Indian Institute of Technology Madras

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COMBUSTION

Lecture 31
Flame Speed Dependencies, G-Equation

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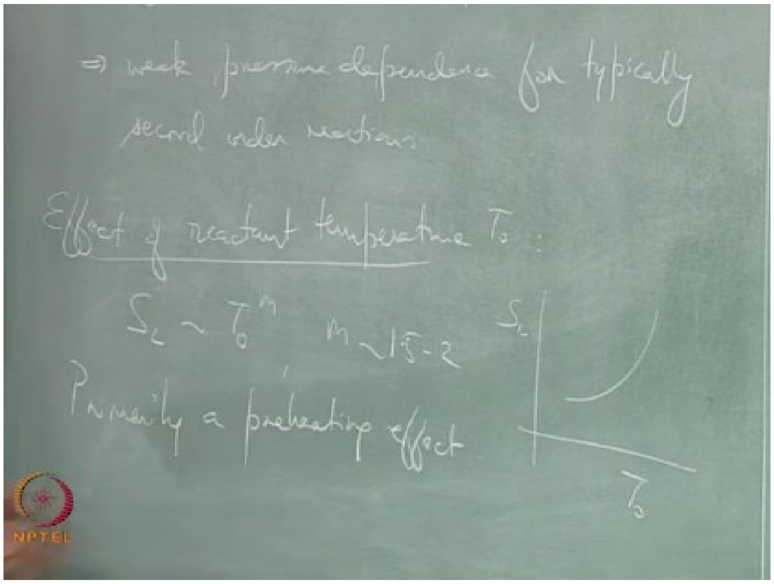

⇒ weak pressure dependence for typically second order reactions

Effect of reactant temperature T_0 :

$S_L \sim T_0^m$, $m \sim 1.5-2$

Primarily a preheating effect

So the last class we were looking at the effect of pressure on the flame speed and what we found was for a nth order reaction for let us say a global reaction the flame speed goes as P to the n/2 n - 2 /2 and this basically gives a week pressure dependence for typical hydrocarbon oxidation combustion reactions with a order close to the global order took close to do so for typically second order reactions then there are lots of other parameters that we have to think about or variables of course when we talk about pressure the next thing we obviously think about is the effect of initial temperature.

So or rather than saying initial temperature as if it is an unsteady problem and in a steady state situation we should be thinking about like a affectivity temperatures of the un burnt reactants okay or far upstream reactants so temperature effect of temperature reaction T0 now of course these things are more like information so you can actually gather these things from most textbooks we will just go through this rather quickly to highlight what the most important aspects are and put it is also important to think about this in physical terms other than just to look at explanations.

So what we are saying here is as far as t notice concern okay the gross effect is like if you now say S_L this goes that goes T_0 to the m let us say where m is around 1.5 to 2 so if you think about this if you now look at S_L versus T_0 we get graphs that go kind of like that right so why is this is mainly a pre heating effect okay see because what you are thinking about is you have the reactants that are approaching the flame in a frame fixed coordinate system and then you have the preheat zone and the temperature has to now raise from there up to the reaction temperature in the reaction zone.

So this effect is primarily a pre heating effect alright so if you were to be thinking about like a PhD qualifiers question the question will not be what happens to the flame speed we are with the reactant temperature the question would be what happens to the flame thickness with reaction time the reactant temperature right so we will we will ask this question differently then what is normally done in the class.

So that for you to think about okay so we say it is essentially a preheating effect now the other thing that you naturally have to think about when you are looking at the effect of anything on flame speed is what is the effect on the reaction rate because you know you see that the flame speed is directly proportional to square root of the reaction rate right, so as a matter of fact we got this n - 2 /2 for the pressure because the reaction rate was going as P to the n and then since the flame speed is proportional to square root of W you have n /2.

And then of course you had a 1 /density in it in a as a factor out so which was linearly in pressure therefore you had this n /2 - 1 that is how you got this so the first thing that you have to think about is the reaction rate what is the effect of whatever parameter you are thinking about on the reaction rate and therefore on the flame speed this is the first step approach the next thing that you have to think about is what is the reaction rate itself depend on and it primarily depends on the flame temperature right.

So what is the effect of anything on the flame temperature and through that on the reaction rate and through that on the flame speed this is how we have to look at this relationship that is very important most of the time but in this case T0 of course affects Tf directly and then Tf effects Wand W effects S_L but in this case you know the Tf effect is significant right when compared to the TF effect the influence the T0 not has on the Tf and therefore on the S_L is marginal this is though this rice is primarily directly because of the preheating effect and much less through the effect through Tf.

