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COMBUSTION

Lecture – 30
Laminar Premixed Flames – Rigorous Analysis 2

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So we have the slope of the temperature profile in the preheat zone leading up to the reaction zone is given by a row you see p TI -T_O/ k. Let us keep in mind that we are actually hunting for u, this is what actually we do not know and this is what we are actually looking for and we are hoping that we will be able to actually get this when we try to use the interface matching condition between the two zones.

So what we have to do next is of course integrate the second equation and then also get a slope from there evaluated at x = 0 + and then equate these two and therefore we expect to get the u that south, that is how we are going to go about this, that is how, that is what is looking down the pipeline we are going to be doing, but at this stage we now have a problem, the problem is that we assume, we suppose that we have T = Ti in both the boundary conditions leading up to x – 0- on the one side and X = 0 + on the other side but we do not know what it is.

All we are basically saying is the temperature has to match and we have to now plug in the value of the temperature Ti over here and we do not know what it is, so how the question basically is how do you deal with the situation of not knowing the temperature, right.

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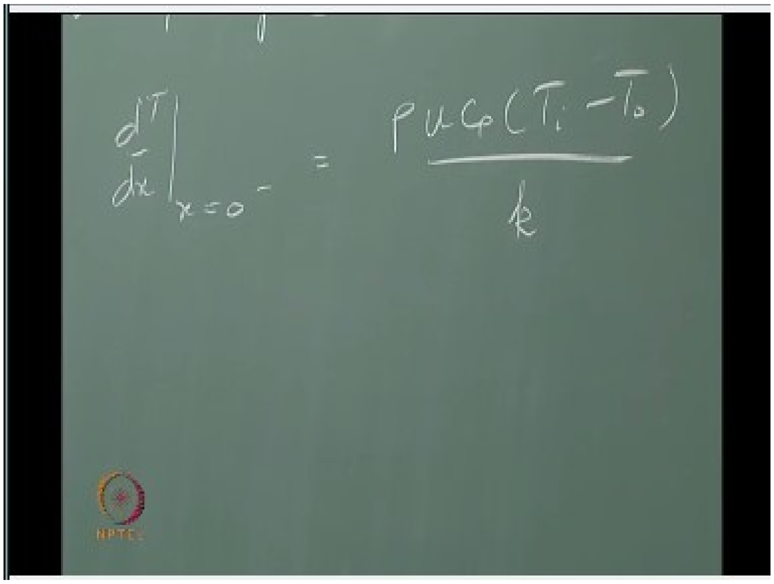

So there are a couple of tricks about this we will talk about, in both the cases we try to now replace this temperature by a known temperature without incurring too much error, so the bottom line basically is without incurring too much error. So what we are going to do from this side looking from, looking from the preheat zone towards the reaction zone at the interface between these two zones is to now say that this is equal to Rho u approximately, ρu CP TF - T 0 divided by K. Why would you do this?

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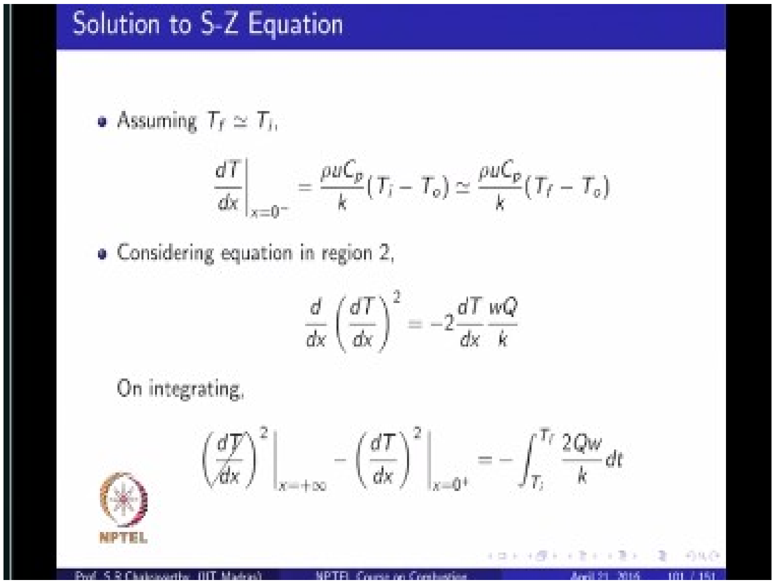

Solution to S-Z Equation

- Assuming $T_f \simeq T_i$,

$$\left.\frac{dT}{dx}\right|_{x=0^-} = \frac{\rho u C_p}{k}(T_i - T_o) \simeq \frac{\rho u C_p}{k}(T_f - T_o)$$

- Considering equation in region 2,

$$\frac{d}{dx}\left(\frac{dT}{dx}\right)^2 = -2\frac{dT}{dx}\frac{wQ}{k}$$

On integrating,

$$\left.\left(\cancel{\frac{dT}{dx}}\right)^2\right|_{x=+\infty} - \left.\left(\frac{dT}{dx}\right)^2\right|_{x=0^+} = -\int_{T_i}^{T_f}\frac{2Qw}{k}dt$$

Well basically the temperatures that we are actually given are TF and T0, TI is an unknown and we are not really making any bones about trying to find it out in the first place, we are trying to actually see if we can replace the unknown by something that is known without incurring too much error. So the last part without incurring too much error is where the crux is so let us look at how TF departs from TI, so the answer is, if you now look at the preheat zone and the reaction zone basically you are having the temperature TI very close to TF, the only difference between these two is the temperature climbs up a little bit more within the reaction zone to level off at a constant slope at the end of the flame thickness.

Alright, so you could say that you are loose there except that the slope is not zero alright, so you have a finite slope, the finite non zero slope that we are trying to look at but it is, it is the value is, this value is pretty small, well if you want to be a little bit more careful about this picture we got to keep in mind that the preheat zone solution is going to actually give you a exponentially increasing solution is what you are looking at.

So effectively we are talking about a value TI that is here and the preheat zone solution would go like this and the reaction zone solution would go like that, right, so that is what we are looking at.

So TR, the point is, the point here we have to keep in mind is this is T0 so relative to relative to t0, so look at this difference or this difference relative to t0 tl is as close to TF, it is not as if like TI is generally close with TF, the question is how close is, it is quite close relative to. That is like you are kind of looking from here and then seeing that those two temperatures are very, very close to each other, alright.

So that is the trick that we are playing in the preheat zone and I will show you how to play a trick in the reaction zone where we do not know ti and we will be integrating it in this region and then, and if you are not anticipating the kind of trick that we are going to play, you must be having your eyebrows raised at this stage, how am I going to actually, how on earth am I going to have ti be replaced by t0?

Okay, because that is what I need to do, okay, because I will be in this region, I am going to go from TI to TF and ti, t0 and tf are what is given, TI is unknown, so in this case I am replacing TI by TF, in that place I would love to actually replace TI by t0. Who of, can I ever do that?

