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Lecture - 55

Droplet evaporation and combustion - Part 2 Equilibrium under steady evaporation of liquid droplet and droplet combustion

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So, that is what we are trying to do now equate the equations A and B, which is the mass evaporation rate is nothing but so from the heat transfer $4\pi r_s \lambda/c_{pg} \ln(1 + B_T)$. Here $4\pi r_s \rho D_{FA} \times ln(1 + B_Y)$. When you equate this, you can see that there, there is no assumption made till now and the main assumption made is the properties are constant.

$$
\dot{m} = \frac{4\pi\lambda r_s}{c_{pg}} \ln(1 + B_T) = 4\pi r_s \rho D_{FA} \ln(1 + B_Y)
$$

We have not made any other assumption like Lewis number $= 1$ or anything till now. Now, when you equate this, you can see that the $4\pi r_s$ cancels and we can write. So, bring this to the left-hand side. So, λ/c_{pg} , So, here c_{pg} D_{FA} .

So, this parameter taken to the left side, this is actually equal to the Lewis number. So, we can write this equation as $(1 + By) = (1 + B_T)^{Le}$ which is nothing but $\lambda / c_{pg} \rho D_{FA}$.

So, if you assume Lewis number = 1, if Lewis number = 1, we can say $B_T = B_Y$; but we have not made assumptions still. So, without making that assumption, we are saying that individually the properties are constant. When the properties are individually taken as constant; that means, that they can be evaluated at some average temperatures. But we have not made the assumption that Lewis number is 1. So, this assumption has not been made.

So, this appears here in this term, we can see that when you want to compare the transfer numbers, we have to compare this like this $(1 + By) = (1 + B_T)^{Le}$.

So, we can calculate, Lewis number may not be 1. See when it will be 1? If the molecular weight of the fuel is almost same as that of the ambient fluid. There are only binary fluids here. If that is the case, then Lewis number will be close to 1 or else it will not be 1.

So, that assumption has not been made. We can keep this and try to work out. So, use this equation, you know what is B_Y. B_Y is Y_{FS} - Y_{F,∞} / 1 - Y_{FS} and B_T, you know c_{pg}(T_∞ - T_s)/h_{fg}. So, when you substitute this, you can find Y_{FS} as a function of T_s or other way also. So, that is what we are going to do this.

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So, using this, mass fraction of the fuel at the interface can be written like this. So, Y_{FS} is written in terms of a T_s here. So, Y_{FS} = $(1 - Y_{F,\infty}) / (1 + B_T)^{L \cdot c}$. So, that is what we are trying to do. So, you can calculate Lewis number based upon the properties.

So, now, if you want to get the value of T_s , you can also write this equation by keeping T_s as unknown. So, this is the equation C, which actually couples the heat and mass transfer. So, that is what we want. So, once you know what will be the equilibrium temperature.

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

So, you know the value of T∞, you know the value of hc_{pg} and Lewis number, then h_{fg} at this, you can take very close to 0. So, this you can even neglect it. So, take it to 0, $Y_{F,\infty}$. So, T_s is an unknown here. So, what we can do is what is the equilibrium temperature for a given T_{∞} , that is a particular temperature which will be T_s and that will obey this equation.

Do you understand? So, when you try to equate these two, there is a particular temperature T_s which will give a value of the mole fraction. See for example, T_s you get the saturation pressure at this T_s , from this T_s . So, once you know the T_s value, you can get the saturation pressure at the T_s. So, this will give you the mole fraction of fuel which is saturation pressure at T_s/p , total pressure p.

Now, mole fraction will lead us to mass fraction and once mass fraction is known, you get this value. So, there is a only particular value of Y_{FS} , when you have a particular T_s so that will obey this equation. So, that is what the equation is.

So, this equation C is very important and that illustrates that the balance between the heat and mass transfer and that will allow us to calculate the equilibrium surface temperature and the corresponding fuel mass fraction at the interface.

Now, we can see that if $T_{\infty} \to \infty$; so, very large value. What happens here then? This denominator will be 0 here; so, $Y_{FS} \rightarrow 1$.

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Now, if you take $h_{fg} \rightarrow 0$ that will happen at critical condition. So, when the pressures are high and you reach the critical temperature and critical pressure conditions, then $h_{fg} \rightarrow 0$. So, we know this.

