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COMBUSTION

Lecture 36 Ignition

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So we were looking at ignition and then we were looking at ignition as a somewhat like an inverse process of quenching not exactly but you look at the numbers to be slightly different but the process is basically have the same idea therefore we could now think about again like a parallel plates what I was saying yesterday is instead of having like a global energy balance we could actually have a local energy balance so let us look at a different approach to do this to probably get the same results again.

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So or similar results so consider a gas between two infinite parallel plates and now what we are saying is at ignition that is one of the criteria that we listed so at ignition we need to have d/dx(-kdT/dx)=wQ where this is actually the should use a different symbol here maybe $\dot{w}Q_R$ so this is the chemical heat release or the heat of reaction. And therefore you could say d^2t/dx^2 which is this is the conduction heat loss that is q, q and that is equal to the chemical reaction rate right.

So that is equal to so if you now assume constant k then you are going to get $-Q_r/k$ you can now write this a \dot{w} as ae^{-E/RT} $Y_f^p Y_o^q$ right, keep in mind that this q is not the same as that so we run out of symbols pretty soon.

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Thermal Ignition
Consider a gas between 2 infinite parallel plates separated by distance <i>R</i> . • At ignition,
$\frac{d}{dx}\left(-k\frac{dT}{dx}\right) = \dot{w}Q_R \Rightarrow \frac{d^2T}{dx^2} = \frac{-Q_R}{k}A \times \exp(-E/RT)Y_F^pY_o^q$
• Let $\eta = \frac{x}{R}$, $\nu = T - T_o$, and $\theta = E \frac{T - T_o}{R_o T_o^2}$. If $\nu << T_o$,
$exp(-E/R_uT) = exp\left[-\frac{E}{R_uT_o}\left(1-\frac{\nu}{T_o}\right)\right] = exp(\theta) \times exp\left(-\frac{E}{R_uT_o}\right)$
• Let $\delta = \frac{Q_R}{k} \frac{E}{R_w T_o^2} R^2 A \times exp\left(-\frac{E}{R_o T_o}\right) Y_F^{\rho} Y_o^{q}$
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Because we use current pretty much the same kind of symbols most of the planets say m and n but that is fine. Now the reason why we have to write the \dot{w} like this is because this is a differential equation in temperature and the temperature shows up here, so it means when you now integrate this strictly speaking we should think about like bringing this down here and then taking it up there and integrating and so on. Now that is of course an involved process so let us actually try to see how we can manipulate this a little bit more.

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So introduce non-dimensionalization η =x/R that is non dimensionalizing the length and now let us suppose the v stands for T-T0 that is a departure from the wall temperature for the gas and let us say θ =E(T-T0)/RT0² this is not the same as or Z_L which factor because we used to have a Tf keep in mind and so obviously then this can be written as Ev/RT0². Now note that we are saying v is quite small when compared to T0 that means we are looking at small departures from T0 for the temperature near the wall and if you have this notion then e-E/RT can be expanded about T0 as exponential of negative E/R from T0+v and that can be written as a exponential of $-e^{E/RT0(1+v/T0)}$.

And then you do a binomial approximation so this would be exponential of e-E/RT0(1- actually should have a parenthesis here, 1-v/T0 and this should be equal to $e^{Ev/RT02} e^{-E/RT0}$ right, and that means this is equal to $e\theta e^{-E/RT0}$ okat, now let us say let $\delta = Q_R/k E/RT0^2 R^2$ well maybe again I mixing up symbols so we should go back and write this as R_U and R_U , RU you have plenty of places where we need to make this correction so and $Q_R/k E/RT0^2 R Ae^{-ERUT0} y_f^p y_o^q$ so just in case maybe you can just go back and put \dot{q} there okay.

So if you now do this go back to your original equation so this is where we were and we did all these things and so finally what you are going to get is we get $d^2\theta/dq^2=-\delta e^{\theta}$ that is really what I like about these non dimensionalization you know it kind of like you have been to haircutting

saloon and got yourself a nice haircut so the governing equation now we can so the king compact right. So for the boundary conditions we have x equals in our new coordinates $\eta=0$ we have to suppose that dT/dx=0 by symmetry and x=R which implies $\eta=1$ we have to have T=T0.