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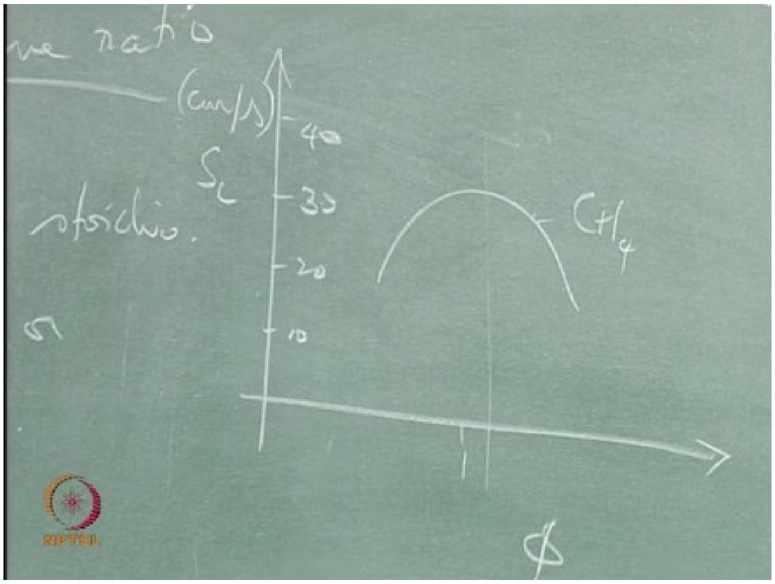

So the influence through Tf is a is less here if you now look at how the Tf itself effects S_L that is the next thing that we should look at effect of flame temperature Tf on S_L of course is significant so here what you will find is these curves are much cheaper so if you now look at Tf this is of course like we are essentially looking at different mixtures having different Tf and what happens to the S_L corresponding to that keeping lots of other things constant so it is a bit difficult to actually think about this experiment but if you now think about this curve is much steeper when compared to this okay.

So a slight change in Tf can cause a significant change in S_L through W that is the reaction rate so now if you if you go back and think about this the first thing that we did was when we wanted to look at the structure of the pre-mixed flame we said the reactants get in and then the temperature rises and then goes to the reaction zone but if you want to just do the a gross order of magnitude balance you would say the reaction rate is evaluated at the flame temperature right we do not have to worry about the variation of the reaction rate with temperature.

We will just evaluate the reaction rate at the flame temperature directly and this justifies that because as Tf changes w changes and as W changes S_L changes there is a direct link between these things so we can we can see this justified experimentally then the most important thing that we should be looking at most of the time effect of mixture ratio so when you say mixture we are always looking at the reactant mixture okay.

In the context of preheat sorry premix flames we are always thinking about the reactant mixture that means the fuel oxidizer mixture right, so here what happens is S_L vs let Us say equivalence ratio and of course you can think about equal is ratio one as stoichiometric and then less than one as fuel lean greater than one as feel rich you should typically look forward to curves that are like that but with a peak little bit off in the fuel rich region okay.

So peak nearly stoichiometric condition or slightly feel rich right now just to also give you some numbers we are talking about laminar flame speed so we are looking at these things measured typically in centimeters per second and these are about let us say 10, 20, 30, 40 these numbers would probably work for maintain lots of other fuels will give you these kinds of curves at much higher values maybe not much higher maybe twice as much or maybe three times as much.

So around that so we are talking about a few to several tens of meters per second sorry if you few to several tens of centimeters per second for the laminar flame speed okay so this is something that you got to keep in your mind and in order to get a feel for things when you do they say experiments or even numerical work and so on.

Now the other thing that we have to worry about is why or why are we having a pig there is slightly shifted off the reason for this is actually again through Tf so look at how the variation happens for the Tf with respect to equivalence ratio right you will find that it picks up near the stoichiometric condition or maybe slightly field rich again and that is because of the CP effect that is the CP.

If you now look at how the CP of the mixture various with Π right you will you will find that the CP affects the Tf and then on top of it think about this Tf is actually sitting in W and on topic and then there is an explicit CP dependence directly on a 44 S_L okay so CP influences Tf + CP directly also influences S_L therefore you will find a further slide shift into the fuel rich region because of this region this is this reason.

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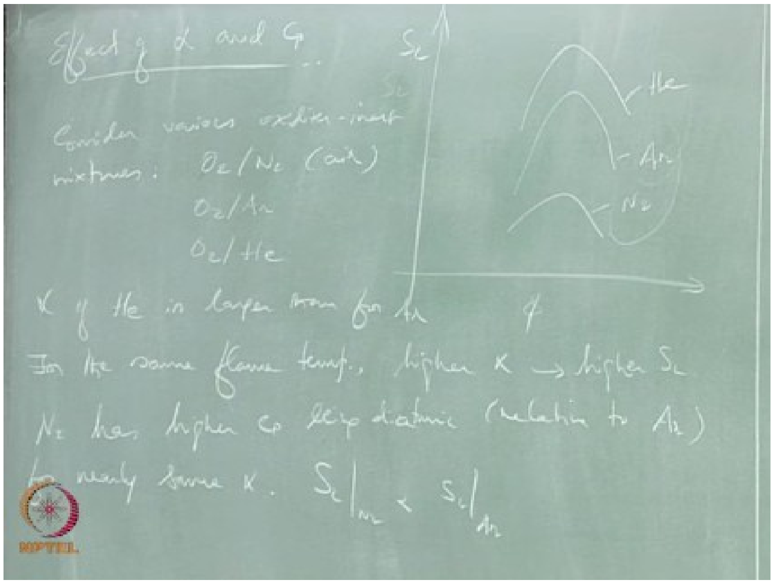

Effect of α and C_p..