So, you take any phase diagram, so this is a critical point, where the h_{fg} is 0. So, all other points, you can see based on your pressure say p_1 etcetera you have these regimes here. So, this is p_2 and so on and this is the critical isobar p_c , you will see that is a critical point. So, the corresponding temperature being T_c , where $h_{fg} = 0$. So, now, in these regimes, where the pressures are lower than the critical pressures etcetera there is a definite saturation temperature say T_{sat}.

Now, here if this is say corresponding h, this is the vapor state. So, this is h_g and this is liquid; so, this is h_f , then there is a difference in this. So, h_{fg} will be equal to h_g - h_f . Now, at the critical point, you will see that $h_f = h_g$; that means, $h_{fg} \rightarrow 0$, when you reach the critical point and h_{fg} \rightarrow 0, then 1 plus this will be ∞ . So, this denominator will be infinity. So, again Y_F will tend to 1.

So, Y_{FS} \rightarrow 1 under two conditions; T_∞ $\rightarrow \infty$ or h_{fg} \rightarrow 0. So, we do not go to this critical point. So, when you are in the equilibrium regime, there should be a definite value of h_{fg} ; positive value of hfg should be prevailed. So, that is very important thing. So, this is first thing you get from this relationship.

Second one is since the mass fraction of the fuel vapor at the droplet surface is a function of T_s , Y_{FS} is a function of T_s , the values of this may be evaluated by solving the equation C. And we need one more equation that will relate the Y_{FS} and T_s . So, that is called thermodynamic relation, which will relate see that is what I have written here.

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

Once you know the value of T_s or at least guess a value of T_s , you will be able to find the saturation pressure p_{sat} at that value of T_s . So, that relationship is called the thermodynamic relation, one of them is the Clausius, there are several relations; one of them which is actually applicable for ideal gases is Clausius - Clapeyron equation.

Clausius Clapeyron equation, we will actually one problem worked example with this. So, now, this is the Clausius Clapeyron equation in which you can see that the mole fraction of the fuel at the interface is nothing but the saturation pressure by the total pressure that is the pressure ratio. Partial pressure equal to exponent of the latent heat vaporization of the fuel divided by the specific gas constant.

So, this is nothing but R_u divided by the molecular weight of the fuel, specific gas constant of fuel into $1/T$; any temperature. So, this p_{sat} at any temperature T, I am going to get that T unknown as a known temperature, but I will get the value of p_{sat} . Now, boiling point of the fuel also is there. So, we see that if temperature $T = T_{\text{boil}}$, what happens? This is 0; so, this will be 1; that means, X_{FS} will be equal to 1.

So, as T, this is surface temperature; say this is surface temperature and this when surface temperature is increased very close to boiling point, as I told you it may not reach the boiling point.

So, it tends to boiling point, then $X_{FS} \rightarrow 1$. So, this is the Clausius Clapeyron equation thermodynamic equation relationship which connects the saturation pressure and temperature; unique relationship between the saturation pressure and the temperature. So, that is the equation. So, this and this if you use this C and this D, if you use, you can get the values of the Y_{FS} and T_s.

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O Interface Quantitie The equilibrium temperature, T_s , for various values of the ambient temperature, may be determined using the below procedure: $410V$ $T_{6} = \frac{4}{310^{k}}$ First a value of T_s is assumed 1. First a value of T_s is assumed
2. Using the thermodynamic relation (equation (b)), the saturation
pressure at T is evaluated pressure at T_s is evaluated. $P_{AB}(1)$ The mole- and mass-fractions of the fuel at the droplet surface \mathcal{R} are calculated. The values of $\overline{B_T}$ and B_V are calculated. $\overline{4}$ 5. Substitute these values in Equation (C) and determine if the equation is satisfied. 6. If Equation (C) is not satisfied, the value of T_s is adjusted and steps 2 to 5 are repeated until Equation (C) is satisfied. $y_{p} = \frac{1}{\sqrt{2\pi}} \int_{x_{p}}^{x_{p}} \int_{x_{p}}^{x_{p}} f(x + (1 - \frac{x_{p}}{2})) \, dx$

The procedure for calculating the equilibrium temperature is as follows. So, you fix the ambient temperature. At any given ambient temperature, we can do this. So, let us do this. First you assume the value, you do not know the value of T_s . So, let us say, you take any fuel.