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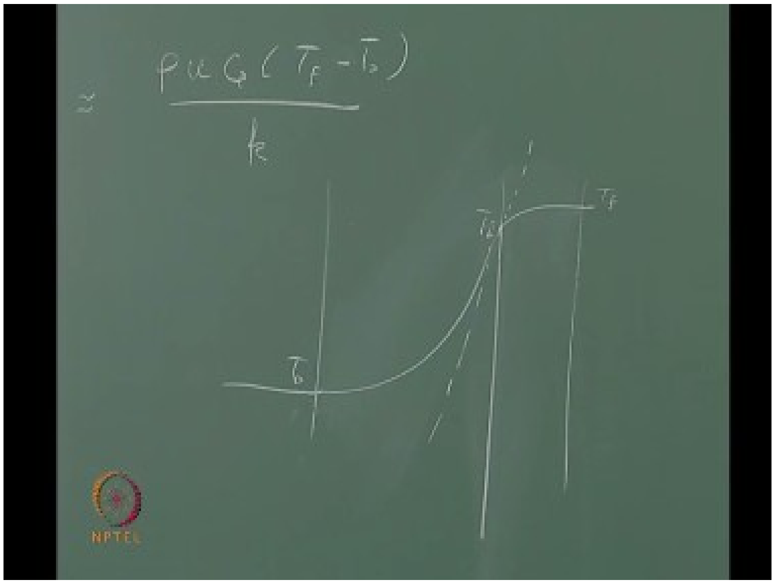

We will, we will see how it works huh, so it is, so wait with bated breath on how we are going to play that trick so let us just go ahead with Rhea, so we now have this, so we will just go ahead with the second equation to integrate it once so the way you want to do that is taking, considering to rewrite it as 2 dt/dx times2 which is like, if you now multiply this equation by twice of dt by DX all the way through then it is possible for us to now write this as d by DX of DG by DX the whole squared = negative 2 dt by DX w q / k, right.

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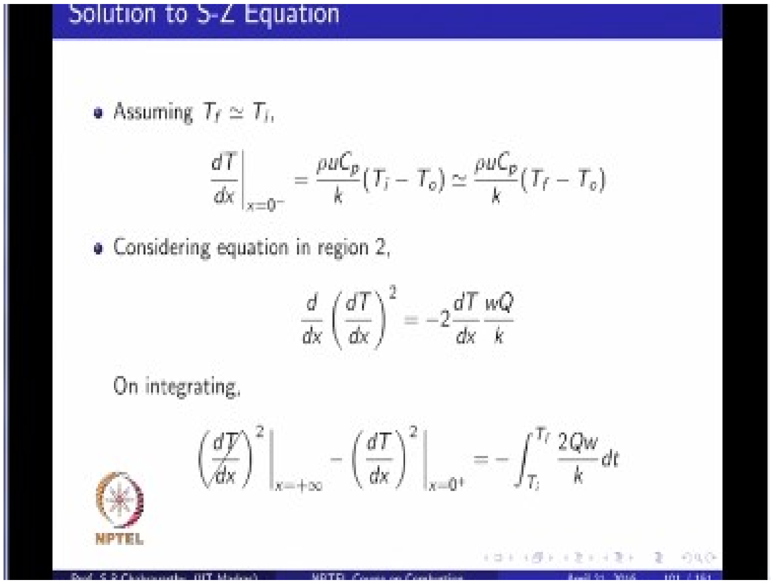

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If you want to just check we can see that if you now differentiate this you get a 2 dt by DX d square t by DX square, so and then the 2 dt by DX gets cancelled on either side. So if you now do this the reason as we can now have exact integrals on both sides so integrating once right from 0 + 0 + to infinity along x, k along x we get dt, dt by DX the whole squared evaluated at x =+ Z. + infinity - VT by DX the whole square evaluated at x = 0 + =, you are going to have this integrated from 0 + to infinity - 2 dt by DX w q / k times DX.

So you could actually say this is not really an integral with respect to X anymore, it is an integral with respect to T, okay, so again you do not have to worry about, and then of course what you have to do is you have to now realize that the limits of the integral have to be substituted in terms of temperature instead of the X location value, therefore we can write this as - integral TI to TF 2 q w / k dt.

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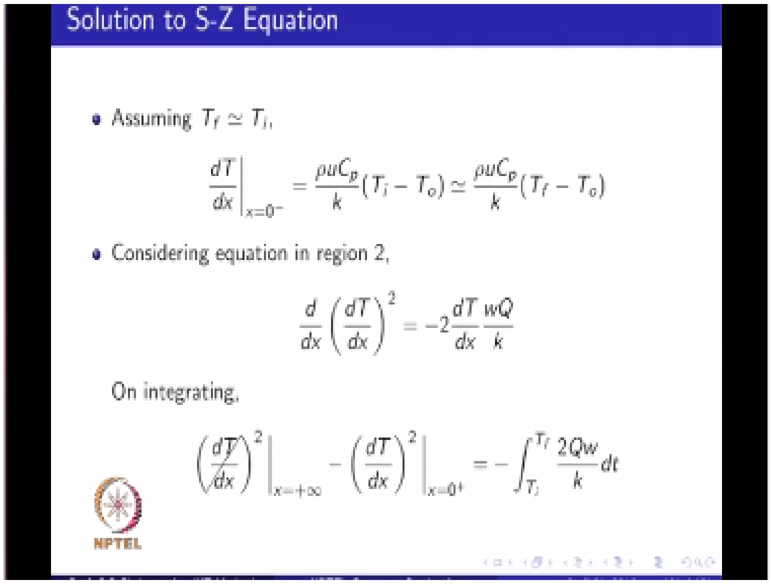

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Now just in case you are one of those people who is impatient about what is going to be the outcome and what or what is it that we are gaining out of this I do not know if you remember I told you that the biggest difference that we are going to get between what you are doing with all these equations rigorously or seemingly rigorously in a mathematical sense when compared to the phenomenological energy balance.

That we did earlier on is we got all the dependencies right the only thing that we are going again is a square root of two okay so the factor square root of two which is different from the thermal logical expression square root of two is 1.4 and force or so you are about forty one percent off in the phenomenological analysis that is still within the order of magnitude you see so 1.4 is both of the order of 1 so, so we there was an order of magnitude estimate so for an order-of-magnitude estimate that was there is it there was a pretty good job so question is where are we getting the square root of two the answer is we are actually having this to showing up here right.

Because we now multiply by 2 dt /dx and then keep in mind that this is going to be a square and I am going to equate this to this right so if I now I am going to have to equate this to this then I have to take a square root so I get the square root of two coming from right here at this particular step okay so now notice that this is going to be zero because you are having your dt/dz go to zero at X as X tends to infinity.

I also want you to point out that we are actually having the X go from here that is the origin and this is very important for us to think about as engineers x equals minus infinity as far as the preheat zone is here whereas x equals plus infinity as far as the reaction zone is here okay so this does not look like very far away when compared to that it is not like we are talking about minus infinity is being here and plus infinity being there and so on,

No that is not what we are really bothered about it okay so infinity is something that is like very kind of flexible it is very contextual right so the reason why we are saying this is actually going to be a very small infinite even compared to that is because you see that you're going to have a steep variation in the reaction rate within this region it is going to rise and fall within the small region and then you have to now take very small steps to capture that steep price and steep fall okay.

So that means to say we are ultimately trying to actually integrate this w with respect to T and you have to get an area under the curve of W as it rises as the temperature changes only a little bit between TI and TF okay and that rise and fall needs to be done over very small steps and if you now keep taking very small steps you pretty much reach you get tired and then you say well I think I have reached infinity if you even if you have not gone too far okay.