Consider various oxidizer-inert mixtures: O_2/N_2 (air)

O_2/Ar

O_2/He

κ of He is larger than for Ar

For the same flame temp., higher $\kappa \rightarrow$ higher S_L

N_2 has higher C_p b/c diatomic (relative to Ar)

& nearly same κ. $S_L|_{N_2} < S_L|_{Ar}$

So this is again mimicking you making T_F trend and a further CP effect we will look at the CP effect directly right away that means we want to keep the Tf constant and see if we can vary the

CP or so that kind of thing so let us just see how that can be done so effect of effect of α and CP right I want to just go back and point out something here in this picture so this curve stops on either side beyond a point as you go from go away from equivalence ratio 1 and this would be a the real lean flammability limit.

And this would be the fuel rich flammability limit means if you now have too much of either feel or oxidizer the flame is not going to propagate and that is called the flammability limit and we will talk about flammability limits separately later on but we have to keep this in mind that this curve is going to actually hold only over a range of Π around one significantly around one it is not like just around one but not too far away on either side okay so going back to the effect of alpha and CP α is of course the thermal diffusivity.

So the way we can actually think about this is also pretty interesting so you can now think about S_L and vs Π you now look at let us say ch4 in air right consider various oxygen oxidizer inert mixtures right so that is like 0 to n2 as an air and O2 organ and 0 to helium all on the same proportions if I keep the proportions the same you should now get pictures that look like that and this is for n2 with oxygen this is for organ and this is for so question is why are we getting this we can think about it in multiple steps.

The first thing that we want to think about this combination both of them are inert gases and monatomic okay so when you say they are monatomic then they are CP's are nearly the same right and the only thing that is different is the density therefore the α changes so CP does not change but the α changes so if you if you look at how the S_L behaves S_L is like 1/ ρ 0 naught square root of KW / CP these are these are the dependencies so k / ρ CP is what we are looking for as α .

So you should now be able to write K/ CP explicitly in terms of α and then you should be able to look at an α effect versus a sepia effect separately that is what we are trying to do so what you are saying here is because the helium is lighter than organ for the same CP α of a helium is much larger when then for organ then for AR and then what happens is you know if you can fix your flame temperature all right that means you can get your flame temperatures to be the same because the CP is the same.

So flame temperature depends primarily on CP as far as this is concerned so for the fleeing same flame temperature higher α Π α R means higher S_L all right so that is the reason why you are going to get a helium diluted S_L to be having a higher value and compared target organ diluted flame speed now then what happens to this combination what you have to think about is here the CP's are different okay.

So between organ and he will nitrogen this is a monatomic gas but this is atomic gas. So therefore the CP is different now n2 has a higher CP being diatomic okay relative to organ is a good comparison with the into because the α are nearly the same age 44 same α so that way you can fix your α somewhat and then say look at the CP effect then what happens is S_L within 2 then becomes lower than S_L with organ right but then when you are thinking about change in CP right.

We started thinking about change in CP even here when we were talking about the SL variation with phi following at variation with fight train and then we were thinking about why was the TF actually varying like that and that we argued it through CP of the mixture as five is varied and therefore there was a strength that is shifting towards.

The fuel rich side so similarly CP is now going to directly affect the flame temperature all right so here what happens is TF also depends on CP so here in the case of SL, SL varies through wand TF and therefore CP effect there and then an explicit CP dependence in the denominator there for you now have a double effect both of them actually adding up together so what happens is typically this gap is larger when compared.

To this gap because you now have both the CP influencing TF and then c be influencing directly okay, so TF also depends on CP and sorry and it is it also effects itself so keep that in mind and then there are some more interesting things that we should be thinking about O before we proceed this is a very interesting thing as an experiment for you to do and we will shortly talk about like a Bunsen burner flame stabilization all right so we will look at what's the condition for flame stabilization in a Bunsen burner for example.

And then we will say okay now I am going to have like a methane air mixture that is burning in a Bunsen flame and then I slowly shut off my nitrogen in the air and then try to introduce organ and then I progressively shut off the organ and then try to introduce helium okay so what happens to flame stabilization so this is like a trick question that is there is typically Austin by qualifiers or exams right so we do not necessarily ask you directly about this that is why kind of reproducing what's there in the textbook right.