For example, say n-heptane the boiling point of this will be say 371 K. So, now, I can assume T_s at the surface can be say 360 K. This is assumption made because I know that it will never reach the boiling point.

So, this is boiling point of n-heptane is 371 K. So, this T_s will be close to boiling point based upon the ambient temperature. See for example, now ambient temperature T_{∞} is say only 350 K. Now, there are scenarios you have to understand this guess is very important.

So, let us take. So, there are three temperatures I have; so, T∞, T_{boil} and T_s. Now, out of the three temperatures, this 350 K, If I will put for this and my boiling point is 370 K; then, the surface temperature cannot exceed this T_{∞} .

So, surface temperature can be guessed as say 340. So, definitely it should be less than the T_{∞} , that condition we have to understand. So, T_s will be less than the T_∞. Evaporation, please understand in the evaporation scenario. I fix the T_{∞} ; now T_{∞} is fixed actually less than the boiling point.

Boiling point is 370 and 350 is the ambient temperature I am fixing. So, evaporation will take place, but the surface temperature will not exceed the boiling point. So, it will not even go close to that because ambient temperature itself is less than the boiling point.

Now, if I say a scenario where the T_{∞} is taken as 400 K which is actually greater than 370 which is the boiling point. Then, I may reach the temperature close to, I cannot exceed boiling point.

Please understand, I may go to 360 K here. So, please understand that T_s can be either less than the ambient temperature T_{∞} , if the T_{∞} itself is less than the boiling point or it may be less than the boiling point, if the ambient temperature is more than the boiling point.

So, this is the important thing you should remember to guess the value of or assume the value of T_s. So, if the situation is 350 K for T_∞, I cannot guess T_s as 360 K because I cannot say that the boiling point is 370 K, I am taking temperature less than that; that is not possible.

So, either seeing the scenario, if T infinity itself is less than boiling point, you have to take a temperature of the surface as it will be actually less than the $T_∞$ which is less than the boiling point or otherwise, if T_∞ exceeds the boiling point, then my surface temperature cannot exceed the boiling point.

So, it should be less than the boiling point. So, that is it. So, you cannot say that now ambient temperature is more, so the droplet surface temperature can exceed that boiling point to reach that, it is not possible.

So, keep that in mind, these two situations and first value of T_s , T_s is assumed based upon this. Then, use the equation D that is the Clausius Clapeyron equation here. Clausius Clapeyron equation is equation D thermodynamic relationship and find the saturation pressure p_{sat} at this Ts. Now, psat is known. So, find the mole fraction.

So, once you know equation D is used again. So, p_{sat} is calculated or X_{FS} is calculated straight away; the mole fraction of the fuel. So, now you know the mole fraction. So, you have X_{FS} is calculated as p_{sat}/p at T_s/p . So, now, you know this. So, what is the molecular weight of the mixture? Molecular weight at the interface will be equal to X_{FS} into molecular weight of the fuel plus 1 minus X_{FS} into molecular weight of the ambient gas A.

Now, you know this now find Y_F ; Y_{FS} , molecular weight of the mixture is known and find Y_{FS} . So, that is what I have told that mole and mass fraction of the fuel at the droplet surface are

calculated. So, straight away the Clausius Clapeyron equation will give you the mole fraction; calculate the molecular weight of the mixture and calculate the mass fraction. So, that is done. Now, you know the mass fraction of the fuel, go back, calculate the values here. So, this B_T and BY, you can calculate and use this equation and see whether this equation is satisfied; correct? So, calculate the values of B_T and B_Y and see whether equation C is satisfied or not because we have guessed the value of T_s , that will give a value of Y_{FS} . But if you calculate Y_{FS} using equation C, that may not be the correct value what you get here.

So, this may not satisfy. So, that is a unique combination of T_s and Y_{FS} which will satisfy the equation C. So, that is not going to be there here. So, you will not get the value here. If you do not get this, then your assumption of T_s is not correct. Now, what you do is the T_s value is adjusted or iterated and the steps 2 to 5 are repeated to get the convergence of equation C, that is equation C should be finally satisfied.

