Fundamentals of Combustion
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Lecture - 57
Droplet evaporation and combustion – Part 4
Species and temperature profiles

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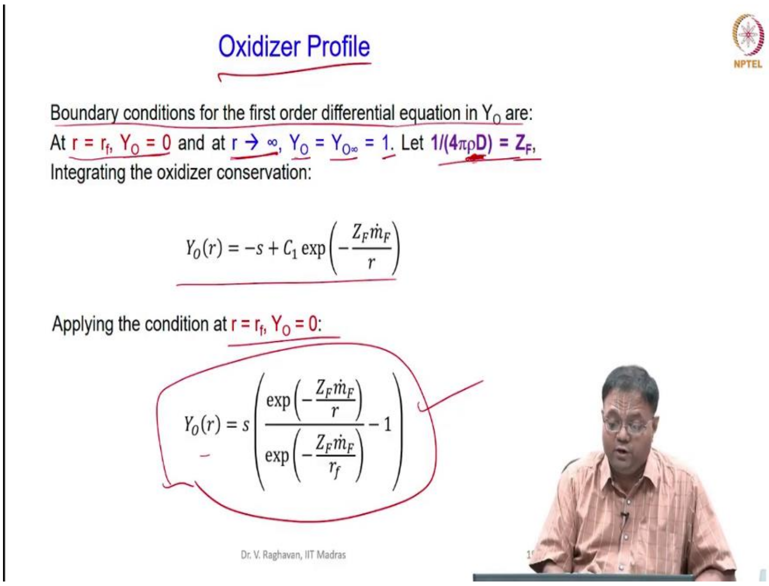

Oxidizer Profile

Boundary conditions for the first order differential equation in Y_O are:
At $r = r_f$, $Y_O = 0$ and at $r \rightarrow \infty$, $Y_O = Y_{O\infty} = 1$. Let $1/(4\pi\rho D) = Z_F$,
Integrating the oxidizer conservation:

$$Y_O(r) = -s + C_1 \exp\left(-\frac{Z_F \dot{m}_F}{r}\right)$$

Applying the condition at $r = r_f$, $Y_O = 0$:

$$Y_O(r) = s\left(\frac{\exp\left(-\frac{Z_F \dot{m}_F}{r}\right)}{\exp\left(-\frac{Z_F \dot{m}_F}{r_f}\right)} - 1\right)$$

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So, here boundary conditions for this. So, the boundary condition for the first order equation in Y_O are at the flame, from the outer region from the flame to infinity. So, at $r = r_f$, $Y = Y_O = 0$; at as $r \rightarrow \infty$, Y_O is the $Y_{O,\infty}$ which is now taken as 1.

Now, again the property $1/4\pi\rho D$, which is already defined as Z_F, I am keeping that same here because the ρD is constant here. So, ρD for fuel or ρD, for the oxidizer are the same. So, it is only Z_F. So, that is already defined. So, that variable is used here.

So, same type of solution I get, some small change here. You can see this. Now, apply the boundary condition $Y_O = 0$ at $r = r_f$. So, when I substitute here $r = r_f$, I will get $Y_O = 0$, constant can be evaluated.

$$Y_O(r) = -s + C_1 \exp\left(-\frac{Z_F \dot{m}_F}{r}\right)$$

Now, other quantities are known to me. So, the constant is evaluated and put back here I get the profile for oxidizer. So, that is Y_O at any r equal to s times $\exp(-Z_F\dot{m}_F/r)/\exp(-Z_F\dot{m}_F/r_f) - 1$.

$$Y_O(r) = s\left(\frac{\exp\left(-\frac{Z_F\dot{m}_F}{r}\right)}{\exp\left(-\frac{Z_F\dot{m}_F}{r_f}\right)} - 1\right)$$

So, this is the profile. Now, you can verify this. So, when you put $Y_O = 0$ you will get that is r_f. Then actually if you put r_f here this and this will cancel and become 1 and 1 - 1 = 0. So, Y_O will become 0.

Now, one boundary condition is used here. Then I will use one more boundary condition, which is nothing but as $r \rightarrow \infty$, $Y_O \rightarrow 1$. If I use that condition when I put r_∞ here, so, this will be $1/\infty = 0$. So, this is $1/\exp(-Z_F\dot{m}_F/r_f) - 1$ that will be equal to here, it will be 1.

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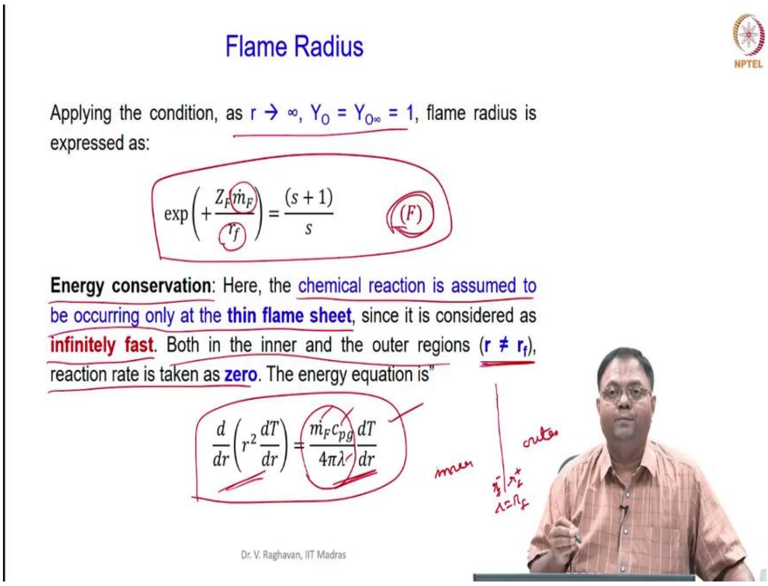