But we also tried a couple this with the flame stabilization issue rig up an experiment where we can vary the dell you and type from nitrogen to organ to helium and ask progressively what happens the flame shape in a Bunsen flame and look at it look at it stabilization and so on so effectively we are playing with the SL while you are trying to do that in relation to like the flames with the flow speed.

We will talk about that later on so keep this in mind proceeding with chemical effects.

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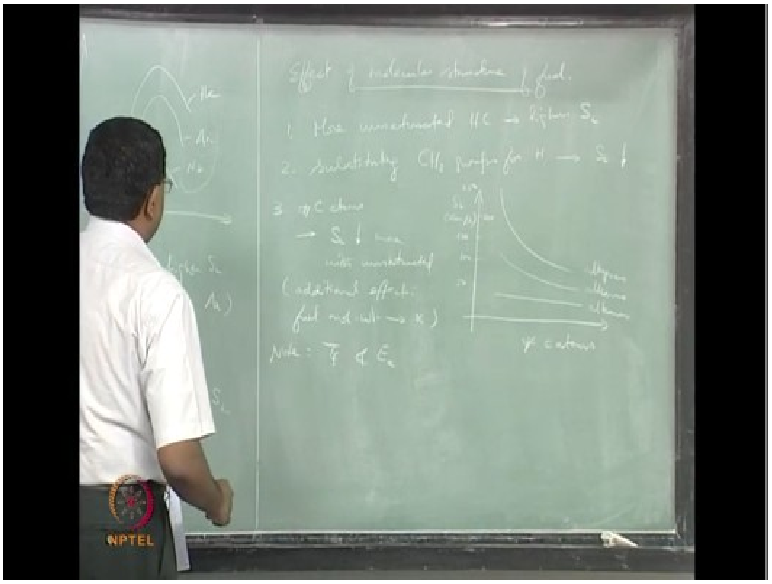

So effect of molecular structure of fuel typically few last words what's of interest the oxidant oxidizer is always air most of the time in what you are talking about or at least oxygen with any diluents now what we find is to two things we have to think about one more unsaturated set you created hydrocarbon higher is SL unsaturated means you have like double bonds and triple bonds right so it is not like alkenes we are down talking about alkenes alkynes those kinds of things they would they would have typically much higher SL.

When compared to when you have when you have only have single bonds then the other thing that we should think about is a substituting methyl groups for hydrogen right leads to a SL decrease that means like for example when you now have maintained you have four hydrogen atoms right so instead of that you now say they take one of the hydrogen's and then you have ch3 ch3 that becomes attained right and then you can now have like chcl3 or CCL a Sorry CC CC kch ch 3 twice and then c CH 3 thrice.

So you can progressively replace your hydrogen atoms by methyl groups and then form larger molecules with more carbon atoms and progress in correspondingly hydrogen atoms as well in the methyl groups what this can lead to is two things one it implicitly also increases the number of carbon atoms okay, so if you now directly look at what happens to the SL as a function of number of carbon atoms right what do you have to do is look at straight-chain hydrocarbons like maintain attain propane butane pentane.

And so on all of them N prefer from propane onwards you ought to think about like N propane and or n-butane N pentane and so on right from beauty on-words you ought to think about like straight chains the other way is like if you know take a methane and then start attaching methyl groups you do not you progressively you do not you do not you know begin to get like for the but are you do it does not have to be N butane it could be like an is butane that means like you have a branched methyl group even if you have straight chains as the number of carbon atoms increase the flame speed decreases provided.

We are talking about alkenes and alkynes with the case of in the case of alkenes there is hardly much of an effect so if you know if you know look at the number of carbon atoms you can look at like a curve that looks like this for alkenes curve that looks like this for alkenes the curve that looks like that for all kinds and these numbers are pretty interesting so this is like centimeters per second like for example you would have something like 50, 100 ,150 ,200 and 250and so on keeps you see this now of course.

When you are now talking about alkynes you are looking at a triple bond so obviously you need to have at least three two carbon atoms for a triple bond to be formed in between so this is like acetylene and you can see that acetylene has a very high flame speed for two reasons one the number of carbon atoms is less and it is unsaturated it is highly unsaturated so both of them contribute to a high flame speed.

So three is number of carbon atoms leads to SL decrease more width and unsaturated and one more thing that you have to think about is when you now have a increase in the number of carbon atoms there is a molecular rate effect that is coming in okay so additional effect is filled molecular weight pre- molecular weight right and so this actually influences your α for the mixture and through that you also one thing is the reactivity right.

