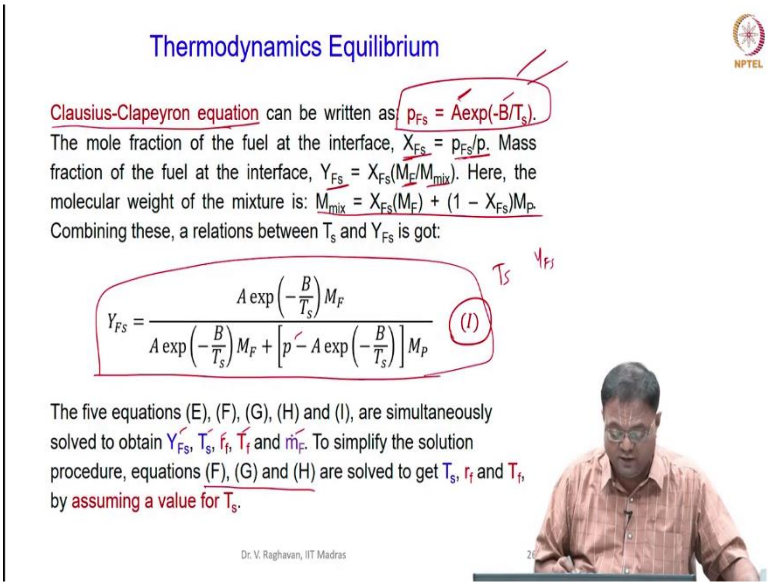
Fundamentals of Combustion
Prof. V. Raghavan
Department of Mechanical Engineering
Indian Institute of Technology, Madras

Lecture – 58
Droplet evaporation and combustion - Part 5
Evaluation of mass burning rate and worked examples

(Refer Slide Time: 00:14)



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:

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

T_s Y_{Fs}

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.

Dr. V. Raghavan, IIT Madras

Here, as this in a simple form I can write p_{FS} that is the saturation pressure of the fuel at the interface or partial pressure of the fuel at the interface both are same, saturation pressure is the partial pressure if the you take at one atmosphere or you have to divide it by the total pressure. So, this is equal to $A\exp(-B/T_s)$, where the A and B are specific constant for a fuel.

When you have a particular fuel this A and B are the constant for the fuel. So, we can write the Clausius-Clapeyron equation in this form also. So, here actually you can easily understand that the A and B are written in terms of h_{fg} molecular weight and so on. Now, when I write the Clausius-Clapeyron equation $p_{FS} = A\exp(-B/T_s)$, then this is9 a convenient way to do this.

Once I know the partial pressure; partial pressure by this total pressure will give you the mole fraction, then mass fraction is got by finding X_{FS} into molecular weight of the fuel divided by molecular weight of the mixture, molecular weight of mixture is calculated again here like X_{FS} into M_F that is the mole fraction of the fuel at the interface into molecular weight of the fuel plus 1 minus mole of fuel is nothing but the products into molecular weight of the product.

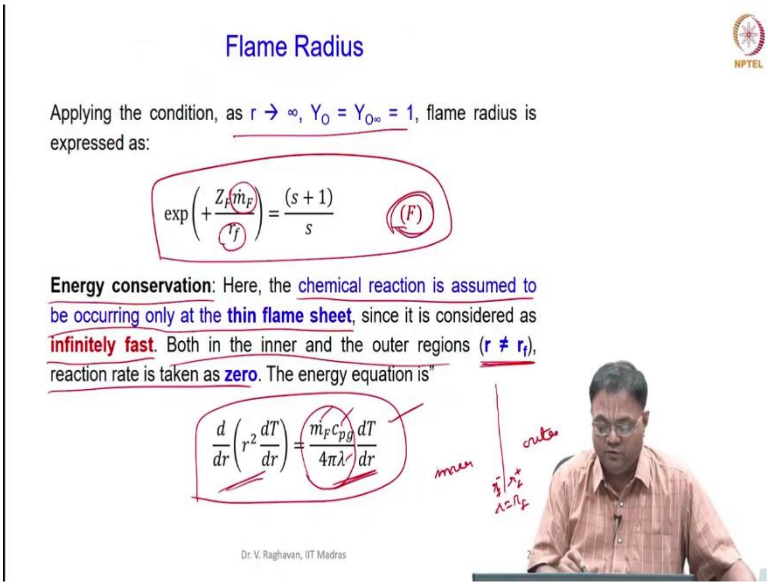
So, if I do this and substitute it back, I get mole fraction to mass fraction. So, once I do this, then these can be combined, for example, this equation can be combined, this Clausius-Clapeyron equation, then the definition of the mole fraction, mass fraction, molecular weight of the mixture etcetera and I get this equation

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

Here, you can see clearly that p is known here T_s is not known and Y_{FS} is not known. So, that will be the equation I. Now, I am relating T_s thermodynamic equilibrium will only relate T_s and Y_{FS} so, that we have achieved here

In a simple way I have done this here, so, you will see that there are five equations E, F, G, H and I and we can solve simultaneously to find the unknowns Y_{FS}, T_s, r_f, T_f and $\dot{m}_F$. But actually you know this equation is very complicated, exponential variations are there in this equation. So, what we will do know normally to simplify the problem, we will only take the F, G and H

(Refer Slide Time: 03:03)



Flame Radius

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

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

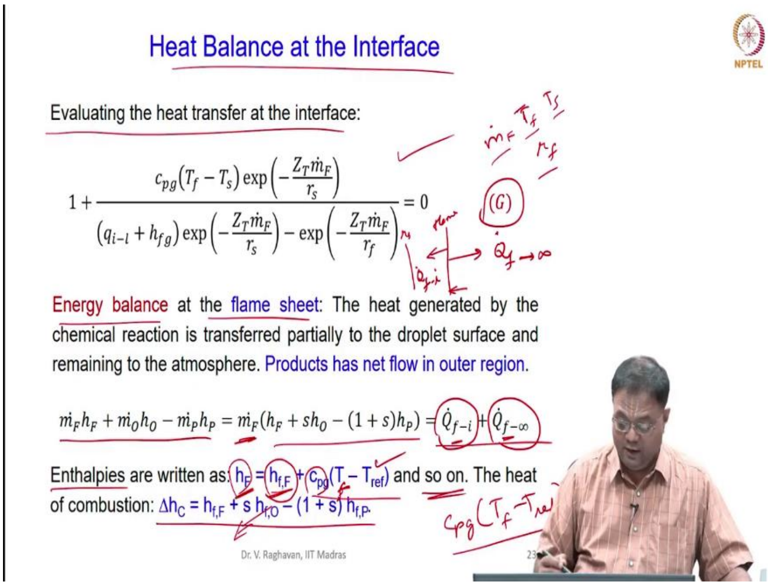
Energy conservation: Here, the chemical reaction is assumed to be occurring only at the **thin flame sheet**, since it is considered as **infinitely fast**. Both in the inner and the outer regions (**$r \neq r_f$**), reaction rate is taken as **zero**. The energy equation is"

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

Dr. V. Raghavan, IIT Madras

So, the unknowns in the F, G and H we will again see quickly. If we take the equation F it has unknown $\dot{m}_F$ and r_f.