Flame Radius

Applying the condition, as $r \rightarrow \infty$, $Y_O = Y_{O\infty} = 1$, flame radius is expressed as:

$$\exp\left(+\frac{Z_F\dot{m}_F}{r_f}\right) = \frac{(s+1)}{s} \qquad (F)$$

Energy conservation: Here, the chemical reaction is assumed to be occurring only at the **thin flame sheet**, since it is considered as **infinitely fast**. Both in the inner and the outer regions (**$r \neq r_f$**), reaction rate is taken as **zero**. The energy equation is"

$$\frac{d}{dr}\left(r^2\frac{dT}{dr}\right) = \frac{\dot{m}_F c_{pg}}{4\pi\lambda}\frac{dT}{dr}$$

inner

outer

r_f^- r_f^+

$r=r_f$

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So, when I use this, I get another equation which I called F. So, this is another equation which will involve flame radius. Now, please understand that it has two unknowns here; flame radius as well as this $\dot{m}_F$. So, I get this. So, maybe I can say that I will write flame radius in terms of $\dot{m}_F$. So, everything I can write up in terms of $\dot{m}_F$. So, this is the second equation I have generated.

$$\exp\left(+\frac{Z_F\dot{m}_F}{r_f}\right) = \frac{(s+1)}{s} \qquad (F)$$

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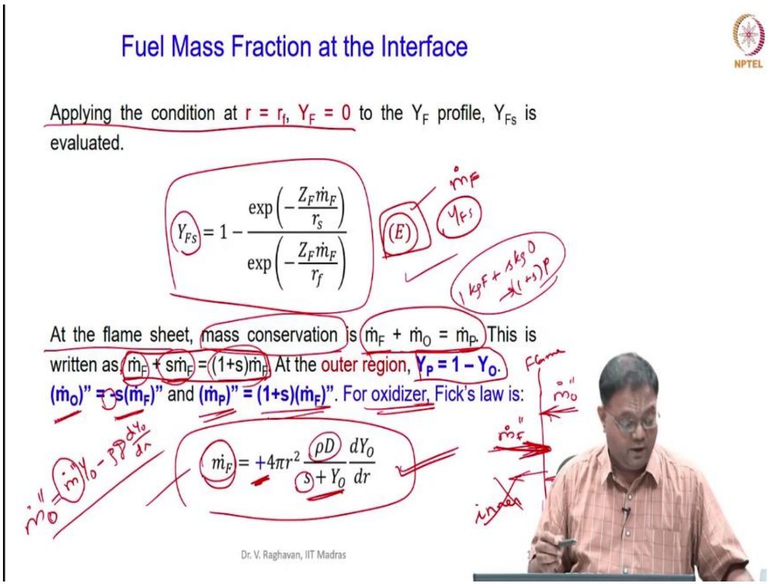

Fuel Mass Fraction at the Interface

Applying the condition at r = r_f, $Y_F = 0$ to the Y_F profile, Y_{Fs} is evaluated.

$$Y_{Fs} = 1 - \frac{\exp\left(-\frac{Z_F \dot{m}_F}{r_s}\right)}{\exp\left(-\frac{Z_F \dot{m}_F}{r_f}\right)} \quad (E)$$

At the flame sheet, mass conservation is $\dot{m}_F + \dot{m}_O = \dot{m}_P$. This is written as $\dot{m}_F + s\dot{m}_F = (1+s)\dot{m}_F$. At the outer region, $Y_P = 1 - Y_O$. $(\dot{m}_O)'' = -s(\dot{m}_F)''$ and $(\dot{m}_P)'' = (1+s)(\dot{m}_F)''$. For oxidizer, Fick's law is:

$$\dot{m}_F = +4\pi r^2 \frac{\rho D}{s + Y_O}\frac{dY_O}{dr}$$

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The first equation what I have generated is this. Y_{FS} in terms of $\dot{m}_F$. So, that is equation E. Now, I am writing r_f in terms of $\dot{m}_F$ or other way whatever you want you can keep. So, there are two unknowns here again. So, I have created a second equation. So, two equations are created by considering the species conservation in inner and outer regions. Now, I will do the energy conservation.

Again, I have energy conservation to be done in the inner and outer region that will generate two more equations. So, two equations are now generated. One is the equation due to the species conservation in the inner zone another one is the that is the fuel conservation. Second one is the oxidizer conservation in the outer zone then I have got this second equation. Now, energy conservation.

Please understand that there is a thin reacting zone, the inner zone, the outer zone. So, only at r = r_f, infinitely fast reaction is complete. So, that means, just left side of this; so, this r_f. So, I will say r_f just left side of this, I will say r_{f-} and just right side of this I will say r_{f+}, the thin zone just to the right of that I will say r_{f+} just to the left of that let us say r_{f-}.

$$\frac{d}{dr}\left(r^2 \frac{dT}{dr}\right) = \frac{\dot{m}_F c_{pg}}{4\pi\lambda}\frac{dT}{dr}$$

You will see there will be no reaction because reaction is complete within the thin zone. So, this is very important that reaction is occurring infinitely fast; that means, when you just step out of the thin zone you will not have any reaction. That means, chemical reactions are assumed to be occurring only in the thin flame sheet, which is very fast. So, other than r = r_f, when r is not equal to r_f then reaction rate is taken as 0.

Only at the location of r = r_f reaction is started and finished; 0 thickness, infinitely fast. So, very thin, thickness of the reaction tends to 0 as the reaction rate tends to infinity. So, in both outer and inner regions you will see that reaction rate is 0. So, the energy conservation is very simple second order equation which is written in this. So, this is a diffusion term and convective term.

You can write the $d(r^2 dT/dr)/dr$ it will be equal to, actually it will be 4π which come this side and λ, here λ also should come inside, but we have taken everything to the other side because we have treated c_{pg}, λ, m_F etcetera are constant. So, some constant dT/dr. So, diffusion and convective terms are there.

Now, please understand that this equation is second order equation involving temperature. So, we can basically go and integrate. So, boundary conditions we have to appropriately use, but please understand that there are two regions inner and outer region. So, same governing equation can be used to solve both boundary condition for the second order differential equation in temperature.

