Combustion in Air Breathing Aero Engines
Dr. Swetaprovo Chaudhuri
Department of Aerospace Engineering
Indian Institute of Science, Bangalore

Lecture - 28
Laminar Premixed Flames VII

After this we have just studied discussed the dependence of prey of flames speed on different parameters like automatic flame temperature of the fuel mixture, of the pressure on things like Thoman Law on like transfer properties. But you now we are ready to look into the chemical structure of flames.

So, in this topic what we discuss is that the thing that we want to discuss is that, so far we have essentially talked about an idealized flame structure where we consider the preheat zone and the reaction zone. And the preheat zone does not contain any reactions and then the reaction zone which occurs in a very thin layer at very high temperatures. So, this was the assumption of the flame structure for analysis that we have should done.

But now we will show that we will consider a case where that this idealization is really a simplification and the actual flame structure might be more complex than what we have just seen.

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Now, this is the thing that we will go into this the difference between the asymptotic versus chemical structure. So, as we just discussed that the asymptotic structure is the broad it is a broad convective diffusive region and it is a non reactive region. In the asymptotic viewed the most part of the flame is essentially non reactive. So, it is only within the narrow diffusive reactive zone at the downstream end of the flame we have reactions.

And we consider this as a result of the one step overall reaction and which has got very high activation energy and which result a very localized heat release and localized reactions. We have not considered at chemical activation as such. And we have considered if at all there is in a chemical activation that is also due to the thermal in nature and that is purely governed by Iranians kinetic because the reactions are promoted at high temperature.

But in actual when you consider a real flame structure with detailed chemistry, of course we can consider that. So far we have considered detailed chemistry only in the flame work of a homogeneous mixture. And that went into this kinetics classes and oxidation mechanism of fuels. So, where all our discussions was actually focused or concentrated in the for a homogeneous reactor. And the difference between a homogeneous reactor and a flame is that in flame you have got strong diffusion going on; strong diffusion of heat, strong diffusion of species going on.

So, the flame is different from a homogeneous reactor in a fact that there are strong transport phenomena involved. So, what happens when this transport phenomena involved is basically what we have to consider is that we here in this we will essentially combine or understanding in the oxidation mechanism of fuels chemical kinetics with just concluded asymptotic analysis or this high activation energy small thin reaction zone analysis.

But this is a very key step to, I mean this is a very important and settle the fact is that-yes our one step high activation energy theory is very important because it gives the very good idea of what the flames speed of the laminar flame speed it will depend on. It depends on temperature, it depends on Lewis number, and it depends on your Zeldovich number etcetera. And we find from (Refer Time: 03:52) those are actually right. So, the analysis is correct to some extent, predicts many of the things correctly. But at the same

time if you want to understand how exactly that the conversion of this fuel molecules, fuel and oxidizer how the conversion of these happens into products and how does that conversion release the heat, then we have to consider the detailed reaction mechanism and do the analysis of this laminar 1 d laminar flame with these detailed reaction mechanism.

And that will tell us a wealth of information about how the reactions are actually participating and how the reactions are actually participating in cognizance with the transport phenomena, with the different diffusion processes. And how the fuel change the flame structure from the ideal behavior. So, this is a very very important part, and this is very important to understand real combustion processes which happens in an engine. Even though this we are doing this for a one step flame we can do these analyses for a complicated flames that exist in the engine. And this will serve as a baseline for essentially doing that.

You see the whole purpose of this course is to not analyze the combustion, we will do that, but the whole purpose with the whole in the whole course we are not analyzing the combustion phenomena inside an engine. We are preparing our steps, we are preparing our tools, we are preparing our knowledge, and we are preparing our viewpoints which will enable us to understand that. So, that is very important.

And once you understand that we will be able to design this. So, that is very important this is how scientific progress happens. So you analyze, you take up a very complex problem and you remove its all this surrounding external flails and you go to the bare skeleton and then you try to analyze that. And then that is what we are doing. We have complicated of a whole flame inside a combustion chamber its very complex.

So, we are considering, we can we can consider that we are considering pieces of that with certain idealization that it is locally planner it is locally laminar. And then we are analyzing that piece of the flame and we will see that here how actually the reaction how actually the fuel oxidizer reacts with oxygen to basically gets converted into products.

That we did first mathematically. Of course, when we did mathematically we have to consider a basically an idealization of one step chemistry and certain other idealizations. But now when you do that with the detail phenomena you solve for everything essentially and you will find that how this, what are the similarities and what are the

differences between the asymptotic structure and the actual chemical structure, but this is very important.