If T=T0 then a v=0 if v=0 then θ = right, now let us now do something like a linearization so take e^{θ} as 1+ θ that means you do a Taylor expansion and chopped off things that are going square and so on, so if you do this then that is pretty straightforward what this means is $ed^2\theta/d\eta^2 + \delta\theta = -\delta$ so you just go back and plug either the e^{θ} as 1+ θ in this and expand out and take the term with the θ to the left hand side so that you have a differential equation that looks a lot more familiar when compared to what we are used over what we have been having and therefore θ equals let us say a1 $\sin\sqrt{\delta\eta}+a2 \cos\sqrt{\delta\eta}-1$ right, so you have the complementary part and the particular integral there and therefore you get $d\theta/dx$ from here as $\sqrt{\delta}[a1 \cos\sqrt{\delta\eta}-a2 \sin\sqrt{\delta\eta}]$.

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So if you now supply the boundary conditions the symmetry boundary condition implies that you now plug your $\eta=0$ and the sine term goes away and then you now say that $d\theta/dx$ D should be equal to 0 which is the same as dT/dx=0 that means that the cosin is actually going to one before a1 should be equal to 0 and at the wall $\theta=0$ this means $0=a2\cos$ is coming from the cos δ -1 right.

So from here we get $a2=1/\cos\sqrt{\delta}$ and θ now becomes $\cos\sqrt{\delta\eta}/\cos\sqrt{\delta}-1$ right, so with this what this means is we need look at what is θ is T-T0 e over this right, so for the solution what we are looking for is ignition that means we need to have some ignition energy that is there that is going to raise this temperature from T0 to whatever value that will create the reactions will happen significantly therefore obviously T has to be greater than T0, so θ has to have positive solutions right.

So one of the things that we have to look for is of course η is a variable so that that is varying and you have to make sure that you have to have this one for the e range of heaters that we are looking at between 0 and 1 should be greater than 1 right. But more than that what we have to worry about is so we need θ greater than 1, right but more than that what we have to worry about is so we need θ >1everywhere for ignition more than that we need theta to be bounded okay it is one thing to actually have a sorry greater than zero right.

So more than more than theta just being positive we also want to make sure that theta does not really blow up right so also, also the solution becomes unbounded for cosine square of Δ going to zero so if the denominator goes to zero in even in the first term then you are in trouble which implies that square root of Δ this π by two right or we can say Δ =PI²/4 right so if this is the case then you do not have a steady state solution so no steady state solution no steady state solution exists for this value.

And a bow now unlike problems that have this kind of a governing equation at least for the homogeneous part where we would be looking for oscillatory situation and Eigen values having multiple values right so obviously you can say that cosine $\sqrt{\Delta}$ is it going to be is going to be 0 when $\Delta = \pi/2$, $3\pi/2$, $5\pi^2$ and so on but that is not what we are interested in right so as you now have the Δ actually keep on increasing you now reach this value and that is bad enough we do not have to worry about the next value it is going to reach the next value those things are not basically physical anymore what we are interested in is like let us say the first value why are we interested in that because Δ for you what we are looking for is the capital R² as your as your size.

So long as your size is less than a certain critical value you are now going to have more loss when compared to the heating by the chemical reactions and at ignition what we are saying is this equality happens so this equality begins will happen for a certain minimum critical value of capital or over here and there for a corresponding Δ beyond which ignition will happen and again this instant this equality would not hold good because you will now have more heat release due to chemical reactions than the conduction at the walls and then the reaction grows and then you now have an ignition right before the critical value of capital R or below the critical value of capital R.

And correspondingly a less value of less than the critical value of Δ you are going to have the heat loss to be greater than the chemical reaction therefore ignition would not happen right therefore what we are basically looking for is this implies that Δ critical as has a minimum value for ignition right now if you go back and look at this Δ and let us not worry about how this Δ is really formed let us now begin to look at the dependencies so looking at dependencies of Δ courage right and this is always something that we have been thinking about we always have to have our square.