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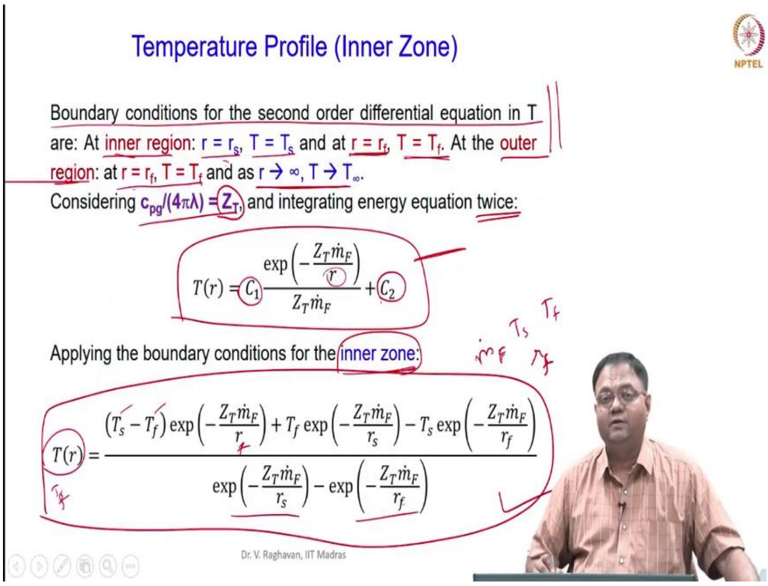

Temperature Profile (Inner Zone)

Boundary conditions for the second order differential equation in T are: At inner region: $r = r_s$, $T = T_s$ and at $r = r_f$, $T = T_f$. At the outer region: at $r = r_f$, $T = T_f$ and as $r \to \infty$, $T \to T_\infty$.

Considering $c_{pg}/(4\pi\lambda) = Z_T$, and integrating energy equation twice:

$$T(r) = C_1 \frac{\exp\left(-\frac{Z_T \dot{m}_F}{r}\right)}{Z_T \dot{m}_F} + C_2$$

Applying the boundary conditions for the inner zone:

$$T(r) = \frac{(T_s - T_f)\exp\left(-\frac{Z_T \dot{m}_F}{r}\right) + T_f \exp\left(-\frac{Z_T \dot{m}_F}{r_s}\right) - T_s \exp\left(-\frac{Z_T \dot{m}_F}{r_f}\right)}{\exp\left(-\frac{Z_T \dot{m}_F}{r_s}\right) - \exp\left(-\frac{Z_T \dot{m}_F}{r_f}\right)}$$

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Now, there are two regions as I told you. Inner region at r = r_s, equilibrium surface temperature T = T_s prevails. At r = r_f, T is the maximum flame temperature, T_f, and an outer zone starting from r = r_f you have flame temperature and as r → ∞, T → T_∞. So, these are the boundary conditions at the both zones, inner and outer zones.

Now, let us define the properties $c_p/4\pi\lambda$ as Z_T, Z_T that is the basically you can see that c_p by that the properties that 1/4πρD etcetera we have taken as Z_F. Here, we have taken the coefficients. The properties club together we have taken as a constant, Z_T.

Now, integrate this 2 times; second order equations you can integrate 2 times and I get 2 constant, one for each time. Then this is the profile I get, general profile and in this if I apply boundary conditions corresponding to any zone I will get equations.

$$T(r) = C_1 \frac{\exp\left(-\frac{Z_T \dot{m}_F}{r}\right)}{Z_T \dot{m}_F} + C_2$$

So, let us take inner zone first. There are two constants. To eliminate two constants, I need two boundary conditions. So, taking inner zone the boundary conditions what I am going to use are at r = r_s, T = T_s. So, when I say here I will put r = r_s then at T say here r = r_s I will say T = T_s. Then I will form one equation involving c_1 and c_2, where the left side is T_s and right-hand side r will have to be r_s. So, in one equation constant is c_1 c_2. Second equation will be at r = r_f, T = T_f and substitute here r = r_f, T I will put T_f.

Now, please understand that T_f is not known, r_f is also not known, but I will form again equation corresponding to with the c_1 and c_2, where I will have variables like r_1 or r_f and T_f or T_s, all the three are not known to me yet.

Now, I get the equation. So, when I solve for c_1 and c_2, these two boundary conditions in the inner region then I get the profile for temperature given here. It is a very big profile So, you can see T_s - T_f into exponent of -Z_T which is the property constant m_F by r plus T_f into exponent of minus Z_T m_F by r_s minus T_s into exponent of Z_T m_F by r_f.

$$T(r) = \frac{(T_s - T_f)\exp\left(-\frac{Z_T \dot{m}_F}{r}\right) + T_f \exp\left(-\frac{Z_T \dot{m}_F}{r_s}\right) - T_s \exp\left(-\frac{Z_T \dot{m}_F}{r_f}\right)}{\exp\left(-\frac{Z_T \dot{m}_F}{r_s}\right) - \exp\left(-\frac{Z_T \dot{m}_F}{r_f}\right)}$$

Now, please see that the temperature profile basically in the inner zone consists of T_s and T_f because now for the surface the influence of the T ambient is gone, T_∞ is gone. So, T_f and T_s, that is the driving force here. So, that we have seen here. Now, this is the equation, I get the big equation for the inner temperature profile.

But please understand that the unknowns here again are $\dot{m}_F$. $\dot{m}_F$is not known, T_s is not known, T_f is not known and r_f is not known only r_s is known here. So, anyway we will try to use some boundary condition some more boundary conditions and use this equation in order to get this.

Basically, we are going to see the other boundary conditions also. We have to generate five equations. This itself have four unknowns. So, these are also profiles. Once unknowns are known then the profile can be plotted, that is the idea here.