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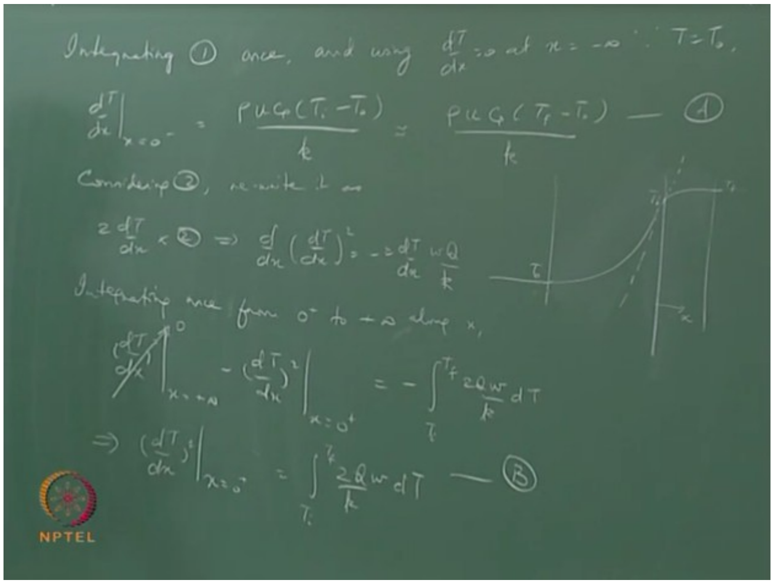

Integrating ① once, and using $\frac{dT}{dx}=0$ at $x=-\infty$ ∵ $T=T_0$,

$$\left.\frac{dT}{dx}\right|_{x=0^-} = \frac{\rho u C_p (T_i - T_0)}{k} \simeq \frac{\rho u C_p (T_f - T_0)}{k} \quad — \text{Ⓐ}$$

Considering ②, re-write it as

$$2\frac{dT}{dx}\times ② \Rightarrow \frac{d}{dx}\left(\frac{dT}{dx}\right)^2 = -2\frac{dT}{dx}\frac{wQ}{k}$$

Integrating once from 0^+ to $+\infty$ along x,

$$\cancel{\left.\left(\frac{dT}{dx}\right)^2\right|_{x=+\infty}}^{\,0} - \left.\left(\frac{dT}{dx}\right)^2\right|_{x=0^+} = -\int_{T_i}^{T_f}\frac{2Qw}{k}\,dT$$

$$\Rightarrow \left.\left(\frac{dT}{dx}\right)^2\right|_{x=0^+} = \int_{T_i}^{T_f}\frac{2Qw}{k}\,dT \quad — \text{Ⓑ}$$

So that, that is essentially asymptotic for you so this is what is called as a inner zone this is what is called as an outer zone this, this zone has a different length scale when compared to that so we are what, what, what we mean by length scale is a characteristic dimension over which we would watch so that is exactly what we what we are talking about when you now saying that this is actually going to 0 there so which means we now say dt/dx the whole squared x equals 0 plus is equal to integral TI to TF 2 qw / KDT so q is the heating value K is the thermal conductivity those are like properties of this system so W is the one that varying with temperature okay.

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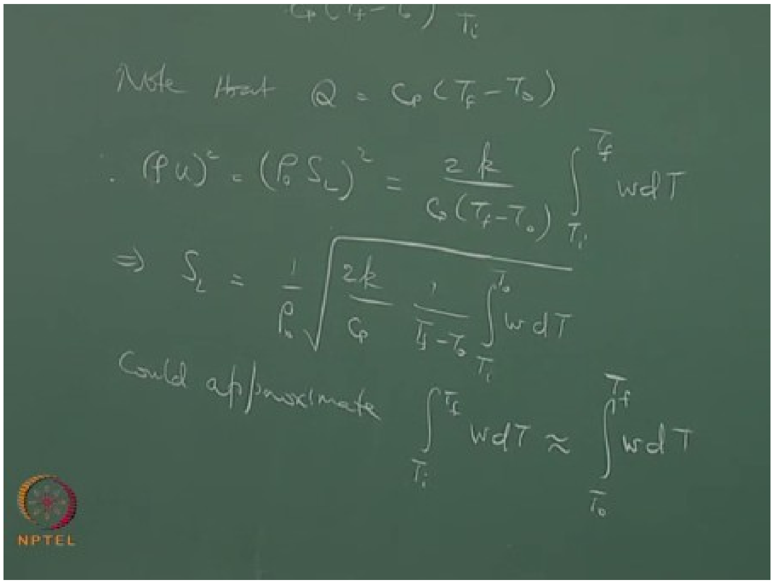

Note that $Q = c_p (T_f - T_o)$

$$\therefore (\rho u)^2 = (\rho_o S_L)^2 = \frac{2k}{c_p (T_f - T_o)} \int_{T_i}^{T_f} w \, dT$$

$$\Rightarrow S_L = \frac{1}{\rho_o} \sqrt{\frac{2k}{c_p} \frac{1}{T_f - T_o} \int_{T_i}^{T_f} w \, dT}$$

Could approximate $\int_{T_i}^{T_f} w \, dT \approx \int_{T_o}^{T_f} w \, dT$

And so this integral essentially is of W with respect to temperature keep that in mind so let us call this B versus let us call that capital A and we now want to actually equate a and B accept a is actually the derivative at x equals 0 minus whereas this is AB by is actually square of the derivative at x equals plus so we have to equate this with square of that okay so a squared equals P implies we now say ρ u the whole square c p^2 see how I am actually squaring things throw you actually what would indicate the mass flux so you want to just keep it together see p^2 TF-T_o.

The whole square divided by k square equal to 22 / k integral t2 TF as a matter of fact we should have thought about trying to get rid of TI in favor of T not right here because we did that when we were trying to get a while getting B we should actually try to get rid of TI we will do it in a minute okay so that is what we should be looking at but now the cats out of the bag we will now try to figure out.

If you that it is not going to be very difficult for us to replace TI/ t^o without much error so that is something that I am going to show you or talk about pretty soon so here we go how to simplify this a bit further so ρ u the whole squared equals 2 k q/CP TF-T_o integral now note that Q equals CP, TF -T_o right for this is actually the adiabatic energy balance so this, this is the heat released in the chemical reaction which is essentially the difference the negative of difference in the ∑ of standard heats of formation of products to the standard heats of formation of the reactants.

And this is actually the sensible enthalpy rise of the mixture between initial and final temperatures right and in fact to be able to notice this made a mistake I guess, I guess so you have a CP^2 $TF-T_o$ not the whole squared so it is mainly to actually cancel this off that we try to replace TI /TF in a back then okay so you might what you might you might think both ways you cv if you did if you got rid of TI there you should have got rid of TI here but if you did not get rid of here.

I hear why did you get rid of ti, ti there okay so we wanted to get rid of TI there because we want to cancel this and we could still go on with this okay so keep going on and see where we where we want to make a change so therefore ρ u squared equals well now for the first time introduce this notation not SL^2 square this is basically notation we could basically say ρu is a constant in one-dimensional steady state right.