(Refer Slide Time: 03:11)



Heat Balance at the Interface

Evaluating the heat transfer at the interface:

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

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.

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

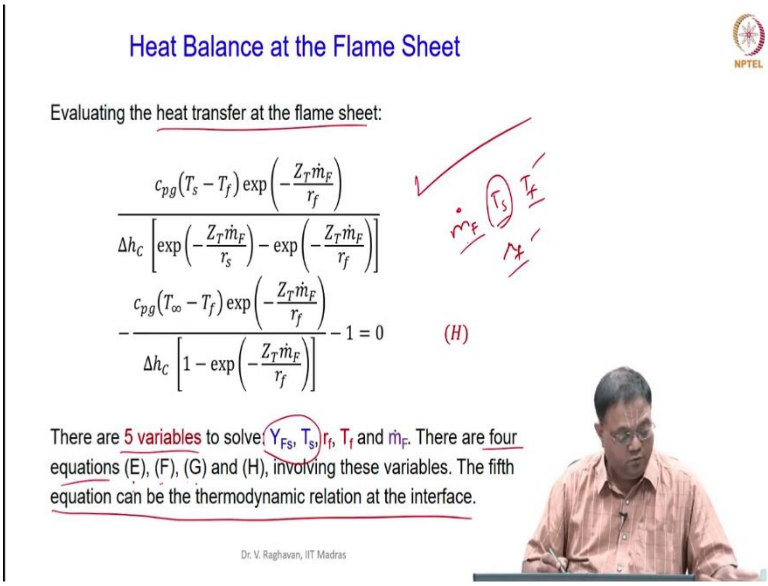
Enthalpies are written as: $h_F = h_{f,F} + c_{pg}(T - T_{ref})$ and so on. The heat of combustion: $\Delta h_C = h_{f,F} + s\,h_{f,O} - (1 + s)\,h_{f,P}$.

Dr. V. Raghavan, IIT Madras

23

Then, G has unknown, I have written here $\dot{m}_F$, T_f, T_s and r_f.

(Refer Slide Time: 03:19)



Heat Balance at the Flame Sheet

Evaluating the heat transfer at the flame sheet:

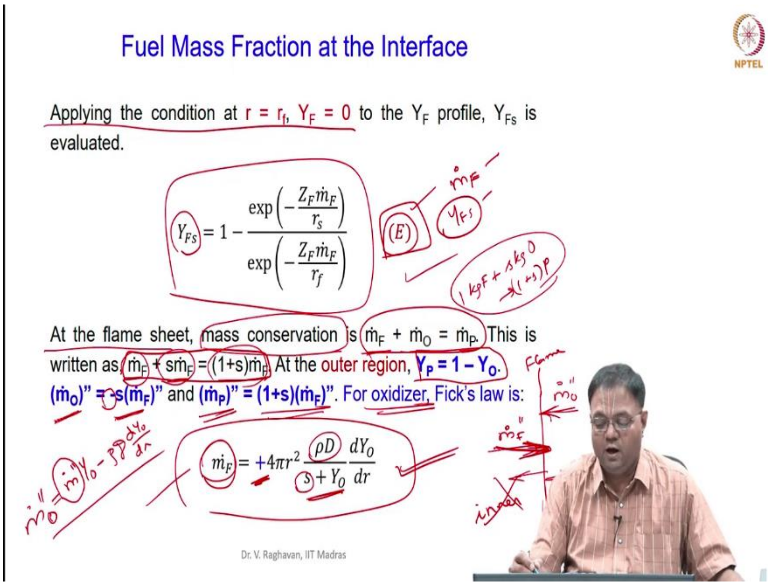
$$\frac{c_{pg}\left(T_s-T_f\right)\exp\left(-\frac{Z_T\dot{m}_F}{r_f}\right)}{\Delta h_C\left[\exp\left(-\frac{Z_T\dot{m}_F}{r_s}\right)-\exp\left(-\frac{Z_T\dot{m}_F}{r_f}\right)\right]}-\frac{c_{pg}\left(T_\infty-T_f\right)\exp\left(-\frac{Z_T\dot{m}_F}{r_f}\right)}{\Delta h_C\left[1-\exp\left(-\frac{Z_T\dot{m}_F}{r_f}\right)\right]}-1=0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

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.

Dr. V. Raghavan, IIT Madras

Then, H has $\dot{m}_F$, T_s T_f and r_f. So, you know this. Now, I will select three equations that is E, F and G. I can solve three variables.

(Refer Slide Time: 03:45)



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.

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

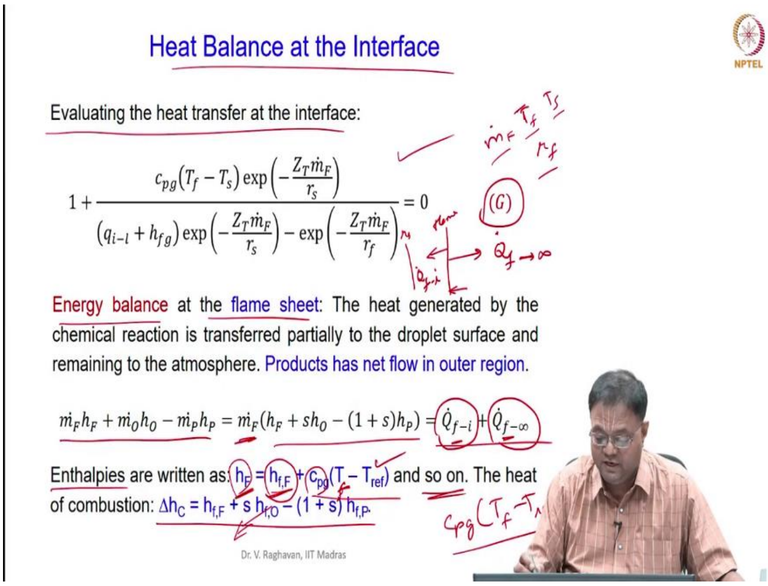
At the flame sheet, mass conservation is $\dot{m}_F + \dot{m}_O = \dot{m}_P$. This is written as $\dot{m}_F + s\dot{m}_F = (1+s)\dot{m}_F$. At the outer region, $Y_P = 1 - Y_O$. $(\dot{m}_O)'' = -s(\dot{m}_F)''$ and $(\dot{m}_P)'' = (1+s)(\dot{m}_F)''$. For oxidizer, Fick's law is:

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

Dr. V. Raghavan, IIT Madras

So, if you take the common unknowns are there for example, in this E $\dot{m}_F$ and Y_{FS} are there, so, two unknowns here $\dot{m}_F$ and Y_{FS} and F, E I leave it so, F I will take first, F has $\dot{m}_F$ and r_f.

(Refer Slide Time: 04:04)



Heat Balance at the Interface

Evaluating the heat transfer at the interface:

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

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.