So that means you it affects the reaction rates the other thing is the molecules are getting heavier and heavier so it influences your alpha and from there your we are beginning to get an effect on the SL so these two things compound and mix for example our settle in to be highly reactive so that is the reason why people say if you are working with something like an oxy-acetylene torch like in welding applications and so on you got to be give it careful should agents a bit careful may be quite careful okay on safety considerations because it is highly reactive and infect I should point out that here we are not looking at ATF effect of TF note TF and as a matter of fact even the activation energies for let us say global reactions of oxidation of most of these fields are comparable right.

So this is not necessarily like a TF effect at also then the other last point that I would like to make is about reactivity so a good comparison that is made is for example if you now have silicon hydrogen bond versus silicon carbon bond like si -H 4 similar to CH war right si-H 4 would probably have like a large reaction already called flame speed okay, so this because this bond is actually quite reactive when compared.

To let us say for example if you now progressively replaced the carbon atoms in methane with silicon right and you go all the way to having si-H 4 versus you can say I am sorry SI CH 3 h 2 and so on so if you do not have some such thing that would be less reactive so if you now have like a silicon carbon bond that is going to be less reactive and compared to silicon hydrogen bond so these are things.

That you can well pickup from textbooks not a very not very difficult but what you have to keep in mind is to highlight two or three things one have a feel for numbers okay, you are talking about tens or a few tens to several tens typically.

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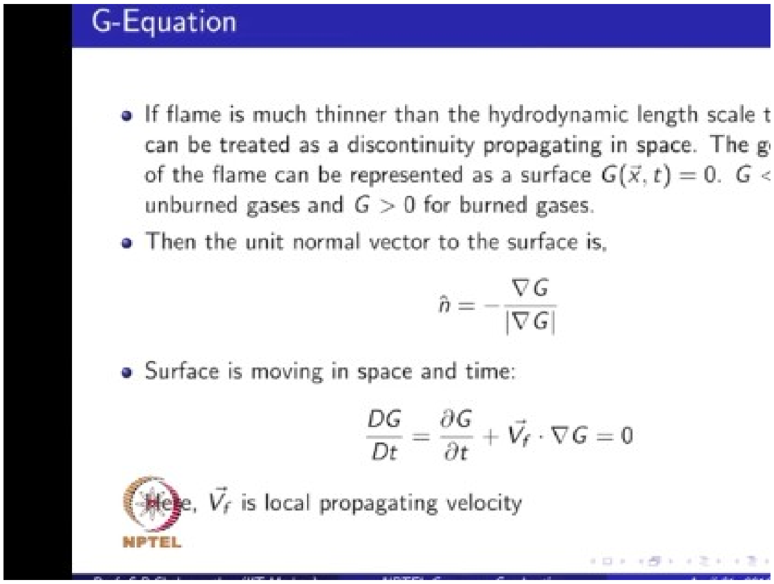

G-Equation

- If flame is much thinner than the hydrodynamic length scale t
  can be treated as a discontinuity propagating in space. The g
  of the flame can be represented as a surface $G(\vec{x}, t) = 0$. $G <$
  unburned gases and $G > 0$ for burned gases.
- Then the unit normal vector to the surface is,

$$\hat{n} = -\frac{\nabla G}{|\nabla G|}$$

- Surface is moving in space and time:

$$\frac{DG}{Dt} = \frac{\partial G}{\partial t} + \vec{V_f} \cdot \nabla G = 0$$

Here, $\vec{V_f}$ is local propagating velocity

For most same speeds in some in terms of centimeters per second you can also look at some of these having a few hundreds of centimeters per second that is one thing the second thing always look for the effect of any of these things through TF okay, because that is a big effect there are only a few exceptions for example T not there is a direct effect of preheating arm and then there is a direct CP effect that you can think about and TF does not really influence significantly when you are thinking about different fuels are in with different carbon chains.

So there is a molecular effect and so on that that is coming to picture so some of these are exceptional but most of the time whatever TF does whatever parameters they think I am thinking about SL would try to follow that most of more mostly so and then keep this shape in mind this and then of course what happens when you know progressively diluted with different gases of different monatomic diatomic gases and then also when you have different molecular weights or densities and so on.

So this is this is pretty interesting as well now with this what we should now try to do is a slightly different framework once we now know how to deal with how to get the flame speed then how do we deal the premix flames.