So ρ u is the same as ρ^o, u^o okay ρ u is also equal to ρ infinity, u infinity, alright so the reason why we are saying so many things is the way we want to actually look at this as the laminar flame speed SL stands for the laminar flame speed ok is always relative to I should not say always but you have to specify this the laminar flame speed is relative to the unburnt reactants okay when you now say ρ^o SL that means to write the laminar flame speed is relative to the unbolt reactants.

That means to say you now have a flame that is propagating into the reactants and the question is you could be actually sitting on the flame and getting the reactants to come into you at the same speed or the other thing that you can think about is you now have the flame that is go propagating and then the products are actually flowing out you see now if you are actually looking at the flame speed relative to the products.

You will get a different speed when compared to if you are looking at the flame speed with respect to the reactants because the reactants and the products are having different speeds themselves therefore it is always quite important for us to note what the flame speed we are talking about and usually we are talking about aflame speed with respect to unborn still reactants alright but ρμ is a constant so the less controversial term is what is called as a mass burning velocity.

So mass burning velocity or mass burning flux if you can you can, you can call it different ways laminar mass burning flux is essentially you and it did not matter whether you are actually talking about it with respect to unbound mixture reactant mixture all the burnt products because it is going to be ρ is constant you see so we are talking about a flame speed then it is, it is it has to be specified that we are talking about it with respect to unburned reactants.

So there we are so you could you can now write this as 2 k/CP TF-T_O integral TI to TF wdt and we are now going to say so SL is equal to 1 over ρ_o K over CP all up to k / CP 1 over TF –T_o integral TI to T_o wdt, now could approximate I am saying could I am not saying should okay we could approximate integral TI to TF wdT as ∫ T0 To Tf wdT without much error because this is an integral and what we are talking about is if you now look at how the W goes right we are looking at essentially the area under this curve well not exactly this curve this is that would be Wdx we are looking at WdT this is W with respect to this temperature variation right.

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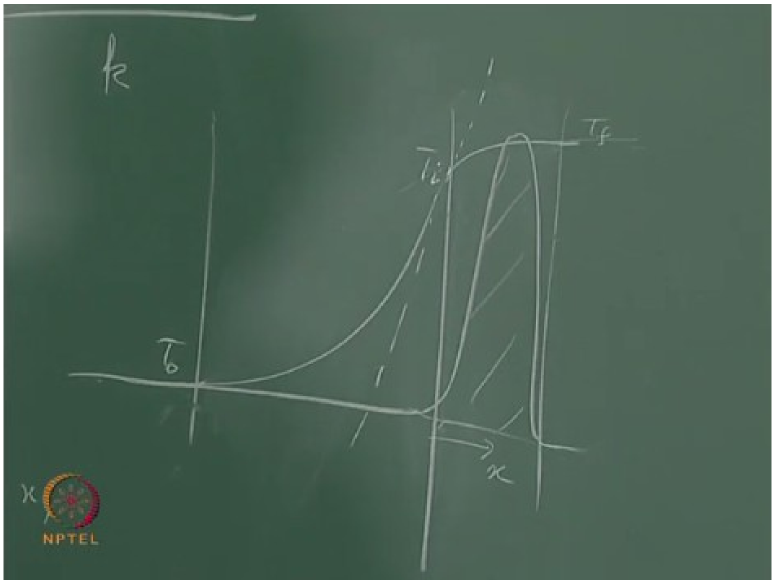

And you can you can easily see that the W is actually 0 outside this region so you might as well actually start integrating from any temperature upstream you would not really care there is hardly going to be any contribution of W there okay so therefore it is because it is showing up within the integral then it is possible for us to actually replace TI / T0 otherwise it would have been much harder in this kind of situation like algebraic it that would be much harder there is no way you can justify that but this is reasonable is pretty good why would you want to do this you do not have to do this as I as I will show you soon.

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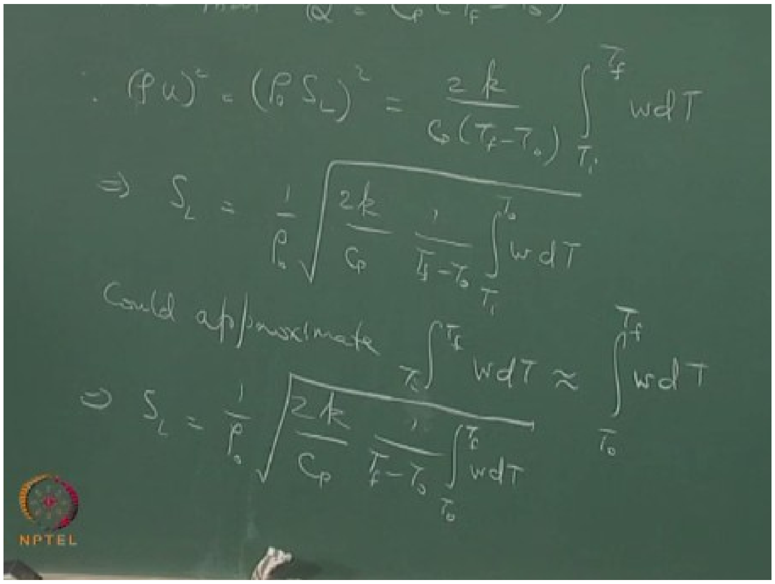

$$\therefore (\rho u)^2 = (\rho_0 S_L)^2 = \frac{2k}{C_p(T_f - T_0)} \int_{T_i}^{T_f} w\,dT$$

$$\Rightarrow S_L = \frac{1}{\rho_0}\sqrt{\frac{2k}{C_p}\,\frac{1}{T_f - T_0}\int_{T_i}^{T_f} w\,dT}$$

Could approximate $\int_{T_i}^{T_f} w\,dT \approx \int_{T_0}^{T_f} w\,dT$

$$\Rightarrow S_L = \frac{1}{\rho_0}\sqrt{\frac{2k}{C_p}\,\frac{1}{T_f - T_0}\int_{T_0}^{T_f} w\,dT}$$

But why would you want to do this what would we get out of seeing this you see that 2k / CP 1 / Tf – T0 ∫ T0 to Tf WdT.

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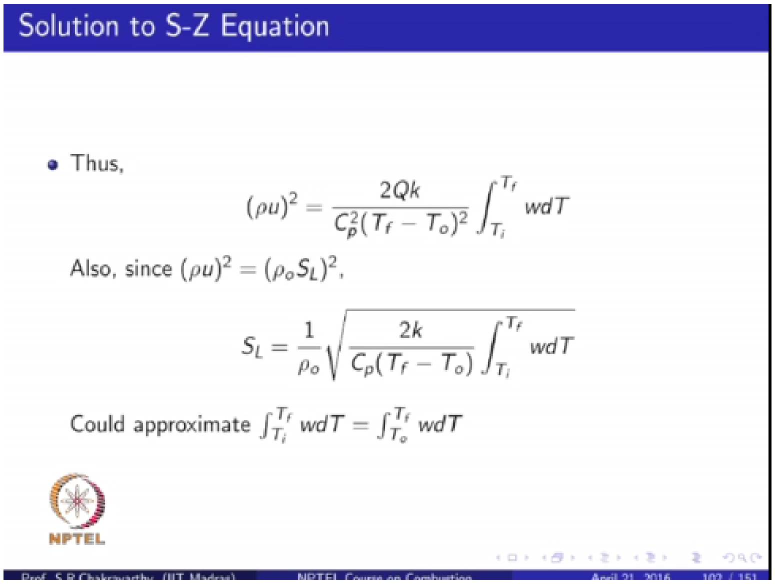