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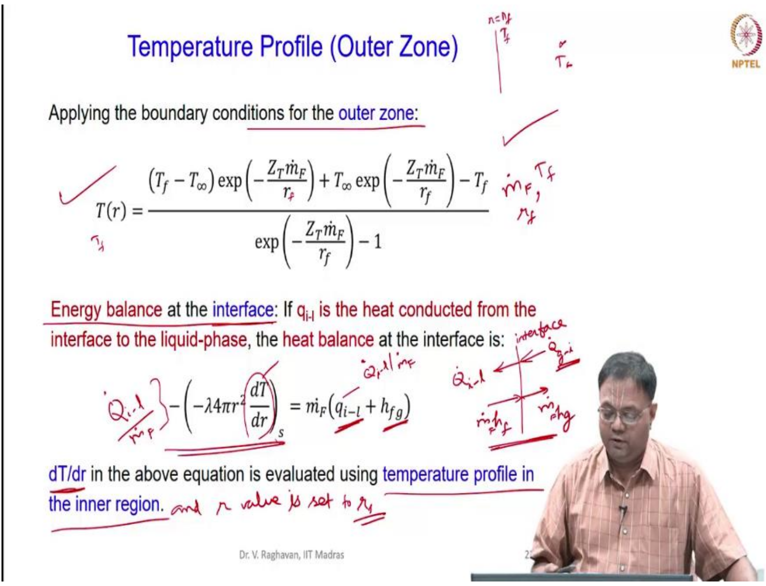

Temperature Profile (Outer Zone)

Applying the boundary conditions for the outer zone:

$$T(r) = \frac{(T_f - T_\infty)\exp\left(-\frac{Z_T\dot{m}_F}{r_f}\right) + T_\infty \exp\left(-\frac{Z_T\dot{m}_F}{r_f}\right) - T_f}{\exp\left(-\frac{Z_T\dot{m}_F}{r_f}\right) - 1}$$

Energy balance at the interface: If $q_{i\text{-}l}$ is the heat conducted from the interface to the liquid-phase, the heat balance at the interface is:

$$-\left(-\lambda 4\pi r^2 \left(\frac{dT}{dr}\right)_s\right) = \dot{m}_F\left(q_{i-l} + h_{fg}\right)$$

dT/dr in the above equation is evaluated using temperature profile in the inner region. and r value is set to r_f

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Now, same thing you do for outer zone. The same profile, this equation is valid for the inner zone as well as outer zone but the boundary conditions are different. Based upon the boundary conditions the constants c_1 and c_2 are evaluated.

So, by substituting the inner zone conditions $r = r_s$, $T = T_s$, $r = r_f$, $T = T_f$ we have evaluated this profile. Again, please understand that once all the variables all the five variables what we are talking about are known then the profile can be drawn.

Now, outer zone again you have to use the boundary conditions, outer zone that is at the flame outer zone at the flame $r = r_f$, $T = T_f$, flame temperature as $r \rightarrow \infty$, $T \rightarrow T_\infty$. So, these are the two boundary conditions to evaluate the two constants. The same profile you take, but now substitute $r = r_f$ in the right-hand side, put $T = T_f$ here. So, the same first equation what we got we get here.

For the first inner zone, the second equation will be there as the first equation here. Then, when $r \rightarrow \infty$, here you put r_∞. So, this will be 1, 1 by this etcetera then you will get another equation in c_1 and c_2.

So, solving c_1 and c_2, I get the profile for the outer zone as T. Now, you can see that the outer zone T_f and T_∞ are the two temperatures involved. So, T_f - T_∞ exp($-Z_T m_F/r$) + T_∞exp($-Z_T m_F/r$) - T_f.

$$T(r) = \frac{(T_f - T_\infty)\exp\left(-\frac{Z_T\dot{m}_F}{r}\right) + T_\infty \exp\left(-\frac{Z_T\dot{m}_F}{r_f}\right) - T_f}{\exp\left(-\frac{Z_T\dot{m}_F}{r_f}\right) - 1}$$

So, this is the equation. Now, we can check the boundary condition. See you can go back here. You will check the boundary conditions here. So, if you say $r = r_s$, now, this will be T_s, I will put $r = r_s$ here. So, here r_s and when you put r_s here then $T_s \exp(-Z_T m_F/r_s)$ plus. So, $-T_f$, $+T_f$ that will cancel. T_s into exponent of this $-T_s$ into exponent of this will come, but T_s we can take common outside and the exponent of $Z_T m_F/r_s$ here and $-(\exp(-Z_T m_F/r_f))$. So, this will cancel and I will get $T = T_s$. So, when you go to other conditions where $r = r_f$ if you substitute here T_f will come, and you are putting r_f here.

Then you can see that T_s this $+ T_s(\exp(-Z_T m_F/r_f)$ and $-T_s \exp(-Z_T m_F/r_f)$ will cancel. Then here you can get T_f take commonly out and $T_f(\exp(Z_F m_F/r_s)$ and $\exp(-Z_F m_F/r_f)$. So, this will cancel and we will get $T = T_f$. So, the profile is matching the boundary condition basically.

Similarly, here you get the outer zone. Outer zone you have flame $r = r_f$, T_f is the temperature here and as we go to infinity you get T_∞. Now, you substitute here and see if you put say T as $r \rightarrow \infty$ basically you can put this will be infinity. So, this will be 1. So, $T_f - T_\infty + T_\infty$ into; so, T_f T_f cancels basically T_∞ into exponent of this divided by this.

So, T_∞ into one minus this will come. So, if this minus 1 will come. So, this exponent term will cancel exponent term -1 will cancel and get T_∞. So, if you substitute $r = r_f$ here in this $r = r_f$ you will get T_f in the left-hand side. You can see whether you will get it. So, the main crux here is now we have developed the profiles, but the profile cannot be plotted because I do not know.

Here also you can see the unknowns are m_F, T_f and r_f. These are the three unknowns present here. Since after evaluating all the unknowns we will be able to plot the profiles, but how do you generate the equations? These cannot be used now. So, already we have created two equations. One relating the Y_{FS} and the m_F another relating the r_f and m_F.