And since you have these dependences here that is going to now have a pressure dependence show up through the concentrations so you are going to have a peep over in show up here and of course we have a key to the e to the minus e / r UT not showing up t0 and you have a $t0^2$ at the bottom right $t0^2$ now this should be depends on so let us say equal to equal to a constant right.

Now the constant here that we are talking about is π by 2 in this analysis and as I said let us not even worry about the next values and so on but in reality this constant is empirical it is not it is not exactly this that is because we are losing a lot of things first of all your kind of assuming a momentary steady state here that this does equals that just this particular point.

But they will all said it is a dynamic process you have an unsteady process essentially and then we are not really worried about the variation in the temperature with time when the ignition is happening so we assumed a steady state process and then looked at when it is violated so this, this formulation is somewhat limited in the way it is done but the most important thing that we are looking for is the dependences on pressure and temperature the pressure of the system.

And the initial temperature of the reactor that is what we are looking at and therefore we simply say this should be equally a constant or if you now have this, this greater than a constant then you will have ignition or if you want avoid ignition like for example you want to now say I have a very narrow tube. And they are reacting mixture that is being sent through the tube and I want to make sure that I did not get ignited then theory critical should be less than this constant value right so that is typically obtained empirically that is actual value if this.

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So here what we can see is that our then squared goes as on ever PN beeping sorry p to the n keep that in mind and also you now have slightly complicated T⁰ dependence okay now let us also now look at what is the situation if you now have like a spark ignition okay so what we have done is something like a thermal ignition where we are trying to heat up otherwise so but spark ignition is slightly different.

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You need to have electrical energy put in there and spark ignition is something that is very commonly adopted in many ignition situations of practical in practical systems so our goal here is to fold one is looking at something like a are critical similar to this and I will show you that a similar dependence can be obtained by looking at the global energy balance similar to the wave you are doing for the quenching so find minimum ignition energy right so what we are looking for is if you now have a spark that is coming up and you now have a flame that is now growing from here spherically locally spherically that is how it is going to happen.

So strictly speaking we should be looking the day is a critical radius for the spherical flame that well that will sustain growing propagating instead of giving away the heat that is liberated during this ignition to the surroundings so if you are only think about this let us suppose that as I said long ago you fill this room with reaction mixture okay and then you pray that you are not going it is not going to get ignited and what happens when it gets ignited right or why is it so is reaction going on and it is not getting ignited there is a question that we are asking before the answer is according to the arena is law because it is actually at some temperature the reactions are going on okay but the reaction rates.

So low that the heat release rate is so low that it is just getting conducted away to the surroundings from where it is happening right so therefore what we are basically looking for is what is the energy that is being supplied by the spark that will actually ignite a critical size of this flame ball whose surface is so large now that the chemical energy release that is happening in this is sufficient to overcome the heat loss to the surroundings right so that is what we are essentially looking for so the flame will not propagate if the radius of the spherical spherically propagating flame is less than a critical value.

And the idea is very similar to what we have seen so far so that is a at this stage QR .= s QL dot and that is to say w heat releases o a reaction rate times heat of reaction that is heat release rate times 4/ 3π or squared sorry cube should now be equal to conduction conductivity times π ups or squared that is the surface area x TF - T⁰ t divided by orchid that is to say we are now basically assuming that locally the temperature is high alright but then this gives rise to a temperature fall just outside this ball and now therefore you have a heat loss in fact if this is your T⁰ let us do this on this side.

And this is your TF you could actually take a cylindrical column let us suppose that you now think about like a hollow cylinder that means a cylinder of wall thickness right so you have an inner a dinner diameter and an outer diameter inner radius outer radius and the temperature inside is uniformly TF okay and now you tend the outer radius to infinity okay so it is kind of like a hole in the middle of nowhere right and then the whole is with added TF and far from here is actually teen on you should now be able to do a conduction problem for this particular situation.