Solution to S-Z Equation

- Thus,

$$(\rho u)^2 = \frac{2Qk}{C_p^2(T_f - T_o)^2}\int_{T_i}^{T_f} w dT$$

Also, since $(\rho u)^2 = (\rho_o S_L)^2$,

$$S_L = \frac{1}{\rho_o}\sqrt{\frac{2k}{C_p(T_f - T_o)}\int_{T_i}^{T_f} w dT}$$

Could approximate $\int_{T_i}^{T_f} w dT = \int_{T_o}^{T_f} w dT$

What do we have this is in fact very similar to the first expression that we obtained phenomenological except for two things one the square root of two factor that have been saying we will get and as a and we are right there getting it starting from this point onwards we get this 2 and then of course it is a square therefore you get a square root of two in the final answer the next is a little bit more important which is originally we simply said we had S_L = 1 / ρ0 ∫2 KW/ sorry did not have the 2 KW / CP and the question was what was the W if you simply had a kW/CP.

Then we assume that that the W was actually privileged over the entire flame thickness Δ and as if it is video is a constant all right but that is not very the case the W varies significantly within this distance in fact it is actually lying very low up until the reaction zone and then Shockley increases and then decreases within a very narrow region call the reaction zone so the major effect of the rigorous mathematical exercise is to recognize that W varies within the reaction zone.

And take it is variation as it is so we are not really replaced we are not really plugging in a w that is a constant and then the question that we had was what would be the constant and we now came up with this came up with this combination call W0 ∞ right where W0 ∞ refers to evaluating the W the reaction rate with reactant concentrations far upstream and the flame temperature downstream right that is W0 ∞ was referring to and that would actually give you the most the highest value that was there as possible.

Whereas if you now have an integral like this what does this look like reason why we wanted to substitute for Ti To this integral was to actually see how what this looks like this is now beginning to look like more of an average you see, so this is an average reaction rate between the two temperatures the limit temperatures T0 for the reactants in Tf for the products so if it is possible for us to actually take an average reaction rate then whatever we got previously with a square root of factor 22 thrown in is what the rigorous analysis gives us based on the Schvab Zeldovich formulation right.

Okay so can we do a little bit better is it possible for us to not necessarily make this approximation okay and then we just plot on saying that let me actually see how this Ti kind of thing is going to work out T is what happens though we want to see if we can evaluate this integral that means we now have to explicitly take in account the dependence of W own temperature and what is that dependence that dependence is essentially given by the Iranian law where we are now saying W is now going to be Ae- E / RuT times concentrations of the reactants.

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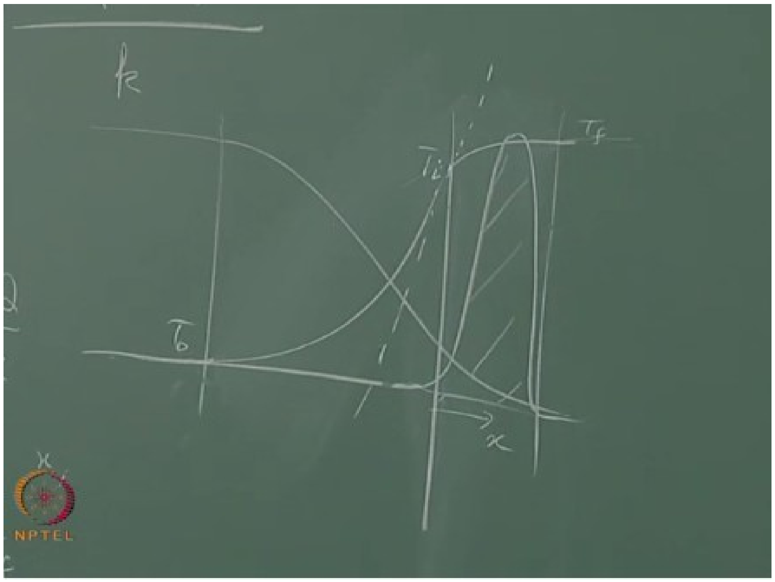

Now keep in mind that the concentrations of the reactants are actually going to fall like this and the AE to the – e/ RT times the concentrations is now going to give rise to a certain variation with temperature which is a bit peculiar so as a simplification we want above the only about variation with respect to temperature which means we will as a first step we will now say for a 0th order reaction.

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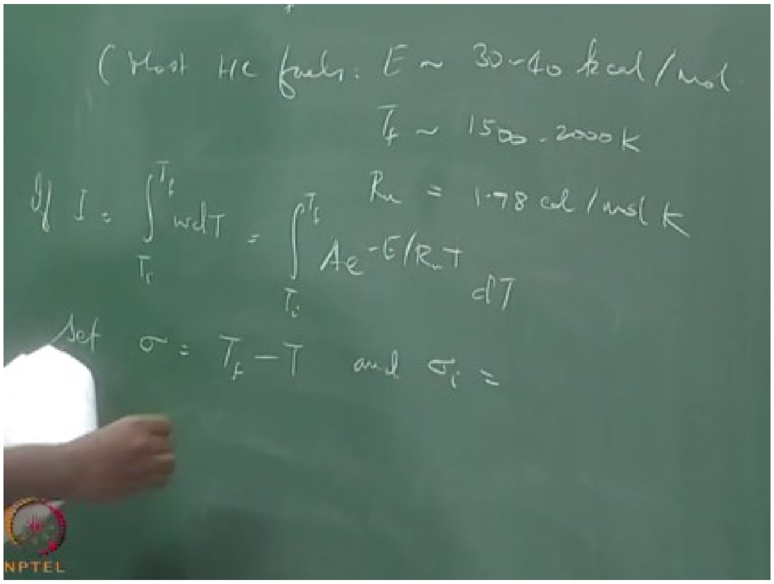

(Most HC fuels: $E \sim 30\text{-}40$ kcal/mol

$T_f \sim 1500\text{-}2000$ K

$R_u = 1.98$ cal/mol K

If $I = \int_{T_i}^{T_f} w\,dT = \int_{T_i}^{T_f} A e^{-E/R_u T}\,dT$

Set $\sigma = T_f - T$ and $\sigma_i =$

W = A E / R UT and that is it of course all along we have been using W instead of ω is the number of moles per unit time per unit volume okay that is how the reaction rate is going to be whereas W is actually the number of kilograms per unit time per unit volume and therefore the difference is you know you know you know have to have a molecular weight shown in here but we suppose that a contains there as well.

So let us not worry about that explicitly but whenever you are using W or ω or any of these things you have to be very careful about the units okay and this is this is many times where you get into troubles with numerical calculations so keep this in mind we are still working on a mass basis and this is this is all we are going to have for a 0th order reaction that means we are not going to worry about how the concentration varies along all right.

Which means we are what are we actually looking for since we have done the phenomenological expressions right we have we have some physical intuition about words what to expect if you are going to do only the 0th order reaction not worried about the reactant concentration did decrease into the reaction zone then all we are basically looking for is this is going to look like the average is the peak value W0 ∞ / β that is a correction that we are basically aiming for okay.