So, we have created two equations. One equation is r_f and m_F are related and here I have related Y_{FS} and m_F. Now, three more equations are required. Now, we have generated profiles for inner and outer zones for temperature, is there any way to use these profiles to get the two more equations? For that I will first do the energy balance of the interface.

So, interface. What is the energy balance here? I said we have drawn it already. So, that will be Q gas to interface; Q gas to interface and that will be taken inside here. So, Q interface to liquid and vaporization occurs. So, $\dot{m}_F h_f$, $\dot{m}_F h_g$. Now, dividing by the mass, this small q_l is nothing but $Q_{i-l}/\dot{m}_F$.

So, that you can; so, this $\dot{m}_F$ into this. So, $\dot{m}_F$ you can say actually here, the fuel is actually generated out. So, $\dot{m}_F$. So, when I do this Q_{i-l}, $\dot{Q}_{i-l}/\dot{m}_F$ that will give you the heat which is going into the interface, to the liquid phase. And this is the heat which is required for this, h_{fg}. $(h_g - h_f)\ \dot{m}_F$ that will be the heat which is required for phase change.

So, that is coming in through the conduction from the gas phase to the interface which is written as this. This is the $\dot{Q}_{i-l}/\dot{m}_F$. So, this is the term. Now, this is interface boundary condition, heat balance at the interface. See we are taking the boundary conditions, additional boundary condition I am trying to create here where derivative of temperature is present.

And since it is done in interface, I can calculate this dT/dr. dT/dr of the above equation can be evaluated using temperature profile for the inner region that is this. So, this equation I will take, differentiate it with respect to r. So, I will get dT/dr.

Once I get this value I can substitute there and I set this dT/dr in the above equation is evaluated using temperature profile inner region and r value is set to r_s because I want the derivative at the surface.

So, you take this profile, inner profile and differentiate this with respect to r. So, dT/dr then there will be r terms that r you set as r_s. So, that will give you this equation. Substitute back here and try to get the equation that is what we are trying to do.

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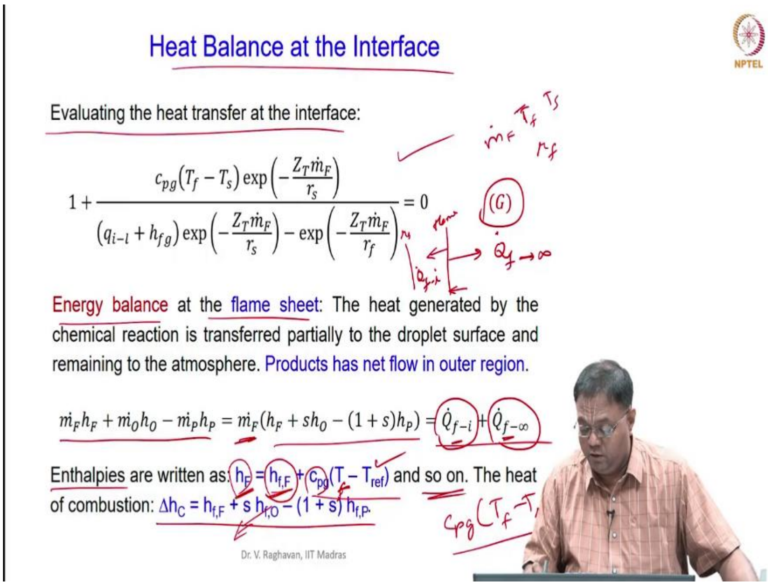

Heat Balance at the Interface

Evaluating the heat transfer at the interface:

$$1 + \frac{c_{pg}(T_f - T_s)\exp\left(-\frac{Z_T \dot{m}_F}{r_s}\right)}{(q_{i-l} + h_{fg})\exp\left(-\frac{Z_T \dot{m}_F}{r_s}\right) - \exp\left(-\frac{Z_T \dot{m}_F}{r_f}\right)} = 0$$

Energy balance at the flame sheet: The heat generated by the chemical reaction is transferred partially to the droplet surface and remaining to the atmosphere. Products has net flow in outer region.

$$\dot{m}_F h_F + \dot{m}_O h_O - \dot{m}_P h_P = \dot{m}_F(h_F + s h_O - (1+s)h_P) = \dot{Q}_{f-i} + \dot{Q}_{f-\infty}$$

Enthalpies are written as: $h_F = h_{f,F} + C_{pg}(T - T_{ref})$ and so on. The heat of combustion: $\Delta h_C = h_{f,F} + s\,h_{f,O} - (1+s)\,h_{f,P}$.

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So, this is the equation which is representative of the heat balance at the interface. So, this is the equation. You can see the unknowns are $\dot{m}_F$, T_f, T_s, r_s.

So, r is known or r is r_f here. So, these are the unknowns in this. These are the unknowns in this; flame temperature, surface temperature, r_f and $\dot{m}_F$. So, the third equation we have generated. So, already two equations; one for the inner region species conservation, fuel conservation, outer region oxidizer conservation by using the balances.

We are trying to get now here after getting the temperature profiles we are trying to put the heat balance at the interface based upon that I get this equation. So, this is third equation I can generate. Now, let us do the heat balance at the flame sheet. Next is the energy balance or heat balance at the flame sheet, this is flame.

Now, how the heat balance occurs here? So, whatever be the chemical energy converted into thermal energy. So, this is here. So, whatever be the chemical energy which is released out as thermal energy that will partially be transferred. So, this is the flame. So, this is the surface. This is r_s. So, partially it will go here like that from the flame, this is the Q dot flame to interface.

$$-\left(-\lambda 4\pi r^2 \frac{dT}{dr}\right)_s = \dot{m}_F\left(q_{i-l} + h_{fg}\right)$$

So, partially it will go towards interface to heat up there or to supply the heat for the droplet and partially it will go away. This is Q flame to ambient, it will be lost away. So, it will go away. So, this should balance what? The chemical energy release, which is nothing but, delta h_c. So, this is $\dot{m}_F$ into this. So, these can be the enthalpies if you properly write you can consider.

