at these acoustics business in seriously, because in the most of the practical systems are confined in nature and the confinement brings into some of these challenges.



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So if you put everything together, so that our topic of discussion would be in a broader sense

turbulent combustion. So we will look at both their basics and theoretical aspects along with the modeling aspect. So that means when you look at these two turbulent combustion with their modeling aspect, everything requires theoretical discussion on the basic flame type that means on laminar, premixed and non-premixed flames which will do first.

So that means to do this first discussion would be on laminar flames and after laminar Flames will move to turbulent Flame. So before doing that turbulent flame one has to make some discussion on turbulence. So that is the whole point but there are complexities in combustion also and how do we look at it?



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So there could be a different ways of complexities. Number one the complexities come from the kinetics or the chemistry. If you have more detail kinetics or you are burning a particular fuel, which is really complicated than that can be representative some thousand of reaction steps. Then the chemistry can become a real issue. Then geometric complexity so the real life burners or combustors, they are having a lot of small, small components.

So, geometric complexity could be one of the features there could be complexity due to flows. So, and the finally multiscale issues. So again, just to give you a glimpse of that simple candle burner, which is one of the simplest burning system and if you go in the growing complexity level in this

direction, this is your gas turbine combustor. So everything is sort of happening here. So that is in a growing complexity situation and you have a lot of scale lot of different physics they are taking place in that particular combustor.



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Now we look at some of these basic flames like Zero Dimensional flames. So here all variables vary with time. Okay, so you have a few linear. So one of the things is that your temperature is and you look at this is a function of temperature and this is the reaction. I mean source term in temperature equation and this is the Species Mass Transfer equation and this is the source term or reaction Source term.

And this comes because of your multiple reactions steps. So this is where your zero-dimensional means there is no geometric complexity, flow variables are only with time so that complexity is also not there but the kinetics brings in the complexity here through this reaction. So, what are the important component here? Even, if you look at a Zero Dimensional film where everything is PSR kind of model that means perfectly stirred reactor kind of model.

So they vary only with time fuel and air so one thing is the complexity comes due to kinetics as I said and the second thing is that now not only the kinetics, your kinetics is also connected with your temperature equation or the thermochemistry. So these are the two important things even for

a simple flame they become quite important.

STEAD (All Va	Y 1D LAMINAR FLAM riables Vary with x on	MES ly)
atr v v	No fluid mechanics: flame The flow field is imposed. $Pu = -P_0 a^2$ $Pv = P_0 a^2$	elet equations only.
Kinetics	Thermo-chemistry	Transport

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Now, you can go to a steady 1D laminar Flames here variables vary with X only so that means no fluid mechanics. You have some sort of an; so air and fuel they are coming in so you get a flame sitting there. And here one can write a momentum balance:

$$\rho u = -\rho_0 a x$$
$$\rho v = \rho_0 a r$$

Where, a is a strain rate. So it is only varying in One direction and one can write these things. So, in the previous case, we have seen that even then there are so that means the fuel and air they are coming in contact. There is a flame sitting here. So kinetics will be there thermochemistry or the kinetics and thermodynamics. The connectivity will be there. There will be one more important things which will now come into the picture is the transport because now they are transported so that complexity. Now, we will see how things get complicated.

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Now this is another laminar flame which one can see in your gas burner or regular laboratory-scale burner which is but multi-dimensional. So here variables could depend on different direction that means X Y or Z. Now the important thing could be kinetics then obviously your thermochemistry transport. Now when you talk about multi-dimensional that mean things will vary with X Y Z another important behavior which will come into the picture is fluid mechanics. So, that means when after another Physical process when they get involved it will make systems more complicated.



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Now you come to a situation where you have a turbulent and confined flame here things are transient in nature at the same time they depend on all X Y Z. So, this is a turbulent flame in a laboratory scale this is your real problem comes from an oil and gas industry where I mean refineries, you can see this kind of flame. Things which will be involved kinetics because the combustion is taking played there is a transport process.

There is a thermochemistry, fluid mechanics because these are turbulent now top of that your turbulence will come into the picture so that will bring in some extra effort to be handled or the scales then since these flames are so turbulent and scales there could be radiation. There will be huge radiative heat which would be emitted from these flames and finally say most of the times if you are burning hydrocarbons and all these things there could be soot particles which are the black particles.

Now, you can see how things get complicated as soon as you move to a laminar situation to a turbulent one. Even a confined flame is kind of involved with so many different processes which makes things complicated.



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Now, when you go to turbulent confined plan, this is an example of your gas turbine combustor. Here, you have all this information kinetics transport, thermochemistry, fluid mechanics turbulence, radiation, soot depends on a particular mixture and fuel and fuel what temperature or not soot may arise or may not but what could arise in a different kind of complexities one is the acoustics that means because of some of the instabilities this may trigger in.

Then heat transfer at the walls and all these things and then finally because of the wall heat transfer there could be thermal loading on the combustor walls, liners and everywhere. So those materials can also expose to some sort of a small deformation where your fluid structure interaction will become also important fluid structure interaction.



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By implication for the models and different codes you have so many parameters kinetics transport, thermochemistry, fluid mechanics, turbulence, radiation, acoustics, heat transfer, FSI. So everything one has to be kind of handled how one can handle that? So, one of the best code or the models for a real application are not always the best code and models for individual problem. So, you may have everything incorporated in one particular model.

But that could not be the best one for your application you want to deal with but it is a good one for realistic situation. Then the limiting part of the code would be the weakest element of all of them especially for real application. So, one has to identify the weakest element now depending on the expertise one can see the weakest link at different places and accordingly he has to or she

has to resolve those things.