So, what we find is that in the chemical structure if you just highlight these points. We find that that is the termination reaction is temperature sensitive. Well, this is from our knowledge in the further from the reaction mechanism oxidation mechanism of fuels. We find the termination reaction is temperature insensitive why because its activation energy is essentially 0. So, temperature reaction becomes more and more sensitive when it is a activation energy increases. As we have seen later, as you seen in the previous kinetic class. And it can occur in upstream diffusive zone.

And as a result reactions can take place or the internal structure. So, when a reaction has activation energy to be very small, there is no at all no requirement that it will only happen at very high temperature. So, this certain reactions of course there are many other reactions like the branching reactions have a very high activation energy. And those are excited or others occur at large rates only when the temperature is small, but that does not mean all reactions have a large activation energy.

And that is where a very good example of this is the termination reaction which is temperature insensitive, unit can occur in the upstream diffusive zone and reactions can take place throughout the entire flame structure. And this termination reactions can be highly exothermic. For example, this reaction will see that H plus O 2 plus M, this c body termination reaction HO 2 plus M is very highly exothermic and there is substantial heat releases in the preheat zone.

Now, chemical activation through radicals produced at downstream high temperature and that back diffuse to the preheat zone. So, you see that in this termination reaction stage H plus O 2 plus M going to HO 2 plus M. This most important key thing is this H radical. So, do you need this two termination reaction to occur, and for these two release the substantial amount of heat you need this H radical presents. So, H radical is a very key element here is a very key atom here and this presence will control the reactions.

But the thing is that in a homogeneous reactor the H radical has to be produced simultaneously in to attack this oxygen molecule. But here what can happen is that even if it being produced later in a downstream region, this downstream region H that is

produced can back diffuse and come up and react with an upstream oxygen molecule and to form this HO 2 plus M and release a substantial amount of heat.

So, that is what is different when you have diffusion processes it couples you this earlier molecules with the later molecules and can still enable you to have the reactions between them; so the personal diffusion. So, in homogeneous systems these radicals are produced by original fuel oxidizer species. So, the initiation reaction for a flame and for hydrogen for a homogeneous system can be very different.

So, that is what makes this chemical structure understanding very important.

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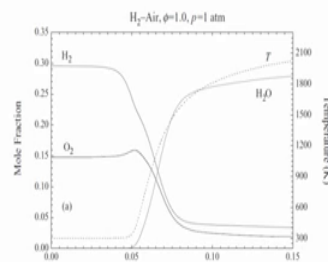
So premixed, the hydrogen air flame if you consider the diffusive structure so this is once again the flame, this is the flame, this is in infinite w in finite domain, this is stabilized and here you have a fuel plus of air mixture coming of the fuels here this hydrogen and air is oxygen plus nitrogen that is air 20 percent in 79 percent. And this is a high temperature product.

So, now these high temperature products are formed and then washed out. So, this is the 1 D blue mixed hydrogen flame and this is the diffusive structure. You see that now this is the flame location we can say essentially this is from here to here is our flame. So, you can consider this from here to here is our flame location. And this is the structure on we heat plot, on this double y axis figure we plot on the left hand side we plot the mole

fraction of different species of hydrogen and oxygen and water. In our right hand side we plot the temperature and this is the hydrogen a stritiometric hydrogen air flame, at a pressure of 1 post fear.

And so the hydrogen or oxygen comes. So, nitrogen is not plotted for diffusion and then it of course its consumed and then it goes down. But you see that this consumption has a unique behavior, and of course water is produced at the end of all the reactions and the temperature increases like this. So, these started line it presence temperature. What you see that once immediately that the thing that is interesting is that if you consider a definition of a thickness that is which is inverse of the gradient, essentially on the numerator we have the difference between the upstream and the downstream or something like that. You see that the hydrogen has a much thickness is the hydrogen depletion zone is much thicker in comparison to the oxygen. And this is because the hydrogen is a higher diffusivity as a result its gradient is smaller.

As a result of this the hydrogen has the high diffusivity causes this thing to have a thicker broader region and in comparison to the oxygen, this bump actually comes from the fact that this hydrogen depletes very rapidly. And it is nothing to do with any chemistry effects. So, this hydrogen diffusion layer is thicker than those of oxygen and the heat because of its high diffusivity. And the rapid reduction in hydrogen concentration causes a bump in the mole fraction of oxygen. This is not physical just definitional on mole basis.

So, now you will be come into the flame structure, where we look into the different kind of chain branching reactions and the different things.