For example, enthalpy to be constituted as the formation enthalpy plus the sensible enthalpy; sensible enthalpy is we have constant property. So, T minus some reference temperature we take T_f. So, this will be the this. So, this actually know the temperature is T_f also you can write because T_f is the flame temperature.

So, the enthalpy of any species, now, I have taken example of fuel and the enthalpy of fuel will be the heat of formation of fuel h_f of F plus sensible enthalpy which is $c_{pg}(T-T_{ref})$, but T is actually the flame temperature itself. So, $T_f - T_{ref}$; so, this will be the enthalpy of this.

Similarly, you can write for the enthalpy of the other species. See for example, oxidizer, this enthalpy of formation will be 0, but only sensible enthalpy may be prevailing, but please understand that c_{pg} is constant for all. So, for all these terms sensible enthalpy can be written as $(T_f - T_{ref})c_{pg}$.

So, that is what we will have for all the species of the sensible enthalpy. Formation enthalpy will be based upon on which is fuel or oxidizer we will have some values. Now, you can see the delta h_C. Delta h_C is the heat of combustion which is nothing but the enthalpy of formation of the fuel plus enthalpy of formation of the oxidizer which can be 0 actually into s – (1 + s) × enthalpy of formation of products. So, this will be normally 0.

So, this is the expression for the delta h_C. So, using these in this, enthalpy definition etcetera and the definition of delta h_c we can write this equation basically.

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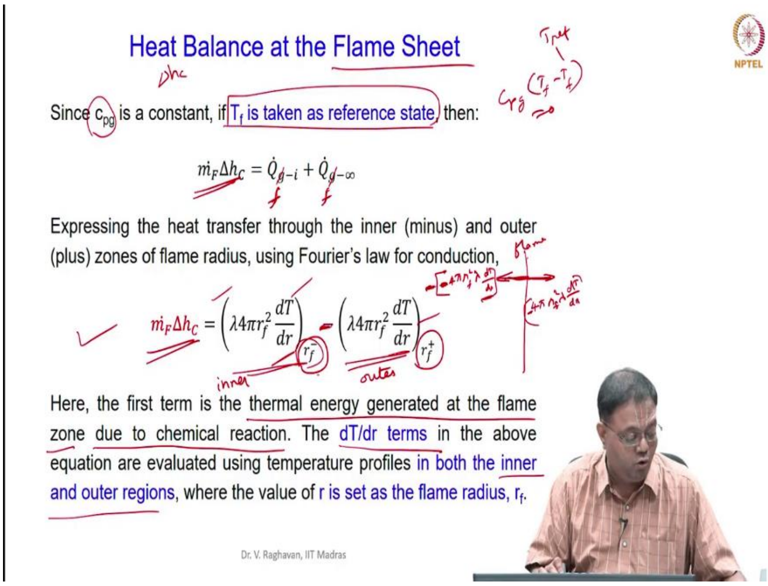

Heat Balance at the Flame Sheet

Δhc

Since c_{pg} is a constant, if T_f is taken as reference state, then:

T_{ref}

$c_{pg}(T_f - T_f) \to 0$

$$\dot{m}_F \Delta h_C = \dot{Q}_{\underset{f}{\cancel{g}}-i} + \dot{Q}_{\underset{f}{\cancel{g}}-\infty}$$

Expressing the heat transfer through the inner (minus) and outer (plus) zones of flame radius, using Fourier's law for conduction,

flame

$-[-4\pi r_f^2 \lambda \frac{dT}{dr}]$

$(-4\pi r_f^2 \lambda \frac{dT}{dr}$

$$\dot{m}_F \Delta h_C = \left(\lambda 4\pi r_f^2 \frac{dT}{dr}\right)_{r_f^-} - \left(\lambda 4\pi r_f^2 \frac{dT}{dr}\right)_{r_f^+}$$

inner

outer

Here, the first term is the thermal energy generated at the flame zone due to chemical reaction. The dT/dr terms in the above equation are evaluated using temperature profiles in both the inner and outer regions, where the value of r is set as the flame radius, r_f.

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But one more assumption what is made here with respect to $c_{pg}(T_f - T_{ref})$ is if we know that c_{pg} is constant. Since c_{pg} is constant basically what happens is a delta h_C will not be affected by T_f. So, T_f itself can be taken as the different state basically.

So, T_f if you take T_f as reference state then the sensible part can be neglected, reference temperature also this is T_{ref}. Now, T_{ref} is also taken as T_f itself. So, this term sensible enthalpy goes away. So, we will only consider this. Now, what happened in this case I can write the left-hand side as $\dot{m}_F$ into delta h_C that is I can see that $\dot{m}_F$ × delta h_C is nothing but the thermal energy generated at the flame zone due to the chemical reaction that is all.

The mass of the fuel which is coming out from the liquid surface that is fully burnt. So, that times delta h_C that will give you the thermal energy which is generated. So, that should be partially conducted back to the inner zone that is r_{f-} represent the inner zone.

So, conducted back to the inner zone and can transported to the outer zone. So, this is the conduction to the outer zone r_{f+}. So, this is the equation what we get. Now, you please see here the Q_{g-i}, gas to the interface if you say the interface, so, this is actually gas, you can also say flame, both are same. Either from gas phase with interface, but here this is actually flame. Flame to this, we have written here flame to the interface and flame to the infinity. So, from the flame sheet, this is the flame sheet, you can see that this conduction when I write this g to i here like this, this will be a negative of $-4\pi(r_f)^2\lambda \times dT/dr$. So, that is going out like this to inner zone. So, minus of minus why I am putting because this is direction from T_f, temperature decreases towards the T_s.

So, this gradient is negative. So, there is a positive heat flow also is in this direction. So, that is positive, but this negative sign is put because this flow happens, it is a vector and happens in the negative radial direction.