And then try to find out what is the heat, heat the heat transfer at the wall you should be able to show that this is what it is right so if you do that then from here of course again so you can cancel this awkward here too from here and then this from there and get x squared so orchid square then is like 3k TF- T⁰/W.QR keep in mind previously we had a w dot which we had to expand in terms of temperature because we are using a differential equation in temperature but here we are not really writing a differential equation in temperature.

The values of the temperature are actually placed as well as specific limits therefore we should not have to worry about expanding this in terms of the rainiest law on the law of mass action clear we can just keep it this way and previously we also said that this QR is nothing but c p x TF $-t^0$ so we do not worry about the TF by T⁰ but keep the CP the bottom and if you now have a cave over CP that can be directly written in terms of α a right.

So if you now find this orchid squared is equal to α similar sl4 / w dot similarly we also had $SL^2=\sqrt{SL}=\sqrt{\alpha}$ w dot or SL squared is α w dot right so if you now take think about our current squared is equal going as α divided by W.SL square is going as α w dot then it can directly get from here you can see that you can see that orchid goes s α over SL as before as before is during quenching

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Right now I want to caution you that you now have a number three here that is coming from the volume to surface area kind of consideration but in reality we do not have this kind of number it is more than that right and I will point that out that this was related to the penetration distance yesterday when we are doing ignition so if you now say we are interested in the energy so if you are opposed if you now say that the ignition the energy that is the spar is going to deposit into

this gas is supposed to go and increase the a critical mass of gas turret to the temperature TF - T not right that is what this is supposed to do that does energy right.

And in fact if you think about this is essentially the statement of the second criterion that we wrote yesterday as a rule of thumb and this is actually relating to the first criterion as a rule of thumb so we are kind of applying both in stages and this M crit now is essentially like alike a pocket of gas of a certain critical mass and therefore it is going to be density times a critical volume and the critical volume is associated with a critical radius that we are looking at so therefore we can now plug the critical radius there so this is nothing but $4 / 3 \pi$ or Squire I am sorry orchid cube you also have a density.

This is this desidensity is for the pocket of gas that is God ignited therefore you are looking at products within this fear right so you need to have a $\rho\infty$ there and CP TF- T₀ and so this implies that ignition let us not worry about the 4/ 3 π let us now begin to look at the dependence and so what we see because we are now looking back again at the our crit going as α over SL as the dependence and therefore this depends on keep the CP all right and write your $\rho\infty$ as P over R ∞ DF right and keep the TF – T₀ all right and then look at our crit or critters nothing but α or SL as a dependence therefore this is going to now go as α over SL³ right.

And in fact putting everything together in terms of how the α depends on pressure and the pressure divine is here itself an S else pressure dependence everything together we will retrieve from here we could deduce that ignition goes as P - 24 n approximately equal to 2 this is 4 if you now go back here you are talking about p to the n is the order of the reaction that means if you are now looking at a global reaction with a law of mass action like this it is essentially p +q right so n =2 is the order of the reaction if you now plug that in there for the SL dependence on pressure you should now get this taking other pressure dependence in this expression into account and this is for typical hydrocarbons right and this actually pretty much gives a good dependence compared to experiments right so if you do not think about how the experimental dependence.

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Tomp: defandence: for increase in 300-450 K range for increase in 300-450 K range Eign f from ~1010 of mJ Eign f from ~1010 of mJ

So experimentally its observed that if you now try to plot your ignition vs. pressure and of course if you know do this on a log-log scale right we should now get a straight line that goes downwards but what we find is typically this the data goes more like this which means this is the P - 2 dependence and the P - 2 dependence is actually fairly well satisfied in the low pressure region and compared to the high pressure high pressure you do not have this fall so that means you do you do have a critical ignition still needed me the ignition energy needed is more than what the pressure dependence would say.