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

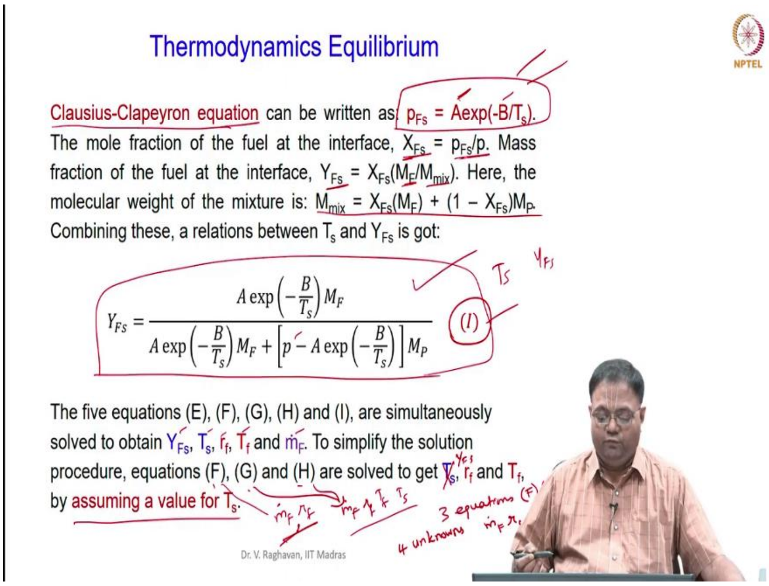
Enthalpies are written as: $h_F = h_{f,F} + c_{pg}(T - T_{ref})$ and so on. The heat of combustion: $\Delta h_C = h_{f,F} + s\, h_{f,O} - (1 + s)\, h_{f,P}$.

Dr. V. Raghavan, IIT Madras

And here, G has $\dot{m}_F$, r_f plus two more T_f and T_s. So, actually go to the next one, H has $\dot{m}_F$, r_f which is unknown in both and the T_f is the unknown generated in this.

So, that the fourth unknown T_s; if I guess the value of T_s, then I have three unknowns what are they? $\dot{m}_F$, T_f and r_f. So, I will guess the value of say in three equations E, F and G, see if we take three equations basically, not this.

(Refer Slide Time: 04:42)



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:

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

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 $\cancel{T_s}$, r_f and T_f, by assuming a value for T_s.

Dr. V. Raghavan, IIT Madras

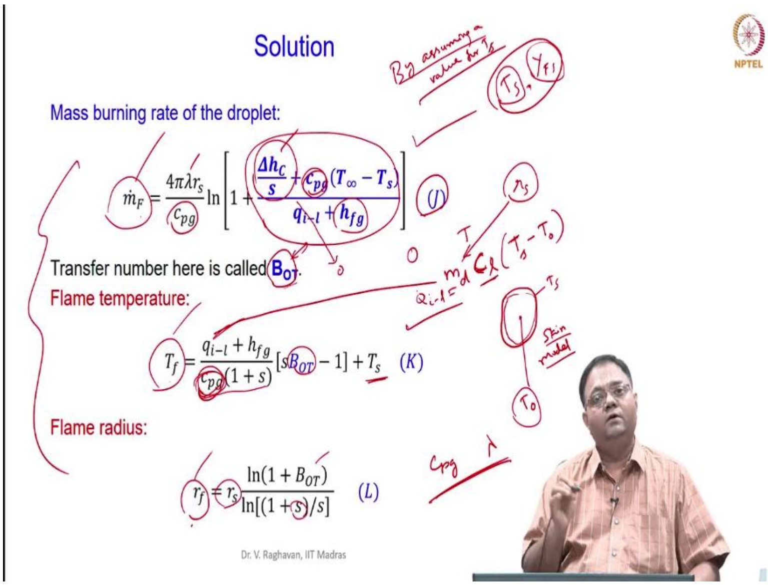
In this, F, G and H, in F I have unknowns of $\dot{m}_F$, r_f then here I have $\dot{m}_F$, r_f, T_f and T_s and here also I am getting the same. So, I have three equations in which there are four unknowns.

Now, please see this, we have we have generated all the five equations here, but simultaneously solving all the equations will be complicated because of the exponential nature of these equations especially that of I.

So, what we will do is we will take the equations F, G and H. So, that is I will just show you quickly, F is here which will relate the r_f and m_F, so, the unknowns here are r_f and m_F. And I go to the next equation which is here G which has four unknowns, $\dot{m}_F$, T_f, T_s and r_f and again H has the same unknowns $\dot{m}_F$, T_s, T_f and r_f.

Now, you have $\dot{m}_F$, r_f, T_f, three you can solve basically. Using these three equations you can solve but T_s has to be guessed. So, what we will do is we will assume the value for T_s and solve these three equations to get the unknowns $\dot{m}_F$, r_f and T_f. So, that is what we are trying to do here.

(Refer Slide Time: 06:20)



Solution

Mass burning rate of the droplet:

$$\dot{m}_F = \frac{4\pi\lambda r_s}{c_{pg}} \ln\left[1 + \frac{\frac{\Delta h_C}{s} + c_{pg}(T_\infty - T_s)}{q_{i-l} + h_{fg}}\right] \quad (J)$$

Transfer number here is called B_{OT}.

Flame temperature:

$$T_f = \frac{q_{i-l} + h_{fg}}{c_{pg}(1+s)}[sB_{OT} - 1] + T_s \quad (K)$$

Flame radius:

$$r_f = r_s \frac{\ln(1 + B_{OT})}{\ln[(1+s)/s]} \quad (L)$$

Dr. V. Raghavan, IIT Madras

So, this solution is got by assuming a value for T_s. When I do that, I get expression for $\dot{m}_F$ as this. So, again you can see the similar expression I am getting what we saw in the evaporation $4\pi r_s$ driving force λ/c_{pg} into natural logarithm of 1 plus some number which I call it a transfer number. So, same similar expression which we have seen in the heat balance equation plus 1 + B; a B number.

Now, please understand this is the B number, $c_{pg}(T_\infty - T_s)/h_{fg}$ that was used for evaporation. Now also, we can see that this may be negligible q dot l can be negligible.

So, in that case know, this additional term you see that is coming due to reaction, so that means, not only the heat transfer from the ambient to the surface, it is now the reaction that also generates a higher heat source for you that is the flame temperature is created here.

So, this B number again ratio of the heat which can be transferred from the ambient can include a flame like this and to the surface and what is taken by the droplet. So, this is the transfer number basically.