So, let us say for heptane itself, the second case let us take T_{∞} is 400 K and T boiling point is 370 K. Now, your T_s can be say 360 K. I am just giving some idea; 360 . So, as ambient temperature increases, your T_s will increase.

So, this iterative procedure to calculate the value of T_s for corresponding Y_{FS} values. So, that is the equilibrium condition at which; so, once you get the T_s and Y_{FS} value, then you calculate using any equation. Like for example, this; any one of this, you can use to calculate the mass evaporation rate. So, accurate value of B_T , if you want to calculate B_T , you will have to know the value of say $c_{pg} T_{\infty}$ - T_s.

So, T_s value should be known to you calculate B_T . If you calculate B_Y , you know this value, again Y_{FS} is required for this. So, once you calculate the correct equilibrium values of T_s and YFS, you can get the mass evaporation rate using one of these equations. So, this is what the procedure which is used to calculate the interface quantities that you have to guess the value of T_s and understand, that I will repeat once again.

When the ambient temperature is less than the boiling point, your T_s should be less than the ambient temperature; when the ambient temperature is more than the boiling point, your T_s should be less than the boiling point. So, it cannot exceed the boiling point.

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Now, again this is the curve what we have basically seen I can do the exercise for several ambient temperatures T_{∞} . So, you can see that the equilibrium temperature T_s for various ambient temperature is shown in this graph. So, these lines; so, this is say, $T_{\infty 1}$, this is $T_{\infty 2}$ and so on.

So, several T[∞] values I get and I plot this. Now, what is this curve? This curve is nothing but the equation C which is this equation; so, equation C. So, when I try to calculate Y_{FS} as a function of T_s etcetera you get this equation. So, this is Y_{FS} as a function of T_s , I plot this. So, I will vary the T_s and try to get this curve Y_{FS} .

Now, this dark line, this dark line represents the equation D; thick black line, this is the Clausius Clapeyron equation. Now, what are the equilibrium temperatures? These intersections are the equilibrium temperatures. Graphically, these are the equilibrium temperatures. So, you can see that the equilibrium temperature T_s values, these are T_s . So, this is say corresponding to; so, for example, this is T_a , $T_{\infty 1}$. Now, this will be the corresponding T_{s1} .

So, T_{s1} corresponding value, this T_{s1} is the equilibrium value for the T∞1, then similarly T_{∞2} corresponding T_{s2} and so on. So, this will be the corresponding equilibrium temperature. The intersection of these curves with this Clausius Clapeyron equation, it will be the T_s .

Now, you can see that as T_{∞} increases the T_s also increases; but please understand that it cannot exceed the boiling point.

So, always I have considered the temperatures basically you can see that always the T_s is less than the boiling point, $T_∞$ itself can be less than boiling point in some scenario. If that is the case, then the T_s cannot exceed T_{∞} itself. So, there are two things which you have to understand in this.

Graphically I am trying to show you the procedure, what you do I have illustrated here like assuming the value of T_s , you calculate the Clausius Clapeyron equation, calculate the p_{sat} and find the mole and mass fractions, then calculate the transfer numbers, then use the equation verify the validity of equation C.

If not, adjust the value of T_s and iterate. Graphically, equation C are several curves based upon the T[∞] value, fixed T[∞] value you get curves for equation C and those curves should intersect the equation D which is the Clausius Clapeyron equation.

Corresponding to that is intersection for a given T_{∞} , we will get the value of T_s . Now, this is about the evaporation, where you try to find the equilibrium values of the surface quantities like T_s and $Y_{F,\infty}$. Once you get that, you will get the equilibrium evaporation rate or steady evaporation rate m dot.

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So, let us move onto droplet combustion. Again, we will assume the problem to be spherically symmetric. So that means, the droplet is spherical and a flame surrounds a droplet. So, what happen if you just ignite the droplet which is evaporating? Then, a diffusion flame is established around the droplet.