So, which gives you an idea of why this combustion process is so complicated because it involves so many processes at the same time and once you have so many processes which are involved at the same time, then things become really complicated. So, these are the complexities of combustion and that we need to handle complexities in combustion.

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And now we will start with some of the basic things like combustion and thermochemistry. So we will develop our discussion or continue our discussion on the basic stop. Then we will make it go into the detail discussion of the complicated things. So what we will cover here, we will look at the basic property then looking at the first law of thermodynamics, enthalpy and some of the basic properties of flame and all these things then finally chemical equilibrium. So these things will look at it.

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So, we can look at this these are the already you should have some background on thermodynamics or some basics of combustion. So you must know there are the property relations there are extensive properties and the intensive properties. So, the extensive properties depend on amount of substance, which are considered for example volume, total internal energy, total enthalpy these are the examples. An intensive properties which are expressed per amount of unit mass so, for example specific volume, specific enthalpy and all these things.

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Then your intensive properties also, you can have air temperature and pressure and extensive

properties are related to intensive one by amount of mass. So, for example,

$$m. v = V$$
$$m. h = H$$

So they are sort of connected the intensive properties and the extensive properties. So, one can look at it.

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Now the other thing which we have already looked at is equation of state. So, you most of the time unless or otherwise it specified will be delivered the ideal gas behavior. So this will give you a relationship between pressure and density, temperature. So an ideal gas behavior is that what it tells you that intermolecular forces and volumes are ignored, so you can

$$PV = NRT$$

So one can say this is our equation? Then PV equals to, you can write in different terms. So,

$$Pv = RT = \rho RT$$

So these are different from one can write the ideal gas law or the equation of state and we can use in different form. (Refer Slide Time: 22:25)



Now there is a specific constant, which is the universal gas constant:

$$R = \frac{R_u}{MW} = 8.314 \frac{kJ}{kmol \ K}$$

Okay and MW is the molecular weight so, most of the things that will show in throughout our lectures will mostly deal with the gaseous state so will require this gas law and we will be using this different gas constant. So somewhere we can use this R_u or R_0 whatever it is. So that is what we use throughout this discussion.

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Now, there will be another thing which one can write is the calorific equation of state so the calorific equation of state which essentially relates the enthalpy and the internal energy to pressure and temperature. So, your internal energy will become the function of temperature and specific volume and h becomes function of pressure and temperature. So, these are my number, now, once we differentiate these two equations 1.4a and 1.4b, so we get:

$$du = \left(\frac{\partial u}{\partial T}\right)_{v} dT + \left(\frac{\partial u}{\partial v}\right)_{T} dv$$

So this is 1.5a and:

$$dh = \left(\frac{\partial h}{\partial T}\right)_P dT + \left(\frac{\partial h}{\partial P}\right)_T dP$$

which is 1.5b so once you do the differentiation, then you get this.

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Now 1.5a + 1.5b you can write:

$$C_{v} = \left(\frac{\partial u}{\partial T}\right)_{v}$$

which is 1.6a and:

$$C_P = \left(\frac{\partial h}{\partial T}\right)_P$$

which is 1.6b, now for ideal gas so for ideal gas:

$$\left(\frac{\partial u}{\partial v}\right)_T = 0$$

And

$$\left(\frac{\partial h}{\partial P}\right)_T = 0$$

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ntegrate 9.1.5 & Just in 1.6->	
W(T) = Wref + f Codt	
(G) (GAT	
h(1) = href That	
ref: reference state	

Now, we integrate equation 1.5 and put in 1.6 so that will get:

$$u(T) = u_{ref} + \int_{T_{ref}}^{T} C_{\nu} dT$$

which is 1.7a and

$$h(T) = h_{ref} + \int_{T_{ref}}^{T} C_P dT$$

which is 1.7b, so here we have some reference so ref stand for some reference state and will define that reference state as we go on.

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Now, what for both real and ideal gases the specific heats which are C_v and C_p they are generally functions of temperature. Now internal energy of a molecule there are how one can look at it, these are essentially the translation energy or vibration energy or rotational and temperature dependent. Monatomic species only translation energy would be involved if it is diatomic or triatomic all three like translation, vibration, translational, and rotational energy will be involved. So, more complex the molecule the greater is the molar specific heat.

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So, now if you go to the ideal gas mixture and we will find out is the mole fraction which would

be:

$$X_i = \frac{N_i}{\sum_j N_j} = \frac{N_i}{N_{tot}}$$

and mass fraction for ith species would be:

$$Y_i = \frac{m_i}{\sum_j m_j} = \frac{m_i}{m_{tot}}$$

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Now for this ideal gas situation for the looking at the mole fraction and mass function one can find out that summation of X_i is always 1 and summation of Y_i is always 1. So, these are the two important properties what one can say 1.10a and b equation number and relationship between X_i and Y_i one can write X_i molecular weight of i by molecular weight of the mixture which is 1.11a and at the same time X_i equals to molecular weight of the mixture divided by molecular weight of the i which is 11b.

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Now how we define the molecular mixer molecular weight:

$$MW_{mix} = \sum_{i} X_{i} M W_{i}$$

And

$$MW_{mix} = \frac{1}{\sum_{i} \left(\frac{Y_{i}}{MW_{i}}\right)}$$

So total pressure one can find out it would be summation of P_i , so this would be 1.12a, b and 1.13. So, we will stop here and will actually continue in the next lecture.