So, the mass burning rate is still the same, similar way we can write $4\pi r_s\lambda/c_{pg}$ into natural logarithm of 1 + B_{OT}, I say B_{OT} because this transfer number is got by combining the oxygen conservation and the temperature. So, I get this. So, this is a famous B number which you can use for the combustion problems. So, this is one.

$$\dot{m}_F = \frac{4\pi\lambda r_s}{c_{pg}} \ln\left[1 + \frac{\frac{\boldsymbol{\Delta h_C}}{\boldsymbol{s}} + \boldsymbol{c_{pg}(T_\infty - T_s)}}{\boldsymbol{q_{i-l} + h_{fg}}}\right] \quad (J)$$

Second is flame temperature. So, please understand this is kept as equation J and flame temperature is again you can see this the heat which is taken by the droplet whether for phase change or for the internal heating divided by the c_{pg} into 1 plus s into s of B_{OT} again B_{OT} comes into play plus T_s. So, this is a positive kinetic which is added to T_s to get the flame temperature. Please understand that in order to predict the flame temperature properly, proper values of the B_{OT} and c_{pg}, B_{OT} basically involves lot of properties here. So, we need to properly evaluate the c_{pg} again. c_{pg} is the only main property here and also the q_l, q_{i-l}, if it is not 0, how will you evaluate the q_l is also big question.

Normally, what we do is we can take this as mass of the droplet whatever be at a given radius, we know the what is the mass of the droplet into c_p into C of the liquid we will say surface temperature to internal temperature, T_o, it is called a skin model.

Skin model what we assume here is the surface is at T_s and leaving a small portion, the bulk of the liquid is at a temperature of T_o. So, it is called skin model. When I use that, I know the specific heat capacity of the liquid into mass of the droplet at a given radius into T_s - T_o, If I do this, I can account for the q. This is actually q dot interface to liquid.

$$T_f = \frac{q_{i-l} + h_{fg}}{c_{pg}(1+s)}[sB_{OT} - 1] + T_s \quad (K)$$

So, this way can do this. This is one of the way I can do this simplified way or you have to solve a differential equation within the liquid to solve for the conduction within the liquid for the temperature distribution. The thin skin model can be used.

So, only a thin portion surrounding the surface will be at T_s other than that everything will be uniform, bulk temperature T_0 so, that heat transfer can be accomplished. So, as the T_0 increases slowly to T_s, then the $q_{i-l} \rightarrow 0$. So, this is another expression which we get.

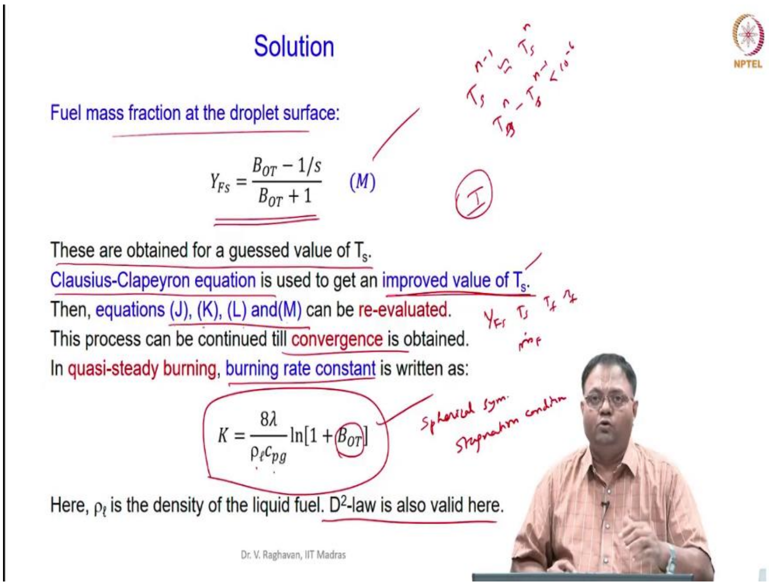
Similarly, the flame radius again you can see that the flame radius depends on the stoichiometric air fuel ratio on the B number r_s times some r_s into sometimes so, it is sometimes, few times the droplet diameter. So, these are the equations which you get. These are the three unknowns which we solve basically.

$$r_f = r_s \frac{\ln(1 + B_{OT})}{\ln[(1+s)/s]} \quad (L)$$

By solving the H, the three equations F, G and H, then here what we have done? We have assumed value of T_s that is the only issue. So, they may not be accurate until you resolve T_s other two unknowns are what? The interface quantities. Until we resolve these two, this cannot be a great. So, because we have assumed the value of T_s and easily solved for the other three unknowns $\dot{m}_F$, T_f and r_f.

Now, we have to correct T_s value based upon the coupling between T_s and Y_{FS} that is what we are trying to do here.

(Refer Slide Time: 11:50)



Solution

Fuel mass fraction at the droplet surface:

$$Y_{Fs} = \frac{B_{OT} - 1/s}{B_{OT} + 1} \qquad (M)$$

These are obtained for a guessed value of T_s.
Clausius-Clapeyron equation is used to get an improved value of T_s.
Then, equations (J), (K), (L) and(M) can be re-evaluated.
This process can be continued till convergence is obtained.
In quasi-steady burning, burning rate constant is written as:

$$K = \frac{8\lambda}{\rho_\ell c_{pg}} \ln[1 + B_{OT}]$$

Here, ρ_ℓ is the density of the liquid fuel. D²-law is also valid here.

Dr. V. Raghavan, IIT Madras

$T_s^{n-1} \simeq T_s^{n}$

$T_s^{n} - T_s^{n-1} < 10^{-6}$

T_B

I

Y_{Fs} T_s T_f r_f

$\dot{m}_F$

Spherical sym.

Stagnation condition

So, here what we do is Y_{FS} fuel mass fraction at the droplet surface can be written like this.

$$Y_{Fs} = \frac{B_{OT} - 1/s}{B_{OT} + 1} \qquad (M)$$

Now, again I am using the 5th equation to do this basically, or one of the equations to do this, again this is not accurate here. Now, what I will do is these are obtained from the guessed value of T_s.

Now, Clausius-Clapeyron equation will be used to get an improved value of this. What is Clausius-Clapeyron equation here? This equation I. So, this will be used, equation I will be used to get the improved value of T_s know.

Now, when I say Y_{FS} and T_s that is the relationship here, once I know Y_{FS}, I can calculate T_s here so, I have calculated using M, I calculated the value of Y_{FS}, now I substitute Y_{FS} here and calculate the value of T_s here so, that will be different value than what we have guessed because of the coupled nature of this.

So, once I do this, what happens is basically I will get all the equations be re-evaluated and until convergence is got. What we did for the evaporation, when I coupled that B_T and B_Y and got the T_s and Y_{FS} value similarly here, we have to couple the T_s and Y_{FS} properly and get this. We have two more equations. One equation is coupled here basically then one more equation is the equation I.

So, the Clausius-Clapeyron equation is used to improve the value of T_s and once you get a iterated value of T_s substitute back and get the values of this J, K, L, M which are the solution and now you will get the iteration. So, slowly if you vary these values, finally, you will not get any more change.

The T_s value for example, got from the previous iteration say n - 1 will be almost same as the value of T_s got from the current iteration or the change between the T_s value at the current iteration minus that in the previous iteration will be less than say 10^{-6} something like that. So, we can say that it is converged.