And of course that that implies a kinetics effect as well that means there is DD reactions do not behave exactly the same way in terms of the global kinetics is concerned and the other thing obviously we are interested in is the temperature dependence and there is some data to that if the temperature dependence like for example if you now say for increase in the three let us say 300 to450 degrees C ray sorry Kelvin range right the e ignition drops from around tens of millions to a few mille joules that means we are looking at numbers like about 40 mille joules 270millions at 300 k whereas when you now go to like 450 k you need only about four millions family jewels kind of thing right. So the temperature the initial temperature has increased the ignition energy required minimum ignition energy required is less correspondingly but you can actually work out how this exact dependences itself from here okay so with this we should conclude ignition and as well we would like to stop talking about premix flames is that essentially what we have done is spent significant amount of time talking about pre-mixed flame deflagration we have not done trim explain detonations starting from where we did the ranking hanging relations.

And we saw that you have one branch is actually four different deflagration to the other branches detonation but essentially the idea is for premix flames right we have you ever we were always assuming that the reactants were approaching the flame in a pre-mixed eight and then we started asking the question how do you how do you know what is the slope of the Rayleigh line and that is actually corresponding to the flame speed and so that actually turns out to be an Eigen value of the system if you now look at how the equations pan out looking at how the preheat zone and the reaction zone is then we constructed the preheat zone temperature profile.

And the reaction zone temperature profile to 20 thought or we just say this is a convective react diffusive zone that is a reactive diffusive zone and then we neglect the other terms that are in unimportant like the reaction zone reaction rate term in the preheat zone and the convective term in the reaction zone and construct temperature profiles match the slopes at the interface and then try to get the flame speed and then we started looking at the dependence of spins the flame speed on physical chemical properties initial conditions or the reactant conditions pressure and temperature.

And so on and then we looked at frame shape show the flame actually gets shaped over a burner and how it gets stabilized and what happens to it at the peak at the tip when you have a flame curvature and a flow divergence effect and then we started looking at flammability limits and quenching criteria and ignition criteria and so on so all these things actually we have been talking about or primarily in the context of pre-mixed deflect laminar deflagration right so it is time we started talking about diffusion flames and so now onwards for the rest of the time or at least for quite some time we should not be talking about diffusion flames we are still primarily in the deflagration regime that is we are looking at low subsonic Mach numbers for the for the reactant flow and therefore we have to go back.

And look at the momentum equation and find that the pressure is approximately a constant because we are now looking at low Mach numbers and low notes and numbers and therefore it just reduces to pressure it is a constant which means we can go back and adopt like the schwabzelda which kind of formulation and where we have to look at the species conservation equation and the energy conservation equation with a flow field that is prescribed unless of course you want to take into account the density variation with temperature which is also the flow field and you can now look at the flow problem loosely coupled with the combustion problem and not necessarily tightly coupled in unlike, unlike in a full compressible manner.

So we will now begin to start talking about diffusion flames now diffusion flames is actually kind of like the classical term for flames that are essentially non premixed so did the modern terminology for this is simply non pre-mixed flames so we have to understand why we are getting these different semantic notions about this what we meant we get

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What we mean by a diffusion flame is here we are now saying that the reactants or just mixing at the flame right it is kind of like you are rushing into the exam hall and you are just studying for the exam right so you are really not prepared so similarly the reactants are not really prepared and what has been by prepared that means you have to actually premix right so if the reactants or pre-mixed then they are ready to react and all they are waiting for is for a temperature rise to happen and then they are going to react right and at a steady in a steady state situation the temperature rise happens because of the flame that has already been established.

And so as the reactants get into the flame they get preheated and then react if that is what the flame is all about that is why that is how we were talking about it but in this case you have aflame all right but the reactants or just mixing at the time they are reacting right so when that is happening then you have to start thinking about which is faster which is a faster process is that the mixing is it going to be quite fast or is it the reactions that are going to be quite fast now typically in a combustion situation what we are interested in is fast eggs or exothermic reactions right this is what we started talking about right at the beginning.