So, negative radial direction. So, this negative of negative I put. So, this is a positive quantity here. Now, if you take this side here you have $4\pi(r_f)^2$ that is the area of cross section into $\lambda \times dT/dr$.

Now, at r_f means this is the; so, again you can see that from this point I will put a negative sign here and leave it, negative sign and leave it. Why you put negative sign here because we know that the temperature gradient is negative, temperature decreases there right. So, the temperature upstream minus the temperature downsream and upstream will be actually negative.

Since this is negative and the heat flows in this direction basically this is the negative terms. So, this negative term comes because of this term here because this has become positive; negative of negative is positive because of the direction of the heat. So, these are vector forms. So, the heat flow, any flow or flux when you have a direction you have to take care of the sign. So, the negative of negative comes because of the negative radial direction. Here in this the heat flow and the radial direction are the same direction, positive radial direction or the same direction. So, this negative sign is to take care of the gradient being negative. So, the chemical heat converted into thermal energy will be equal to this. Partially used to heat the interface or supply the latent heat partially transported away to the ambient.

$$\dot{m}_F \Delta h_C = \left(\lambda 4\pi r_f^2 \frac{dT}{dr}\right)_{r_f^-} - \left(\lambda 4\pi r_f^2 \frac{dT}{dr}\right)_{r_f^+}$$

So, this is very important equation. Now, please understand that I have this equation and now gives the energy balance of the flame sheet. Now, I have two derivatives here. Temperature at the r_{f-}; that means, I have to get that temperature gradient at r_{f-}, I have take the inner profile and here r_{f+} I have to take the outer profile.

Now, the dT/dr terms here are evaluated using the temperature profiles in both inner and outer regions first. So, for this value of dT/dr at r_{f-} I will take the inner temperature profile. This inner temperature profile I will take, calculate the dT/dr and set $r = r_f$ and use this here because at r_f know so, set $r = r_f$ and use this here. In the other derivative I will take from the outer zone.

Here, the outer zone this profile I will take a differentiation of this with respect to the radius and set $r = r_f$. So, I will get the values here.

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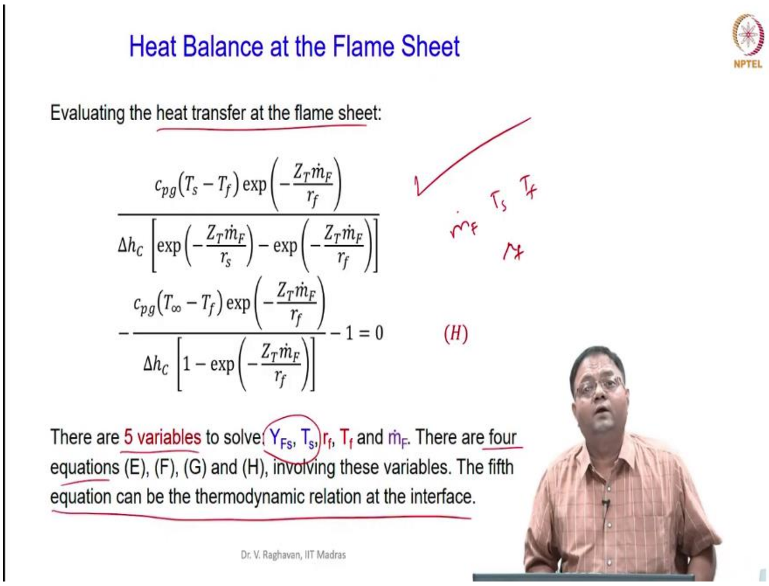

Heat Balance at the Flame Sheet

Evaluating the heat transfer at the flame sheet:

$$\frac{c_{pg}\left(T_s-T_f\right)\exp\left(-\frac{Z_T\dot{m}_F}{r_f}\right)}{\Delta h_C\left[\exp\left(-\frac{Z_T\dot{m}_F}{r_s}\right)-\exp\left(-\frac{Z_T\dot{m}_F}{r_f}\right)\right]}-\frac{c_{pg}\left(T_\infty-T_f\right)\exp\left(-\frac{Z_T\dot{m}_F}{r_f}\right)}{\Delta h_C\left[1-\exp\left(-\frac{Z_T\dot{m}_F}{r_f}\right)\right]}-1=0 \qquad (H)$$

There are 5 variables to solve: Y_{Fs}, T_s, r_f, T_f and $\dot{m}_F$. There are four equations (E), (F), (G) and (H), involving these variables. The fifth equation can be the thermodynamic relation at the interface.

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So, when I do this I get the fourth equation.

$$\frac{c_{pg}\left(T_s-T_f\right)\exp\left(-\frac{Z_T\dot{m}_F}{r_f}\right)}{\Delta h_C\left[\exp\left(-\frac{Z_T\dot{m}_F}{r_s}\right)-\exp\left(-\frac{Z_T\dot{m}_F}{r_f}\right)\right]}-\frac{c_{pg}\left(T_\infty-T_f\right)\exp\left(-\frac{Z_T\dot{m}_F}{r_f}\right)}{\Delta h_C\left[1-\exp\left(-\frac{Z_T\dot{m}_F}{r_f}\right)\right]}-1=0 \qquad (H)$$

So, first equation was due to the species transport in the inner zone that is fuel transport in the inner zone. Second equation was generated using the oxygen transport in the outer zone.

Third equation is generated using the interface heat balance using the energy conservation. Inner temperature profile was used and using that derivative term calculating differentiation of that temperature profile with respect to r and setting r = r_s, I got the heat balance of the interface that was the third equation. Fourth equation is the heat balance at the flame sheet.

So, there we get two temperature derivatives. One for the inner zone, one for the outer zone and use that and get an equation. So, there are now four equations, but five unknowns are there still. So, again please see that this equation has $\dot{m}_F$, T_s, T_f, r_f as the unknowns; basically, there are four unknowns here.