So, once it is converged, then we can say that is the equilibrium temperature corresponding mass fraction is Y_{FS} and the solution is given here for the mass burning rate, flame temperature and r_s, but very critical is the evaluation of c_{pg} and λ.

So, c_{pg} and λ are the values which we have to carefully take and put it here. So, to get the values of see λ and c_{pg} you have to properly take at what temperature etcetera we will take this that will govern the solution.

So, we can see that once you get the convergence, you get proper values of all the quantities the unknowns what we wanted was where Y_{FS}, T_s T_f, r_f and $\dot{m}_F$ so, you got all the values. Now, one more quantity which is interest of us is this burning rate constant.

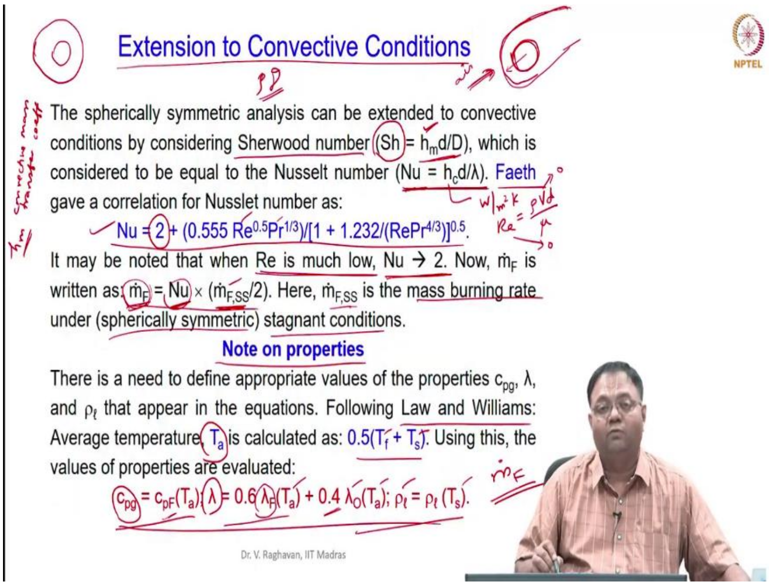
The evaporation rate constant was seen previously, now burning rate constant K which is the same thing like for example, $8\lambda/\rho_l c_{pg}$ $(1 + B_{OT})$.

$$K = \frac{8\lambda}{\rho\ell c_{pg}} \ln[1 + B_{OT}]$$

So, this is similar expression what we get and as I told you D^2 law is valid here because only leaving up the initial ignition part or the final extinction part etcetera for 80% to 85% of the droplet lifetime the burning rate would be a constant. So, we can get the burning rate constant also in this but this is the burning rate which is got at the spherically symmetric condition, that is stagnation condition.

So, in a spray, a droplet will be actually moving so, there will be relative velocity between the droplet and the surrounding air but when this model will be applicable, only when the droplet has reached an almost stagnant condition and also this is separated from the other droplets. So, isolated droplet burning in a stagnant condition. So, that will be the solution what we have got so far.

(Refer Slide Time: 16:21)



Extension to Convective Conditions

ρD

air

convective mass transfer coeff

h_m

The spherically symmetric analysis can be extended to convective conditions by considering Sherwood number (Sh = $h_m d/D$), which is considered to be equal to the Nusselt number (Nu = $h_c d/\lambda$). Faeth gave a correlation for Nusslet number as:

$$Nu = 2 + (0.555\,Re^{0.5}Pr^{1/3})/[1 + 1.232/(RePr^{4/3})]^{0.5}.$$

W/m^2K

$Re = \frac{\rho V d}{\mu} \to 0$

It may be noted that when Re is much low, Nu → 2. Now, $\dot{m}_F$ is written as: $\dot{m}_F = Nu \times (\dot{m}_{F,SS}/2)$. Here, $\dot{m}_{F,SS}$ is the mass burning rate under (spherically symmetric) stagnant conditions.

Note on properties

There is a need to define appropriate values of the properties c_{pg}, λ, and ρ_ℓ that appear in the equations. Following Law and Williams: Average temperature T_a is calculated as: $0.5(T_f + T_s)$. Using this, the values of properties are evaluated:

$$c_{pg} = c_{pF}(T_a);\ \lambda = 0.6\,\lambda_F(T_a) + 0.4\,\lambda_O(T_a);\ \rho_\ell = \rho_\ell\,(T_s).$$

$\dot{m}_F$

Dr. V. Raghavan, IIT Madras

Now, anyway we can try to extend the solution to the convective conditions. See for example, if there is a relative velocity between the droplet and this for example, the atmosphere ambient. For example, now the droplet can have a flame like this, the air can be like this or the droplet can move in this direction or the air can move in this direction and the flame can be formed like this.

Now, please see that there is no spherical symmetry for the flame, but still here the droplet can be assumed to be a spherical because of the low Weber number, it can be spherical.

Droplet can be spherical, but the flame surrounding the droplet may not be spherical because of convection but there is no theoretical solution possible for this, but we can correlate the value so, what basically the convection does to the burning rate is to enhance the burning rate or evaporation.

So, both the evaporation, because if more evaporation occurs, then only burning can be improved. Both the evaporation and the burning rate are increased due to convection.

If you have a spherically symmetric evaporation or combustion, you will have only diffusion dominated transport here, but here convection comes in favour. So, when there is a convective transport, the heat transfer and mass transfer processes are enhanced.

So, we can take into account of say Sherwood number which is nothing, but Sherwood number is Sh which is the convective mass transfer coefficient. So, h_m is convective mass transfer coefficient and that into diameter of the droplet divided by the diffusion coefficient, D is diffusion coefficient.

So, this will tell how much the mass transfer has been enhanced. So, if you only have diffusion dominated, you can see this the driving force was ρD alone for the evaporation. When there is only diffusion, spherically symmetric stagnation environment the only driving force was ρD.

Now, if you take into account of convection, the convective mass transfer coefficient also will come into the play and that the strength of the convection will be determined by the non-dimensional number called Sherwood number. So, the effect of convection is to increase the burning rate or evaporation rate.

So, we considered the Lewis number equal to 1, we can also consider Nusselt number into place. Now, convective heat transfer coefficient, because please understand as I told you both mass transfer and heat transfer are enhanced, but we will assume that the enhancement in the mass transfer and heat transfer are of the same order when there is a convection.

So, we will say h_c is the heat transfer coefficient and d/λ, λ is the thermal conductivity of the gas. So, this Nusselt number, if we assume that the Sherwood number will be equal to Nusselt number or in other words, if the enhancement in the heat transfer is of the same order of that of the mass transfer, then we can take any Nusselt number coefficient and try to get the enhancement in the convection or the convective dominant burning or evaporation.