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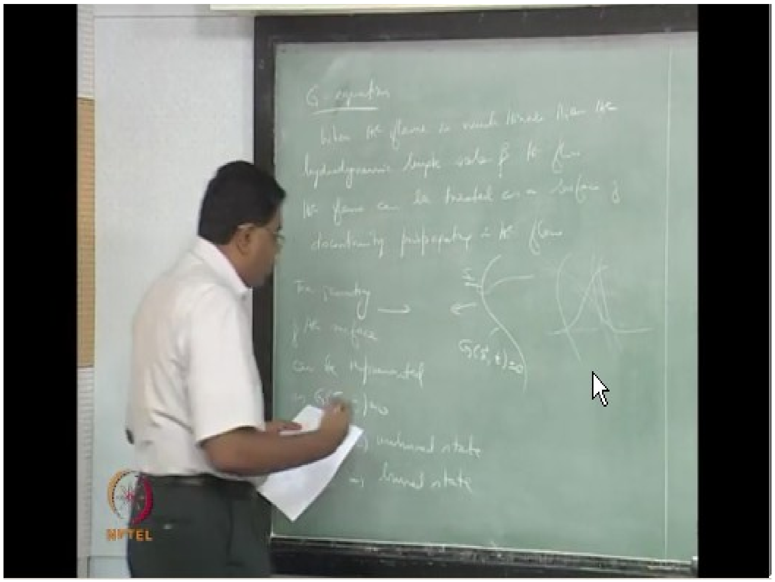

So then we talk about what is called as example, G equations what happens when you are thinking about a G equation is when the flame is much thinner much thinner than the hydrodynamic art length scale of the flow right we can treat this flame as like a surface a soft surface that is propagating in the flow so it is essentially like a surface of discontinuity the flame can be treated as a surface of discontinuity right propagating in the flow that means the flame has a certain propagation speed which we now kind of take for granted.

We have gone through enough of what is happening across the flame within the flame how the temperatures rise the concentrations fall for the reactants lots of things and then we now have the preheat zone the reaction zone we could have like multiple preheat zones for no unity lowest numbers depending upon diffusion length scale versus conduction length scale lots of such things we have think thought about right and then we have also further thought about what are the effects of pressure temperature flame temperature.

All these things but now let us say flame speed is given right if the flame speed is given and you are now talking about a situation where the characteristic length scale of your flow is much larger when compared to the flame thickness okay and the flame is not very thick many times alarm the flame for example is very thin right it is about a few millimeters thick of course it is much it is quite thicker than a shock like if you are thinking about gas dynamics shock that is that is only a few mean free paths thick okay.

You have a sudden change in properties across a very small distance and we are even continuum assumptions are broken down whereas that is not the case with flames but still it is quite thin when compared to most applications however where you come across most applications therefore if you now think about this you now say that's the flame we are just now beginning they were just trying to propagate into a flow right.

Now where was all the preheat zone and all those things it is kind of like you know how to take a magnifying glass hold it against this right and then that is going to kind of look like and soon all the stuff that we drew and so it is almost like locally one-dimension also when you now say locally one-dimensional that means the flame is trying to propagate with its flame speed normal to itself right so the flame could be curved that refers to the flame shape what is what we have been talking about so far is what is called as the flame structure a flame shape is like a much global picture a flame structure is something that happens almost like at a point in the flame along the length of the flame right.

Where you now try to typically resolve temperature and concentration profiles reaction rate profiles all those things across the thickness of the flame so what we are talking about is locally normal to itself it is going to have aflame speed which is now of course going to be in different directions flame speed is a scalar right and it depends mainly on reactant temperatures pressure reacting temperature pressure and the mixture ratio all right and the all the other parameters like what is the α what is the CP and what are the kinetic constants.

What is the order of the reaction all these things right so once all those things are given if you are given a certain mixture at a particular ratio and temperature and pressure SLS fixed as a scalar the flame speed acquires a direction locally normal to the flame shape so dependent upon the shape of the flame is how the flame propagation direction is fixed and many times you would think wait a minute the flame is probably going to shape itself depending upon how it can propagate right.

And I will have to try to find the shape in the first place depending upon how it can propagate if I do not know how it is going to propagate how can I figure out what its shape is and how can I figure out the propagation direction so it is a loop that we have to think about so how do you do this right so the way we deal with this situation is we now say this is actually treated as a surface of discontinuity and we want to mathematically describe.

The surface by a by an equation called G of X vector , T is equal to 0 right so the geometry of the surface can be represented as G of X vector ly equal to 0 X vector referring to the position vector for that particular position there.

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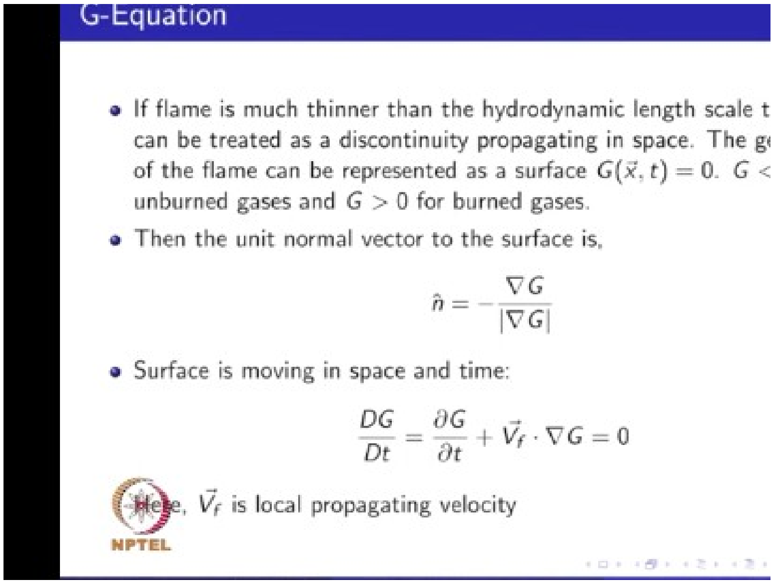