So we are always interested in situations where we have a very high sensitivity of the reaction rate a temperature in turn meaning a high activation energy right and that simply means that the reaction rates are going to be very, very fast once you got the mixing to happen so this is a situation where the mixing is the one that is limiting the entire set of processes in other words if the fuel and air were to mix with the field and oxidizer were to mix with each other then the reactions will happen rather instantaneously or immediately right so mixing is the rate-limiting process in case of diffusion flames and of course the technical sounding term for mixing is diffusion.

So you can say diffusion is the late rate limiting process and therefore the heat that is released from a diffusion flame is not necessarily limited by the chemical kinetics as in the case of premix flames so you would say they are premix flames are kinetically limited in terms of heat release whereas in the case of diffusion flames you should say it is diffusion limited right.

So you are not going to really experience the as much heating there then premix flames is that is essentially the idea so here the mixing between the reactants or mixing off the reactants is the rate limiting process relative to relative to reaction therefore the heat release in a non-prime explained is diffusion limited Oh as opposed to as opposed to being politically limited in a premix flame hence the name diffusion flame for these.

But we will see that there is some exception here I mean we will be able well just keep building this idea and then see where it falters okay so at the moment the idea basically is that diffusion is the rate limiting process and therefore the heat release is diffusion limited rather than or the heat can be released one lead to the extent but to which the reactants can mix then whether they can actually release by chemical kinetics like what is a chemical reaction rate based on law of mass action and so on.

So do you think that we have to think about is are these very common in fact these are actually more common when compared to the premix flames premix flames pretty much have to be contrived many times you have to make somebody has to mix the reactants right whereas diffusion flames at the ones that are happened naturally in nature right.

So if you want to for example light fire to a block of wood or something like that that is essentially a diffusion flame that is going on right and candle flames the best example right so the candle flame is essentially a diffusion flame so that the laboratory if you want to now establish a diffusion flame take go back to the Bunsen burner that we have been talking about but you now shut down the air entrainment along with the fuel at the bottom right and just allow the field to come along and I have the air mixed with the fuel outside and that is if that is a pretty good interesting experiment that you can think about so if we now had a Bunsen burner.

And you now had the bottom ring open pretty much fully and you had this orifice through which the fuel is coming out like a jet and creates a locally low pressure so that the air gets sucked in and in and in trains into the field and then mix us into this tube and then you now have a nice conical blue pre-mixed flame and then you now start slowly trying to move this ring so that the hole is actually progressively closed and you are letting in less and less air and as you get in less and less air you are making this flame more, more fuel rich because you just have more or more fuel and less and less air.

So it becomes fuel rich and we talked about fuel rich premix flames earlier in the context of stabilization and what we understand is two things one as the air entrains at the base of the flame you are going to have a enrichment of this mixture and it is going to be close to the stoichiometric and actually get anchored much more firmly the other thing is for the remaining shoulder of the flame you are going to have a fuel rich products that are coming out and that is going to mix with the reactants and have a diffusion flame envelope right so ultimately when you now close this ring completely.

And you know do not let in any more fuel then what is happening is you have only fuel coming out and then you have mixing of air that is happening and typically what you should find is you now have a diffusion flame that is fairly elongated when compared to a more compact pre-mixed conical flame and this is going to now look not exactly shaped like a cone anymore right it is going to have like it a tear drop kind of shape and it is on blue and blue any longer it is more orange and elevations and pockets and so on that essentially typically or orange flame so what this means is you have inside of the flame you have all fuel outside of the flame you have all oxidizer at the flame you are basically having the to mix. And produce products of course the products are free to diffuse on either side and they are in general getting convicted upwards and of course the whole set of species are actually moving upwards because of buoyancy that is another that is another matter in a gravitational field around and that is and that is partly the reason why you are seeing this, this kind of a shape for the flame and, and also the reason why the flame looks elongated besides.

The diffusion process itself causing it elongate when compared to a compact conical pre-mixed flame so these are lots of these kinds of different thing are happening as you now change this from a pre-mixed flame to a division play which a nice experiment the 24 for you to think about and do so, so the diffusion flame can be commonly come across come across and we will now talk about how to analyze this next class.

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