So, what we try to do here is like this. So, we have a famous correlation given by Faeth which is nothing, but Nusselt number equal to 2 plus some function of Reynolds number and Prandtl number. Please understand that this 2 is definite. If there is any convection, then there will be a certain value for Reynolds number. For the fluid, there will be certain Prandtl number etcetera.

$$Nu = 2 + (0.555\, Re^{0.5} Pr^{1/3})/[1 + 1.232/(RePr^{4/3})]^{0.5}.$$

Now, please understand that if there is no convection or when Reynolds number is nothing, but what ρ × velocity × diameter of the droplet / μ. If velocity is tending to 0, then the Reynolds number will tend to 0. When Reynolds tends to 0, we can see that this term, the second term here will tend to 0, so, Nusselt number will tend to a value of 2. So, when the Reynolds number is very low, Nusselt number will tend to a value of 2.

So, keeping that in mind, we can write the mass burning rate in a convective environment as Nusselt number times mass burning rate at the spherically symmetric condition SS is the mass burning rate at a spherical symmetric condition divided by 2. So, when you multiply Nusselt number, see when Nusselt number is equal to 2 that means, 2 into mass burning rate at spherically symmetric divided by 2, so, mass burning rate will be equal to the spherically symmetric mass burning rate.

$$\dot{m}_F = Nu \times (\dot{m}_{F,SS}/2).$$

When there is a Reynolds number which is not 0 or not close 0, it is higher value, then the second term will wake up and we will have a higher Nusselt number say 10, 15 something like that or may be more than that in that case, you will see that the Nusselt number effect will bring in more mass burning rate compared to that of the spherically symmetric regime. Do you understand?

So, this $\dot{m}_{F,SS}$ is the mass burning rate at a spherically symmetric condition or stagnation condition that is enhanced by the value of Nusselt number which is a function of Reynolds number.

So, this is the way we can correlate, there is no theoretical analysis possible because flow is important, we have not even touched the flow so far. So, when there is a convection, then flow becomes more important and there will be non-uniform distribution of vapours etcetera and spherically symmetric model will not work we have two-dimensions now and so on.

So, a lot of complications arise, but this is only empirically, we are trying to correlate the effect of the Nusselt number or Sherwood number which is taken of same order as the Nusselt number and try to increase the mass burning rate. So, the increase of the mass burning rate due to enhanced heat and mass transfers in a convective environment is taken care by a correlation such as this and modifying the mass burning rate expression using the Nusselt number.

Now, finally, the note on properties. So, as I told you properties values are very important, you assume that is a constant. It cannot be just a constant or we cannot use air properties; there should be some property values we have to take at some average temperatures. So, let us follow Law and Williams in which the average temperature is taken as 0.5 of surface and the flame temperature.

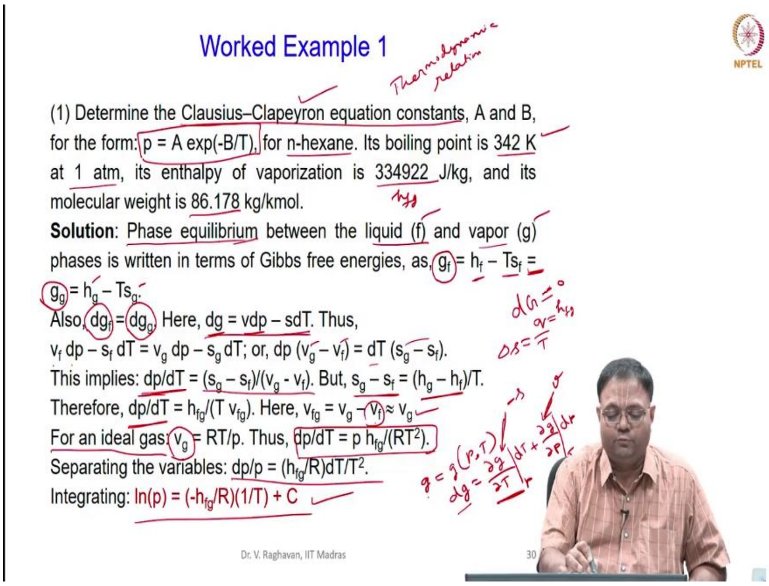
Please understand that ambient temperatures are not considered here. The equilibrium surface temperature and the flame temperature is taken into account again iteration are involved. We do not know the equilibrium temperature so, we assume an equilibrium temperature, calculate the average temperature, then calculate properties as given here, then do the calculations, then iterate.

Now, c_{pg} is calculated as the c_p of fuel at the average temperature. Thermal conductivity is calculated as weighted average of the fuel thermal conductivity 0.6 times fuel thermal conductivity at the average temperature and point 0.4 times oxidizers thermal conductivity at average temperature then the liquids density is taken at the surface temperature.

$$c_{pg} = c_{pF}(T_a);\ \lambda = 0.6\ \lambda_F(T_a) + 0.4\ \lambda_O(T_a);\ \rho_\ell = \rho_\ell\ (T_s).$$

So, if you do this, then you get what you measure in experiments whatever the mass burning rate etcetera, when you use these properties, you get proper mass burning rate values. So, this is note on properties.

(Refer Slide Time: 24:19)



Worked Example 1

Thermodynamic relation

(1) Determine the Clausius–Clapeyron equation constants, A and B, for the form: $p = A \exp(-B/T)$, for n-hexane. Its boiling point is 342 K at 1 atm, its enthalpy of vaporization is 334922 J/kg, and its molecular weight is 86.178 kg/kmol.

h_{fg}

Solution: Phase equilibrium between the liquid (f) and vapor (g) phases is written in terms of Gibbs free energies, as, $g_f = h_f - Ts_f = g_g = h_g - Ts_g$.

Also, $dg_f = dg_g$. Here, $dg = vdp - sdT$. Thus,

$v_f\, dp - s_f\, dT = v_g\, dp - s_g\, dT$; or, $dp\,(v_g - v_f) = dT\,(s_g - s_f)$.

This implies: $dp/dT = (s_g - s_f)/(v_g - v_f)$. But, $s_g - s_f = (h_g - h_f)/T$.

Therefore, $dp/dT = h_{fg}/(T\, v_{fg})$. Here, $v_{fg} = v_g - v_f \approx v_g$

For an ideal gas: $v_g = RT/p$. Thus, $\boxed{dp/dT = p\, h_{fg}/(RT^2)}$.

Separating the variables: $dp/p = (h_{fg}/R)dT/T^2$.

Integrating: $\ln(p) = (-h_{fg}/R)(1/T) + C$

$dG = 0$

$\Delta h = h_{fg}$

$\Delta s = \frac{\Delta h}{T}$

$g = g(p,T)$

$dg = \left.\frac{\partial g}{\partial T}\right|_p dT + \left.\frac{\partial g}{\partial p}\right|_T dp$

Dr. V. Raghavan, IIT Madras

30

Then, we will do a couple of a worked examples. The 1st worked example is determine the Clausius-Clapeyron equation constant.

So, we know that the Clausius-Clapeyron equation was written as p = Aexp(-B/T). So, now, this is saturation pressure and this is surface temperature, T is surface temperature. So, what are the constants A and B for a specific fuel?