G-Equation

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Here, $\vec{V}_f$ is local propagating velocity

Now if you are trying to-do this analytically you could just deal with this surface having this equation right as it is or the other possibility is you can now think of G as a scalar like enthalpy or temperature or any anything okay, just too just like any scalar so it is sort of like if you now have and particularly what's called as a passive scalar that means a scalar that does not influence the flow okay, so if you now kind of carve a scalar quantity that is actually dropped in the flow it just goes with the flow right unless.

It has a propagation speed that it wants to compete with the flow against right so that is the kind of thing that we want to see so if you want to look at it as a scalar that means it is a scalar field that means it should be this it should be defined and described everywhere in your flow field right so if you want to do that then there is a very way of dealing with this that is you can say G less than 0 could refer to the unborn staying and G greater 0 could refer to the bone state.

That means all reactants have a value the reactant field now should be assigned a value of G that is less than zero and the product field should be assigned a value of G that is greater than zero and what happens in the entire field as you now solve for G is the G rapidly rises across zero within a very thin narrow region mathematically speaking it is almost instantaneously happening that is why it is a surface of discontinuity at the at the frame all right that means it is having a value that is less than zero up.

To the flame it is now suddenly jumping to a value that is greater than zero on the other side numerically like if you want to now look do like computation like right okay,discretized approximate numerical calculations you could now think about some values from let us say minus 1 + 1 and look for a contour or a surface.

Where typically when you disguise your space for maybe about two or three grid points you now have a sudden rise in G right so that is like a approximate way of doing the flame but effectively we are looking at something like this so what you want to do is as I said SL itself is scalar so it acquires the direction normal to the flame therefore you need to actually define a unit normal vector unit normal vector.

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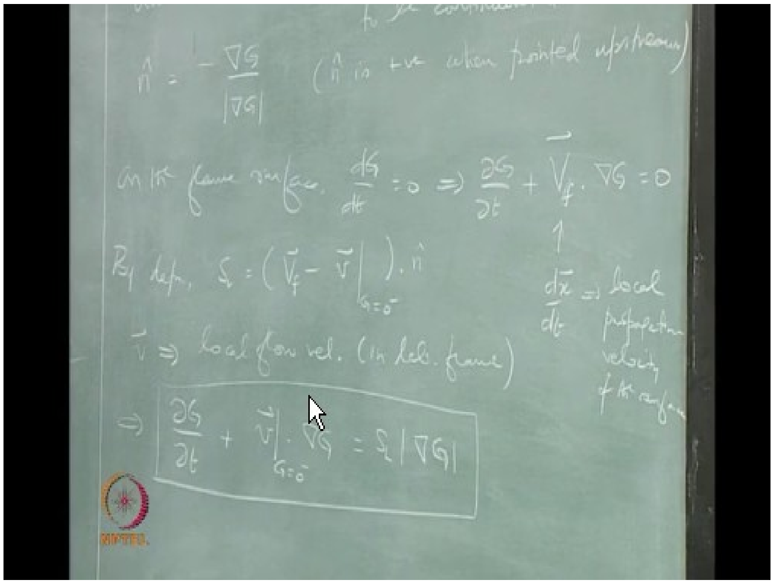

We are of course assuming the flame surface to be a continuous and smooth right that means you say it is important to actually have a continuous and smooth flame as an assumption because at every point you need to be able to define a unit normal so if it is not smooth and it is kind of having like a cusp then you are going to have multiple unit normal at the point which is ill-defined right so you cannot really allow for cusps to happen so that is like saying it is really not smooth but it is still continuous.

But there are situations when actually the flame gets cut right but even when the flame gets cut it actually tries to coil around and then make like a circle and then start consuming reactants that are entrapped within this zone so momentarily you might you might find some discontinuities but pretty soon you are going to get something to be to be made continuous sorts it is not terribly bad assumption so what you are saying is under these kinds of assumptions.

We now say we can define a local normal like _ grad G / Mont grad G and we take n as positive and pointed upstream you need to have a convention on this and in is taken as positive and pointed up screen okay, so then what you do is we want to now have an evolution equation for G how does the G equation evolve or how does the CD surface described by G = 0 evolve right so the evolution equation is obtained by adopting a Lagrangian system the beans you now sit on the flamer you write the flame course.