So is it possible for us to actually show that this average reaction rate is going to be like W0∞ / β that is what we did before when we said if we want to keep in mind the variation of W with respect to the flame thickness and say that it varying mainly within this small region and therefore we scale this distance by as Δ / β that is what we did then we got S_L =1 / ρ0 ∞ KW 0 ∞ / β CP.

So we essentially we are looking for this average integral if you evaluate it as it is without replacing Ti/ T0 is it possible for us to show that this will be somewhat like W0∞/ ∞ is what we are basically looking for we are not looking for further Corrections which are taking into account the reactant concentration decrease with into the reaction zone and still for the corrections with no need lowest numbers which we did before okay because those things are still not possible with whatever we are doing now okay.

So now in this in this case I see that E/ RuTf particularly Tf is typically a large value which is around10 which means it is one order magnitude more than unity keep this in mind because I most hydrocarbon fuels you have E of the order of 30 to 40 kilocalories per mole that is again a mixture of units you are not talking about joules per kg it is calories per mole there, so you got you ought to make the conversion this is typically how the values are given and Tf is anywhere between 1500 to 2000 Kelvin or even upwards and Ru = 1.98 calorie per mole Kelvin right.

So if you now take these values you can you will find that this is of the order of 10 which is quite larger than 1 and we are going to use that fact so what we want to do is if I = ∫ TI to Tf W dT right then this is equal to TI to Tf Ae2 the - e / Ru TdT what we want to do is we want to basically be looking at a variation in temperature only within the small region right that small variation is what we what we want to do so Midas will actually look at the temperature as a departure from Tf rather than the actual value okay.

So when you now talk about departures and you start magnifying that value rather than look at high values and then varying where over a small range there so set your new variable σ s Tf - T and then σi becomes Tf – Ti.

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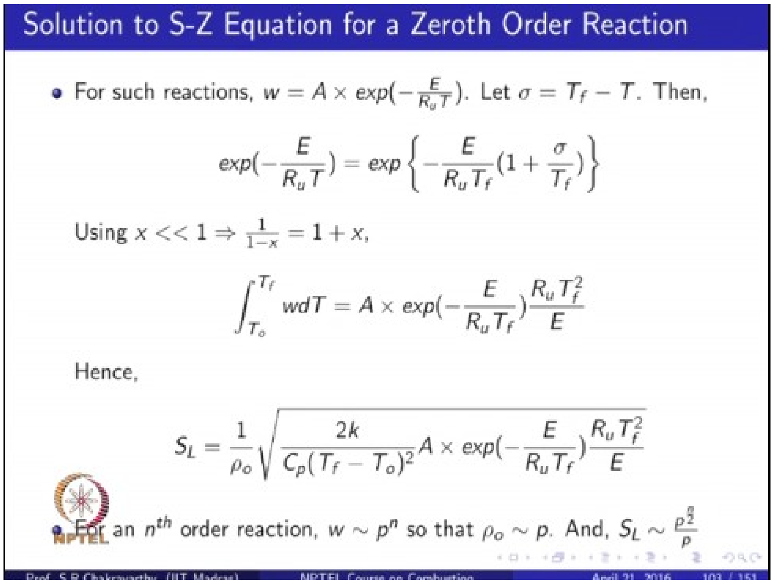

Solution to S-Z Equation for a Zeroth Order Reaction

- For such reactions, $w = A \times exp(-\frac{E}{R_u T})$. Let $\sigma = T_f - T$. Then,

$$exp(-\frac{E}{R_u T}) = exp\left\{-\frac{E}{R_u T_f}(1 + \frac{\sigma}{T_f})\right\}$$

Using $x << 1 \Rightarrow \frac{1}{1-x} = 1 + x$,

$$\int_{T_o}^{T_f} w dT = A \times exp(-\frac{E}{R_u T_f})\frac{R_u T_f^2}{E}$$

Hence,

$$S_L = \frac{1}{\rho_o}\sqrt{\frac{2k}{C_p(T_f - T_o)^2} A \times exp(-\frac{E}{R_u T_f})\frac{R_u T_f^2}{E}}$$

- For an n^{th} order reaction, $w \sim p^n$ so that $\rho_o \sim p$. And, $S_L \sim \frac{p^{\frac{n}{2}}}{p}$

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And of course is now going to go to 0 when T becomes Tf so σ = Tf right and we also have to find out what T is like so T is TF – σ= Df times 1 - σ divided by Tf and we want to note that σ / Tf is much less than 1 right.

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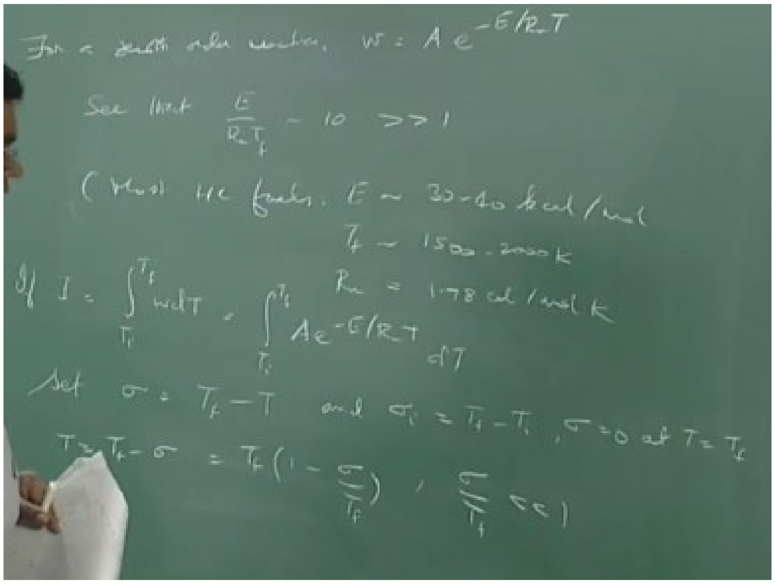

For a zeroth order reaction, $w = A e^{-E/R_u T}$

See that $\frac{E}{R_u T_f} \sim 10 >> 1$

(Most HC fuels: $E \sim 30-40$ kcal/mol

$T_f \sim 1500-2000$ K

$R_u = 1.78$ cal/mol K

If $I = \int_{T_i}^{T_f} w dT = \int_{T_i}^{T_f} A e^{-E/R_u T} dT$

Set $\sigma = T_f - T$ and $\sigma_i = T_f - T_i$, $\sigma = 0$ at $T = T_f$

$T = T_f - \sigma = T_f\left(1 - \frac{\sigma}{T_f}\right)$, $\frac{\sigma}{T_f} << 1$

So σ is a very small value it is a departure from Tf it is not going to be large because T itself is not going to it is gone very only from Ti onwards to Tf and Ti is quite high very close to Tf in the first place so this difference is going to mean that the σ is going to be very small when compared to Tf.