So, we will take a fuel for consideration as n-hexane and its boiling point is 342 K, its enthalpy of vaporization h_{fg} is 334922 J/kg and its molecular weight is 86.17 and the boiling point is the normal boiling point because it is given at 1 atmospheric pressure.

So, how will you calculate the Clausius-Clapeyron equation constant? First of all, we should calculate what is Clausius-Clapeyron equation and try to fit that in this form p = A exp(-B/T). So, Clausius-Clapeyron equation is a thermodynamic relation. Now, if you see this this ensures a local phase equilibrium, liquid vapor equilibrium vle vapor liquid equilibrium. So, liquid is represented at f and the vapor is represented as g.

Now, as I told you when there is an equilibrium, the Gibbs-free energy should be the same, that is we have already seen that dG → 0 or equal to 0 at equilibrium, dG = 0 that means, you can can say that the free energy of the liquid f which is written as $h_f - T(s_f)$ will be equal to the free energy of the vapor g_g which is $h_g - Ts_g$.

Now, not only this any small change in the Gibbs-free energy of the liquid will be same as see for example, if some molecules leave the liquid to the vapor that means, there is a small change in the Gibbs-free energy of the liquid that change should replicate in the magnitude, basically the magnitude of this change should replicate in that of the vapor also. So, this also should be obeyed.

So, when you take this into consideration, dg can be written as vdp - sdT. Please understand as I told you, g is a function of p and T. So, now, dg can be written as $(\partial g/ \partial T)_p \times dT + (\partial g/ \partial p)_T \times dp$. Now, this term $(\partial g/ \partial T)_p$ is nothing, but -s and this term $(\partial g/ \partial p)_T$ is nothing, but v the specific volume. So, when you do this, you get this dg as this.

Now, try to write this dg_f as $v_f \times dp - s_f \times dT$. We know that g is a function of p and T, $v_f \times dp - s_f \times dT = v_g dp - s_g dT$. Now, we rearrange $dp \times (v_g - v_f)$ that is the this is what? This is the specific volume of the gas or the vapor and specific volume of the liquid. So, dT times the entropy change between the vapor and the liquid.

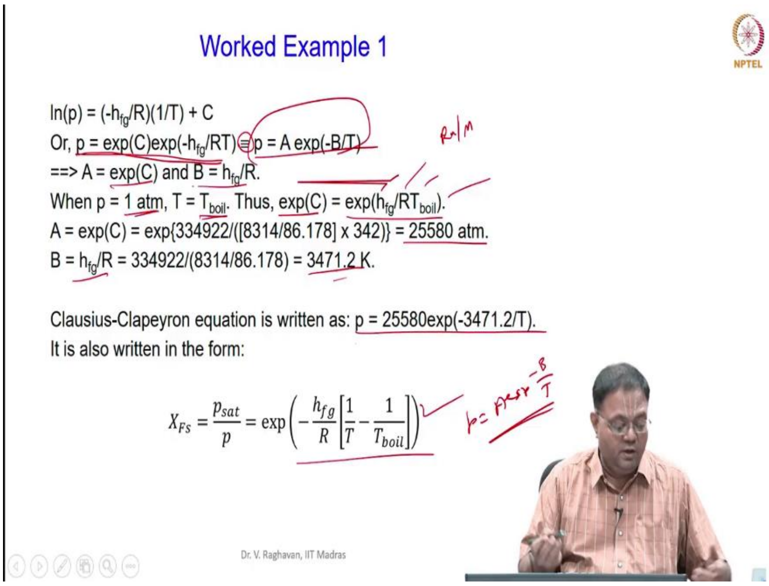
Now, I want dp/dT that is what the Clausius-Clapeyron equation is about. The relationship between the pressure and the temperature. So, that is written as the entropy change $s_g - s_f$ minus the volume specific volume change $v_g - v_f$. But, now you take into account of $s_g - s_f$ can be written as what? s_g delta s so, delta s basically will be equal to q/T. When T is called basically when the phase change T is constant.

So, this q is nothing but the latent heat that is h_{fg} so, this is nothing but h_{fg}/T. So, h_{fg} is $(h_g - h_f)/T$, so, that is $s_g - s_f$. So, when you substitute this, dp/dT can be written as h_{fg}/Tv_{fg} v_{fg} is nothing, but $v_g - v_f$, but you know that the physical volume occupied by the liquid is very low when compared to that of the vapor.

So that means, I can neglect this v_f and v_{fg}, $v_g - v_f$ can be only written as v_g , but if you take ideal gas which is the problem in hand, ideal gas v_g basically can be written using the equation of state that is pv = RT, s, $v_g = RT/p$.

So, I combine everything and write the equation. This is the Clausius-Clapeyron equation the differential form, $dp/dT = p(h_{fg}/RT^2)$. So, now I separate the variables and I try to integrate this that is $\ln p = -h_{fg}/RT + C$, this is the equation I have.

(Refer Slide Time: 29:58)



Worked Example 1

$\ln(p) = (-h_{fg}/R)(1/T) + C$

Or, $p = \exp(C)\exp(-h_{fg}/RT) \equiv p = A\exp(-B/T)$

$\Longrightarrow A = \exp(C)$ and $B = h_{fg}/R$.

When $p = 1$ atm, $T = T_{boil}$. Thus, $\exp(C) = \exp(h_{fg}/RT_{boil})$.

$A = \exp(C) = \exp\{334922/([8314/86.178] \times 342)\} = 25580$ atm.

$B = h_{fg}/R = 334922/(8314/86.178) = 3471.2$ K.

Clausius-Clapeyron equation is written as: $p = 25580\exp(-3471.2/T)$.

It is also written in the form:

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

Dr. V. Raghavan, IIT Madras

Now, I want to fit this p as some A into exponent of minus B by T. So, that is what we are trying to do here. So, ln p is written like this, $-h_{fg}/RT + C$. So, $p = \exp(C) \times \exp(h_{fg}/RT)$ because this is of the form $A\exp(-B/T)$. So, now, we can see what is A? A is exponent C and B is h_f by R that is it.

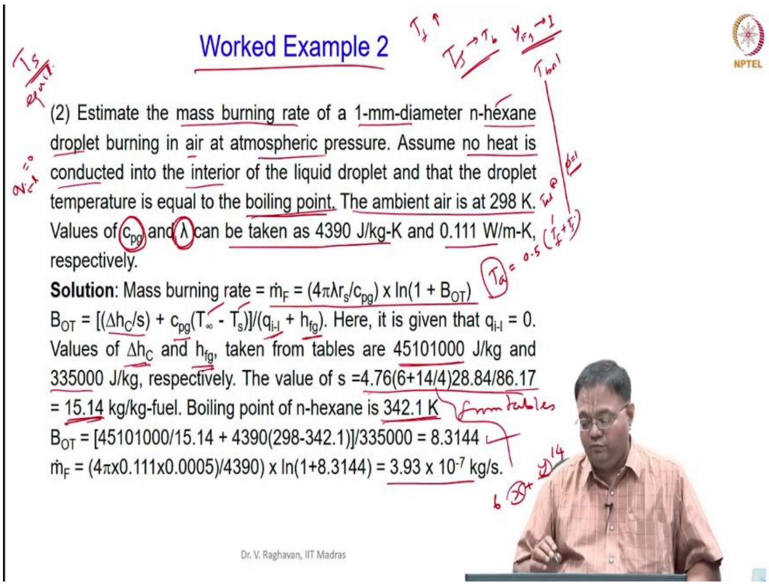
Now, we evaluate. So, for the given liquid hexane, you know that exponent of C is the exponent of this h_{fg}/RT_{boil} so, write this and calculate A similarly, h_{fg}/R calculate this, that is it. So, exponent of C is nothing, but this h_{fg}/RT. The exponent of h_{fg}/RT_{boil}.