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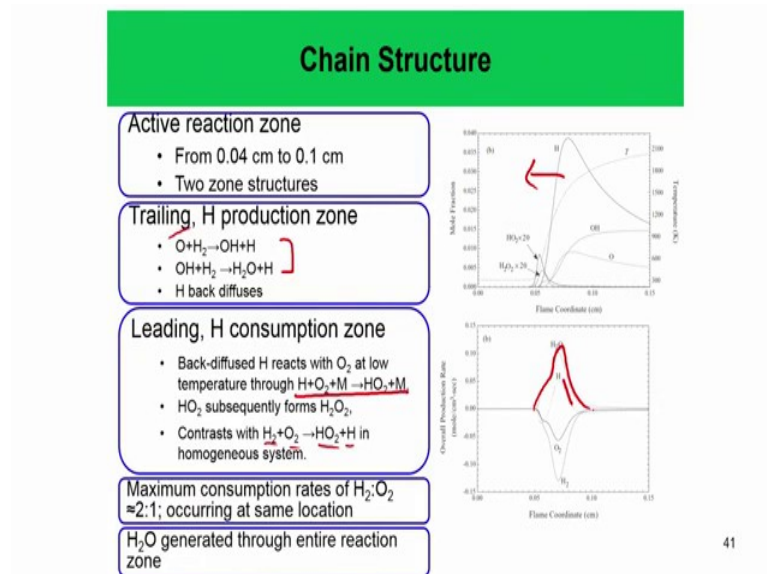
So, the first thing that comes into the mind is that you see; this is the thing. So, the first active species that comes up is essentially this HO 2. So, in this whole thing the first radicals that is formed is that of HO 2 among all the radicals say HO, H OH H 2 O 2 etcetera everything. So, there where then the question is that there where does HO 2 come from.

So, they to answer this that become we go into before we answer this thing we go into essentially analyze what are production and consumption rate of different species. We see that this hydrogen production rate, this hydrogen atom which is the most important active radical actually, you see this is a shape like this.

So, here we have first consumption of hydrogen, we have first consumption of hydrogen atoms and then it has a increase in the production of hydrogen atoms. And this hydrogen consumption essentially coincides with the high production of HO 2. So, somehow hydrogen consumption in HO 2 are being related, are related through some reactions.

So, first lets understand that how H is produced. To understand how H is produced this is by this two mechanisms of two reactions H is produced. H 2 that is the hydrogen fuel is attacked by the oxygen atoms and its produces OH plus H. And of course, H 2 is also attacked by a hydroxyl molecule OH and it produces HO 2 and H. And then this hydrogen is consumed here which is found here and that shows of as this large peak of

hydrogen. But once this is hydrogen atom and once this is formed it can actually back diffuse.

So, once it back diffuses now this termination reaction can happen that is this H plus O 2 plus M can go to HO 2 plus M and which essentially results in the consumption of hydrogen. So, that is why the first we have a consumption of a H atom and then we have a production of H atom, and that gives rise to this unique structure. But, this you see this back diffusion process is very very critical, because once this goes back diffuses it can now react with oxygen to form my HO 2 plus M. And these reaction is extremely exothermic.

And this reaction is exothermic and that is a result of which you have is temperature release, we have a lot of heat release in low temperature upstream regions which is not possible otherwise. In a normal hydrogen oxygen homogeneous system we will have high temperature at a reasonably higher temperature not in this manner. And this is because in a homogeneous system your initiation reaction that is the formation of H is through this H 2 plus O 2 by HO 2 plus H.

So, this is the contrast between our flame structure and the homogenous structure. So, you see that combustion is not only about reactions, it is also about transport of properties combined with reaction. So, this is a very classic example of this. We have seen in the zeldovich analytic the Frank (Refer Time: 15:58) analysis also that transport and reactions are equally important because f 0 square is you think f 0 that is the burning flux is essentially the geometric mean of your reaction and transport properties that is your thermal diffusivity and the reaction rate. Here you see how this different transport that is a back diffusion of H radical our upstream causes this termination reaction to over to pick up at a low temperature. And we can consume the hydrogen and release a lot of heat. And that changes the overall flame structure itself.

And later you will see that when it comes turbulence, the turbulence also changes a flow and of course using previously the stretch it can cause stretch in that corner again changes the flow structure. So, combustion is among having is about different numerous reactions combined with transport, combined with flow properties at different scales. So, that is the most interesting thing about combustion.

Now, we see that water is also generated through the entire zone, because this is the thing about water.