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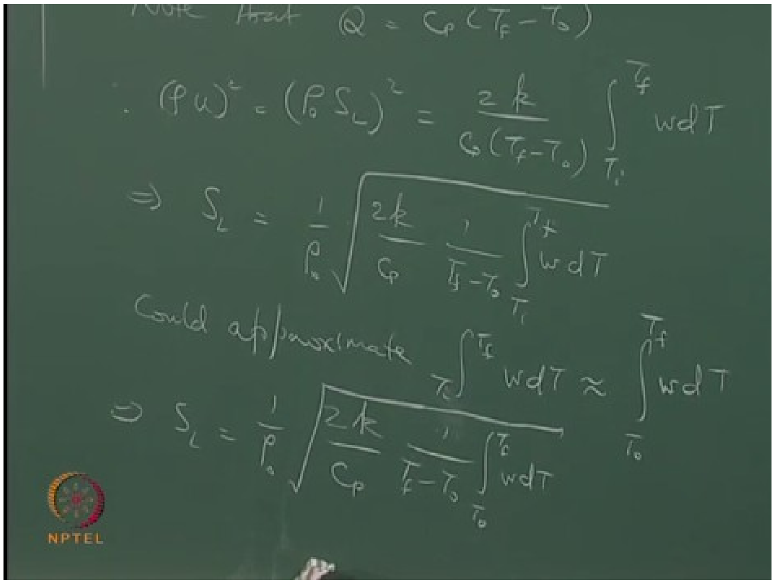

Note that $Q = C_p (T_f - T_0)$

$$\therefore (\rho w)^2 = (\rho_0 S_L)^2 = \frac{2k}{C_p (T_f - T_0)} \int_{T_i}^{T_f} w \, dT$$

$$\Rightarrow S_L = \frac{1}{\rho_0} \sqrt{\frac{2k}{C_p} \frac{1}{T_f - T_0} \int_{T_i}^{T_f} w \, dT}$$

Could approximate $\int_{T_i}^{T_f} w \, dT \approx \int_{T_0}^{T_f} w \, dT$

$$\Rightarrow S_L = \frac{1}{\rho_0} \sqrt{\frac{2k}{C_p} \frac{1}{T_f - T_0} \int_{T_0}^{T_f} w \, dT}$$

So then how is your e to the - e /RT gone get changed or transformed into of σ is exponential - e / RU Tf times 1 - σ / Tf so that is approximately exponential -E / Ru Tf times 1 + σ / Tf. Now these kinds of things are all sort of tailor made for approximations we should we should sort of get an intuition about how these analysis are done, so if you now start thinking about a σ is a small quantity then that is like a sitting duck for a binomial approximation okay, so whenever you have a chance we approximate given within our lives most of the time by the way.

So we do a binomial approximation and then it also gives you this factor which we have a feel for from here right so you get all these things isolated then I is equal to you can plot these things Ti to Tf u the – E σ/ RTf^2 dT whereas our integral s with respect to σ so therefore we should write this as Ae - e / RTf ∫ σ I to 0e to the - e / e σ Tf^2 dσ now that is a little bit of a cumber something over there so what you can do is let not very cumbersome it is possible to deal with this but still if you want to now call to this e / eσ / $RuTf^2$ and βi is eσ i / RUTf then I is Ae to the – e/ RuTf $^{2\,/}$ E it is cup pulled out and 0 βi e-β dβ.

Now this is so what are we expecting what are we expecting to happen what you are basically saying is that we are looking for this integral which is what we start out with to approximate W0

∞ divided by a different better than what we have used here fortunately okay and that β was times Tf – T0 / RuTf ^{2} Tf – T0 is already here so we should be looking for something like Ru e/ RuTa^{2} in the denominator to couple with this in order to get you this Zelda with scaling factor.

And then we should get aw not infinity WR ∞ is essentially the W evaluated at the reactant concentration levels and product temperature levels we are now doing a 0th order reaction which does not depend whose reaction rate does not depend on the reactant concentrations anyway so we do not have to worry about he 0 part of the W0 ∞.

We do not have to worry about evaluating it at the reactant temperatures what we have two reactant concentrations what we have to be looking for is devaluated and the product temperatures which is what this is so this is the reaction rate expression evaluated at the product temperature right and then this is there coupled with the Tf0 Tf – T0 in the denominator you are going to get the Zelda with scaling factor in the denominator.

So this all of all by itself is giving you for what we thought was the average reaction rate giving you W0 ∞ divided by beta so we are fine so all we need is a unity out of this integral sure enough that is what we are expecting to get so this is going to be like 1 - e to the – βi where we are now saying that βi corresponds to σi and σi corresponds to Tf - Ti which is a very small quantity right when compared to Tf.

Therefore we are now going to get rid of it and say this is approximately = 1 then from there on we should now be say saying therefore S_L = 1 / ρ0 ∞ 2k / CP Ae/ RuTf that is W0 ∞ for a 0th order reaction / Tf – T_0 times RuTf ^{2} / e.

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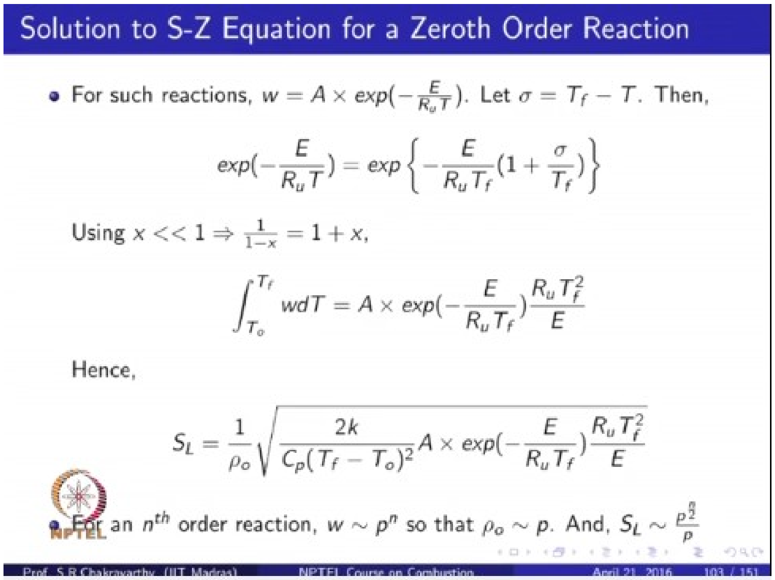

Solution to S-Z Equation for a Zeroth Order Reaction

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- For an n^{th} order reaction, $w \sim p^n$ so that $\rho_o \sim p$. And, $S_L \sim \frac{p^{\frac{n}{2}}}{p}$

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The Zeller with scaling factor showing up the denominator of W0 ∞ so we essentially are getting back the same thing again except for the square root of two let us come out again right. So this is typically how we are able to retrieve the answers that we were expecting for this case what I want to point out just point out not really go through this because we are just spending too much time on this you should look up so this is looking like what we got before right you should lookup how to actually do the rigorous analysis on taking into account the reactant concentrations.

Then what that means is we have to now relax this assumption on a 0^{th} order reaction and notice that W will now depend on the reactant concentrations so for a first order concentrate first order reaction you will have a concentration of one of the reactants coming into picture for second order reaction you are going to have concentrations of two reactants coming into picture, so those things have to be broadened account and then the next thing that we talked about was the lowest number effect okay.

So what you will find this you can actually when we need the lowest number for example we found that and also the reactant concentration you got this W0 ∞ / β^m for the m is the exponent in corresponding to the order of the deficient reactant right and then you also had a low number on in the numerator.