Now, you have to apply the boundary condition to get this. So, you know this expression, now, in this expression, you substitute 1 atmosphere to the left-hand side and the boiling point to the right-hand side, then you can know the unknown constant C. So, now, exponent of C can be evaluated as h_{fg}/RT_{boil} you know h_{fg}, you know T_{boil}. Now, R is nothing, but R_u by molecular weight, molecular weight also is given.

So, in this equation, C is an unknown so, to calculate this C, you have to substitute the boundary conditions which is nothing, but at 1 atmosphere, the boiling point is given to you so, use that temperature and pressure here to get this expression. So, that will give you the A value which is exponent of C and B value is h_{fg}/R which is known to me that you calculate. So, this is the Clausius-Clapeyron equation as I told you I can also write in this form. So, this is the first example.

So, you please understand that writing in this form and in this form $p = A\exp(-B/T)$ this has an advantage like we can simplify this instead of writing in this way, we can write in this. So, p_{sat}/p into exponent of something will come. So, instead of writing this, but both are same, equivalent.

(Refer Slide Time: 32:16)



Worked Example 2

(2) Estimate the mass burning rate of a 1-mm-diameter n-hexane droplet burning in air at atmospheric pressure. Assume no heat is conducted into the interior of the liquid droplet and that the droplet temperature is equal to the boiling point. The ambient air is at 298 K. Values of c_{pg} and λ can be taken as 4390 J/kg-K and 0.111 W/m-K, respectively.

Solution: Mass burning rate = $\dot{m}_F = (4\pi\lambda r_s/c_{pg}) \times \ln(1 + B_{OT})$

$B_{OT} = [(\Delta h_C/s) + c_{pg}(T_\infty - T_s)]/(q_{i\text{-}l} + h_{fg})$. Here, it is given that $q_{i\text{-}l} = 0$.

Values of Δh_C and h_{fg}, taken from tables are 45101000 J/kg and 335000 J/kg, respectively. The value of s =4.76(6+14/4)28.84/86.17 = 15.14 kg/kg-fuel. Boiling point of n-hexane is 342.1 K

B_{OT} = [45101000/15.14 + 4390(298-342.1)]/335000 = 8.3144

$\dot{m}_F$ = (4πx0.111x0.0005)/4390) x ln(1+8.3144) = 3.93 x 10^{-7} kg/s.

Dr. V. Raghavan, IIT Madras

Now, the final example what we will see today is the mass burning rate of a 1 mm diameter n-hexane droplet. Now, burning in air at atmospheric pressure. So, what is given is no heat is conducted into the interior that is $q_{i\text{-}l} = 0$, and that the droplet temperature is equal to the boiling point, very simple. So, this is a very crude assumption what we make actually, T_s where in T_f is very high so, T_f is very high, $T_s \rightarrow T_b$ and $Y_{FS} \rightarrow 1$.

So, these are the assumptions we make correct, this is already seen $T_\infty \rightarrow \infty$ $Y_{FS} \rightarrow 1$. So, that assumption is involved here. So, here, the temperature of the surroundings which is surrounded by a flame is very high so that $T_s \rightarrow T_b$, but it cannot exceed T_b, it will go towards T_b. So, we are saying that it is equivalent to boiling point, maybe actually in a real scenario, it will be few K's below the boiling point.

Now, the ambient temperature is 298 K, but does not have any influence here only for calculating B_{OT} we will use this. Now, we need appropriate values of the properties as c_{pg} and λ and that is given here in this problem and calculated at appropriate temperature.

See for example, if you want to do this problem without knowing these values, you have to first calculate T_a which is nothing, but $0.5(T_f + T_s)$

Now, T_s is simplified for us. So, T_s is taken as T_{boil}. So, that is known. T_f we have to calculate. So, you have to again assume some values for T_f. For hexane, we can take adiabatic flame temperature and since, this is stoichiometric mixing, we can say T_f as T_{ad} at $\phi = 1$, that we can take, adiabatic flame temperature of hexane and air at say stoichiometric value you can take.

Then, we have to calculate this, then we have to use the Law and Williams correlations, these correlations to calculate the values. Once you do this basically, you will get the values of this.

If I have a constraint that T_s, you calculated the equilibrium value of T_s, then you have to iterate. So, the iterative procedure we cannot manually do, that will be very cumbersome, here you have to develop a MATLAB program or any program or you have to at least use an excel sheet to do that.

Now, mass burning rate is a very simple expression like this $4\pi r_s\lambda/c_{pg}\ln(1 + B_{OT})$. Now, we can see B_{OT} is delta h_c by s, delta h_c we have to take from the tables, n-hexane value, similarly, h_{fg} also will take from tables, q_{i-l} is given as 0, c_{pg} value is given. So, there is no issue, you can take this, so, 298 K is given, this is boiling point. It can also be taken from the tables for the hexane. So, delta h_c, h_{fg} are taken from the tables as 45101000 J/kg and 335 kJ/kg and boiling points also taken from the from the tables Stephen Turns tables, you can take those 342.1 K.

Now, if you use these values, what is the value of s? s is nothing, but the stoichiometric air fuel ratio that is 4.76 times a, a is nothing, but here $a = x + y/4$, for hexane, $x = 6$ and $y = 14$.

So, when you substitute this now, you get this value a 4.76a, 28.84 is the molecular weight of the air divided by the molecular fuel so, kg/kg-fuel, 15.14 kg/kg-fuel is s. Now, you use this to get the value of b as 8.3 and mass burning rate as 3.93×10^{-7} kg/s. So, that is the mass burning rate. So, please understand this the problem is heavily simplified. When you want to really calculate the value of equilibrium T_s, equilibrium value of T_s then iterative procedures are required as we have seen, then we have to first guess the value of T_s, then use these correlations to calculate the values, finally, check whether the Y_{FS} what we got from the expression that is the equation E is same as that we got from I, if not, then you re-guess the T_s and redo this calculation so, to get these solutions.

So, everything is iteratively done, but actually for a spherical symmetric droplet evaporation or in a convective condition where you use Nusselt number correlations etcetera iterative procedure can be used to get the appropriate values of this, but anyway proper choice of the properties c_{pg} and λ are required for this. So, this completes the topic on droplet evaporation and combustion.