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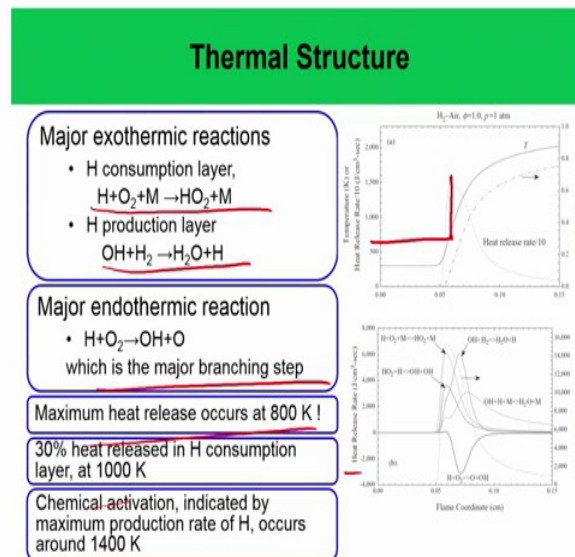
Now, this going back to the thermal structure this was a chain branching structure you see that the major exothermic reactions essentially is this one; that is the H plus O 2 plus M goes to HO 2 plus M and also the hydrogen production layer OH plus H 2 goes H 2 O plus H. And this is here your different heat release rate to contribution this is the heat release rate you see, this is the heat release rate the thing and that the total contribution by different reactions is this one; that is this concepts almost entirely this is the overall heat release rate this dotted line you see. And that coincides very well almost with this termination reaction H plus O 2 plus M, we are going to HO 2 plus M only near the upstream regions.

Whereas, near the downstream region it coincides well with this reaction OH plus H 2 going to H or H 2 a plus H. So, in that upstream region this is the major contribution of heat release and the downstream region, this one is the in the upstream region this is the consider contributor of heat release in the downstream region, this is the major air contributor of heat release. So, if you plot the heat release rate with temperature you see that this heat release essentially peaks at a very low temperature of about say like 700 to 800 Kelvin this is the heat release rate this dotted line and this is the temperature. And it peaks at temperature of what 700 800 Kelvin.

And which is very in contrast with the all the analysis that we have done so far that is where we have assume that large activation energy, it causes the heat release to happen at large temperature. But you see here in this particular case usually this comes from our reaction which has got very low activation energy almost 0. So, as a result of that the heat release comes in low temperature and we changes the whole frame structure.

But this is of course, hydrogen which is a little bit exceptional case. The hydrogen for more hydrocarbon your heat released that indeed occurs at high temperature, and to the c oxidation route and it is not in there. But this asymptotic analysis and this analysis of this high activation energy that we have done so far holds in a better manner.

So, here the major endothermic reaction is this H plus O 2 going to OH plus O which is essentially the chain branching, which is a major branching step and going little hence the leads to the reactions to proceed further. And here the maximum heat release rate as we have said that occurs at about 800 Kelvin and that is the hallmark of this H plus O 2 plus M in the H 2 plus M, the three body termination reaction. And of course 30 percent of heat releases in hydrogen; heat released in hydrogen consumption layer at or 30 at about 1000 Kelvin. So, this is a chemical activation as indicated by the maximum production of H occurs at around 1400 Kelvin. So, this is also that is this one and this one corresponds to about 1400 Kelvin; this is what I want to say here.

So, with that this in this part of the analysis of the laminar flames and laminar flame structure, laminar premix flame and laminar premix flame structure is complete. And of course, you might think that why did we spend so much time on laminar flame analysis the reason once again (Refer Time: 20:13) that laminar flames are essentially units of turbulent flames. We can only understand problem of flames which happens to the engine so well, only if you understand the laminar flame behavior the response that is the laminar flame speed, laminar flame structure, on premix flame structure. And these have basically units of a much bigger thing. So, only when you understand the building blocks well you can use those to construct a big building which is essentially the goal of this course to understand combustion in air breathing aero engines.

So, with that next we will proceed to; so all these analysis that we did for laminar flames for non premix for laminar flames whether it is a non premix flames; so there is for droplet combustion, whether it is for laminar premix flames these are all for steady

analysis right; so everything steady. So, next we will going to like unsteady phenomena where we will look into ignition and extinction. And we will also sometimes we will do a steady analysis to see whether it is possible to in ignite or extinguish a given mixture without going into how they can be ignited or extinguished.

So, that will be taken at the next class, so until then goodbye.

Thank you.