It is going to be pretty hot out there if you are able to bear that ok so you're going to have some fun sitting on the flame right what happens as you sit on the flame and it is doing whatever it's doing you are there roaming you are not nothing is nothing is happening because you're always sitting on the flame right all the fun can be seen only if you know view from outside like in a laboratory fixed coordinate system you can see the flame movement.

So the Lagrangian frame of reference says that on the claim surface right DG over DT equal to zero the reason why we use a ordinary derivative is your space is fixed by the location of the flame on you are on G = zero and the only thing that is varying is time right and then we are saying that the G is going to be invariant in time because you are sitting there nothing is happening while you are sitting there this in fact is what is typically radians capital G over capital D T in an solitarian frame of reference then with respect.

To an already in frame of reference if you now pull yourself outright you will now call this the material derivative right so this would then mean in a lamina frame of reference we have to write this as partial z with respect to time because g partially changes with respect to time besides there is an apparent change with respect to time because of its motion right.

Therefore we have to say a capital V F vector dot grad G = 0 this is essentially partial T partial leave over DT+ V 0 δ of G so this is an operator that is acting on G that essentially is basically trying to say so what is what is VF now VF is nothing but DX robo DG right that is essentially the position vector corresponding to where the G is and it's change in time so that means it is essentially the displacement of the points along the flame taken as derivative with respect to time to get the flame motion.

So this is actually the local so this is like local propagation velocity right now when you say local propagation velocity it is sort of relative to something that is very local it is not thinking about a flow field that is around it is trying to have a relative motion of the flame with respect to flow round right so this then by definition of the way SL this right SL is nothing but the VF minus the flow velocity V vector evaluated at Z equals 0 minus this is corresponds to the upstream reactant velocity at the flame 0 n hat right.

So this is to say that you are going to have a relative velocity between the flame moment and the and the flow that is manifesting as SL if your flow work y ascent writer or you if your reactants require sent then you will I identically have the flame propagation velocity that we talked about as the flames flame speed okay, except we have to now consider the 0 product because you have to look at the local normal propagation otherwise you won't get a scalar out of this vector or you couldn't have made a vector out of the scalar either way you can look at this but so if you now say so we then SC local flow velocity in lab frame right.

That is all earring in frame and from here we can get if you now plug this back here you can get in this equation you can get plus V obtained at g equals0 minus dot grad G equal to SL mod grad G that is substitute for n s _ grad G divided by mod grad G and you should be able to get this right.

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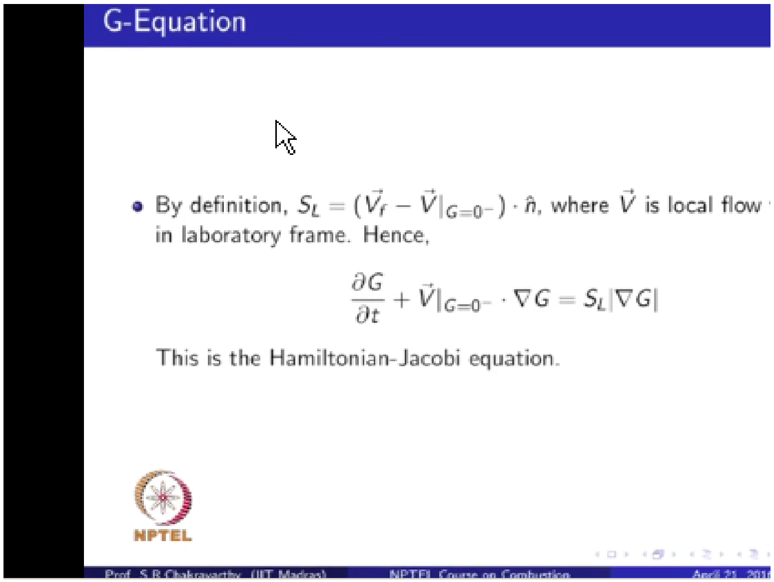

G-Equation

- By definition, $S_L = (\vec{V}_f - \vec{V}|_{G=0^-}) \cdot \hat{n}$, where $\vec{V}$ is local flow in laboratory frame. Hence,

$$\frac{\partial G}{\partial t} + \vec{V}|_{G=0^-} \cdot \nabla G = S_L |\nabla G|$$

This is the Hamiltonian-Jacobi equation.

Prof. S.R.Chakravarthy (IIT Madras) NPTEL Course on Combustion April 21, 201

So this is what is called as the G equation the G equation essentially is an evolution equation for the flame surface as if is a surface a surface of discontinuity across which the temperature changes from the unborn temperature to the burnt un burnt reactant temperature to the burn product temperature and reactant concentrations become zero for particularly the deficient reactant and product concentrations go from zero to whatever is the final product value and so on okay, we will stop here this at this stage I will see you at 3 o'clock tomorrow you.

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