So, what is the next step? how the fifth equation can be created? There are four equation I have used. Now, please understand conservation equations for species, see there are two species. So, only one conservation equation can be used. The other one can be found as 1 minus the mass fraction of the other species. So, one conservation equation is enough for the inner zone and outer zone. For the inner zone we have used fuel, for outer zone we have used oxidizer. So, you got two equations out of that. For temperature we have two profiles for inner and outer and we have the heat balance at the interface providing one, heat balance at the flame sheet providing one more. So, we have consumed all the boundary conditions now. So, four equations are got. Fifth equation is not available. There are five unknowns here. For getting that I need to connect this T_s and Y_{FS}; that means, the fifth equation can be generated using the thermodynamic relationship which is Clausius Clapeyron equation. So, these are the important things. Now go to that.

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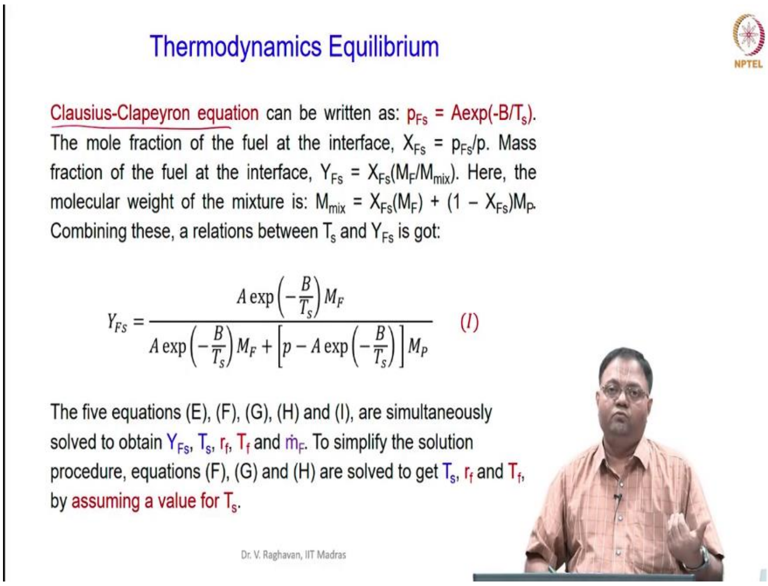

Thermodynamics Equilibrium

Clausius-Clapeyron equation can be written as: $p_{Fs} = A\exp(-B/T_s)$. The mole fraction of the fuel at the interface, $X_{Fs} = p_{Fs}/p$. Mass fraction of the fuel at the interface, $Y_{Fs} = X_{Fs}(M_F/M_{mix})$. Here, the molecular weight of the mixture is: $M_{mix} = X_{Fs}(M_F) + (1 - X_{Fs})M_P$. Combining these, a relations between T_s and Y_{Fs} is got:

$$Y_{Fs} = \frac{A\exp\left(-\frac{B}{T_s}\right)M_F}{A\exp\left(-\frac{B}{T_s}\right)M_F + \left[p - A\exp\left(-\frac{B}{T_s}\right)\right]M_P} \qquad (I)$$

The five equations (E), (F), (G), (H) and (I), are simultaneously solved to obtain Y_{Fs}, T_s, r_f, T_f and $\dot{m}_F$. To simplify the solution procedure, equations (F), (G) and (H) are solved to get T_s, r_f and T_f, by assuming a value for T_s.

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So, Clausius Clapeyron equation as we have seen already which is written in a different form.

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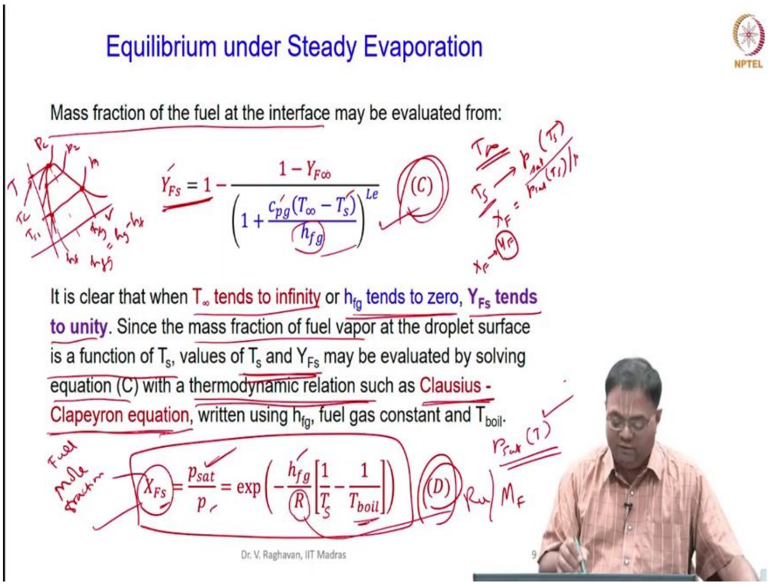

Equilibrium under Steady Evaporation

Mass fraction of the fuel at the interface may be evaluated from:

$$Y_{Fs} = 1 - \frac{1 - Y_{F\infty}}{\left(1 + \frac{c_{pg}(T_\infty - T_s)}{h_{fg}}\right)^{Le}} \qquad (C)$$

It is clear that when T_∞ tends to infinity or h_{fg} tends to zero, Y_{Fs} tends to unity. Since the mass fraction of fuel vapor at the droplet surface is a function of T_s, values of T_s and Y_{Fs} may be evaluated by solving equation (C) with a thermodynamic relation such as Clausius - Clapeyron equation, written using h_{fg}, fuel gas constant and T_{boil}.

$$X_{Fs} = \frac{p_{sat}}{p} = \exp\left(-\frac{h_{fg}}{R}\left[\frac{1}{T_s} - \frac{1}{T_{boil}}\right]\right) \qquad (D)$$

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So, $X_{FS} = p_{sat}/p$ = exponent of this. But you can see this, these are the variables which are known to us. T surface, if you substitute, I get the X_{FS} value but the fuel properties like h_{fg} and T_{boil} has to be given as an input.