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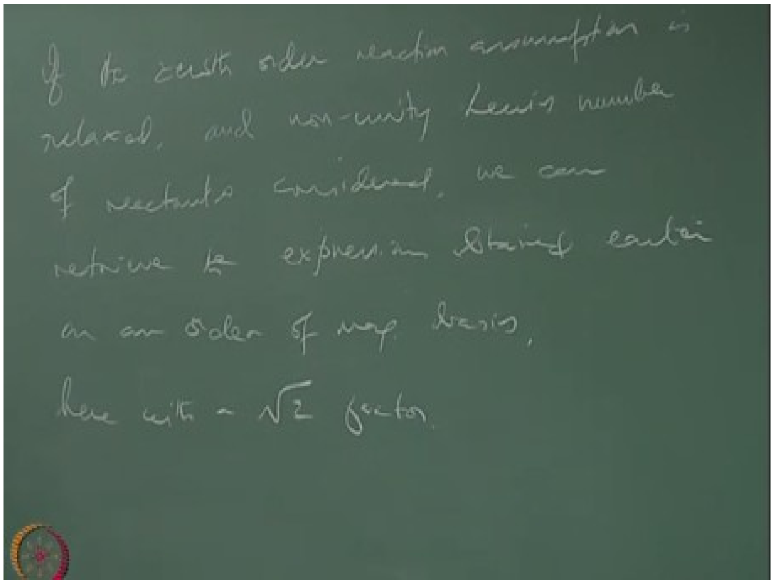

If the zeroth order reaction assumption is
relaxed, and non-unity Lewis number
of reactants considered, we can
retrieve the expression obtained earlier
on an order of mag. basis,
here with ~ $\sqrt{2}$ factor.

So we should be able to retrieve those things if the 0^{th} order reaction assumption is relaxed and non unity Louis number of reactants considered right we can retrieve the expressions to think earlier on a order of magnitude basis here with a square root of two factor right, so we can get this and then what would we suppose then.

So we notice that for let us say for a n^{th} order reaction right w goes is P to the n right because you will have the linear expression times the concentrations as many as the number of reactants are and the order the reaction depends on and for that much order you are going to have each concentration contributing a pressure and therefore you are going to have a P to the n for the nth order reaction for the pressure dependence right.

Now what you have is a not in the beginning right so ρ or ρ0 goes as P I do not want to say p0 because we are assuming the pressure to be constant it does not matter whether it is p0 or p ∞ k we just talking about a constant pressure lower less a constant pressure deflagration here.

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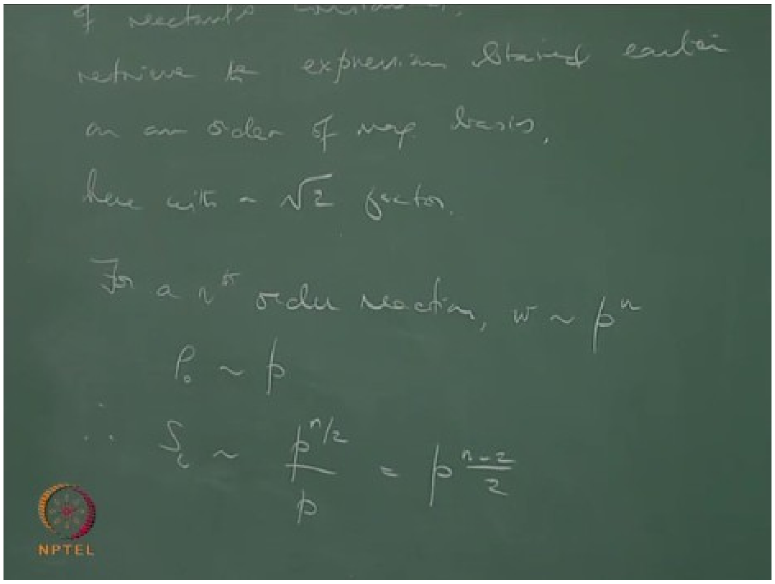

of reactants

retrieve the expression obtained earlier

on an order of mag. basis,

here with ~ $\sqrt{2}$ factor.

For a n^{th} order reaction, $w \sim p^n$

$\rho_0 \sim p$

$\therefore S_L \sim \frac{p^{n/2}}{p} = p^{\frac{n-2}{2}}$

Therefore your S_L is going to go as P n/2 / p n/ 2 coming from having W depends P to the n and then under square root therefore you are going to have this as P to the n- 2 / 2 right or you can say n by 2 - 1 so n / n – 2/2.

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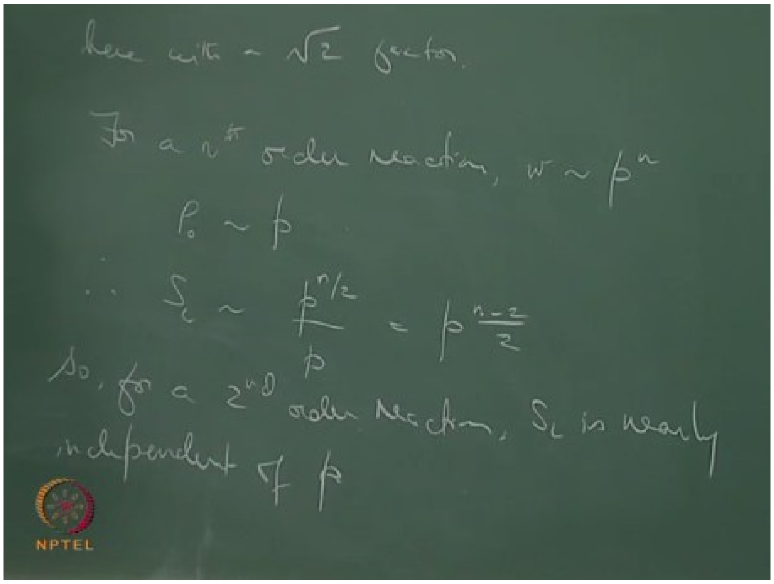

here with ~ $\sqrt{2}$ factor.

For a n^{th} order reaction, $w \sim p^n$

$\rho_o \sim p$

$\therefore \; S_L \sim \frac{p^{n/2}}{p} = p^{\frac{n-2}{2}}$

So, for a 2^{nd} order reaction, S_L is nearly independent of p

So for a second order reaction second order reaction S_L is nearly independent of pressure keep in mind order is a global quantity it is it is valid for a global reaction right or if you are able to actually represent a scheme of chemical reaction steps from a elementary reaction steps in terms of a global reaction so it does not have to be an integer so typically for most what we call a second order reactions let us say hydrocarbon gaseous hydrocarbons oxidation your order of the reaction is going to be somewhat like let us say 1.8.

So John will be exactly two right so the reason why I am saying nearly so we find that there is a weak dependence on pressure, so if you now think about an end that is like about1.8 you see you are going to have an inverse dependence on pressure right that means as the pressure increases the S_L decreases okay that since back to that so that is what we actually observe but it is a weak dependence so we are now beginning to talk about dependences of s1 various factors.

So what we just mentioned was pressure which was obvious what we have not really worried about is how it depends on let us say initial temperatures okay and what we will see is this is primarily the dependency and S_L is going to depend on lot of other factors mainly through W okay so if W is going to depend on initial temperature it will depend through Tf okay so we will now talk about these things in the next class you.

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