So, there is a flame which is established around the droplet and this is the flame. So, this is diffusion flame. Now, you can see that this is also a spherical, I will say spherical again here. So, droplet is spherical, the flame which is surrounding droplet is also spherical. The radius of the droplet at any time instant say r_s and the flame surrounds the droplet and its radius say r_f . So, the ignition source on evaporating droplet will create a flame over the droplet and the flame sustains at radius r_f . So, this is the scenario at a given time instant. So, what happens is fuel

from this droplet surface goes to the flame and the ambient air from the ambient or the oxidizer comes to this and products are formed here.

So, that is what the diffusion flame nature is here. So, you can see this when this burns it reduces the droplet diameter. So, what happens is the same type of this. So, if you say d^2 versus time in this spherical coordinate and if it is a steady burning, steady droplet combustion I say steady burning problem, you can see that there will be a constant rate; the rate at which this burn is a constant.

So, whatever assumption we have made for the evaporation will be there, we can also make few assumptions here. So, when you talk about the structure of this flame it is like this. So, you can see this is the droplet surface r_s and the flame radius r_f . Please understand that this is a very thin flame basically, but I have given a finite thickness here.

In practice, there will be some finite thickness. So, I have exaggerated and shown the thickness here. So, what happens is you can see that the fuel from this mass fraction of the surface Y_{FS} goes and consume it, it is fully consumed at the flame zone. Similarly, oxygen from the ambient is consumed at the flame zone like this.

So, fuel and oxygen are consumed, where the fuel and oxygen are consumed you can see that the product has the maximum mass fraction there and the product actually diffuses in this zone. This is called a zone between the flame and the surface. So, this zone, I call as inner zone between the flame and the surface of the droplet.

The outer zone is obviously the ambient, from the flame to the ambient, it is called outer zone. The product also is transported to the ambient. So, the product which is formed at the flame zone, maximum value is diffused towards the inner zone and transported towards the outer zone.

So, oxygen is actually transported towards this zone and you can see that the oxygen cannot penetrate the inner zone, fuel cannot go to the outer zone because its consumed within the flame zone.

Temperature also is maximum because the reaction is completed in the flame and you can see the temperature decreases towards what is called T_s, surface temperature. Again, please understand like in steady evaporation problem, a steady combustion problem that has a definite value of T_s and Y_{FS} , equilibrium values.

Again, we can say that the equilibrium prevails. So, we will make the assumptions more clear in the next slides. Now, once the temperature is maximum here, it actually decreases towards the surface to reach the equilibrium temperature T_s and towards the ambient, it again decreases to reach the ambient temperature T_{∞} at a far-off radius.

So, this is the structure of the droplet flame and the radial structure profiles. So, fuel from the droplet surface $r = r_s$ basically reaches the flame zone by both convection and diffusion. Fick's law, we have seen that. So, this is like actually the flame separates the part.

For example, the ambient temperature will not have any influence now. In the previous case, evaporation case, only the ambient temperature actually was the driving force for evaporation. In this case, the flame itself is there which has higher temperature. Now, you can see that the surface temperature can be larger than the ambient temperature.

In the previous case, what we told was the surface temperature cannot be larger than the ambient temperature. Then, if the ambient temperature is less than the boiling point, then the surface temperature cannot exceed the ambient temperature; if the ambient temperature is more than the boiling point, then the surface temperature cannot exceed the boiling point.

So, in this scenario, we can see that there is no influence of the ambient temperature because of a high temperature, this is the flame temperature T_f that high temperature zone is there in between the droplet surface and the ambient. Similarly, the oxygen from the ambient is transferred towards the flame and it is consumed completely in the flame zone. So, this is the typical structure.

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Now, like in any diffusion flame the transport processes are going to control the combustion zone; How fast the fuel is diffused; how fast the ambient air comes to the flame zone etcetera will control the flame zone location etcetera. But if you see in this case, additionally the evaporation process also is there; like the rate at which there is heat and mass transfer occurring to the droplet surface that also will be.

So, this is heterogeneous in nature because this has to cause a phase change basically and this process is slower, these processes are much slower than the chemical kinetics. So, that means that I do not need chemical kinetics at all to analyze a droplet combustion problem, especially when it is surrounded by a diffusion flame like this.

So, this problem can be analyzed by considering only transport process in mass and energy conservation equations, as done in the simple chemical reacting system SCRS. We already discussed that.

So, we need not invoke any chemical kinetics here. So, that is one of the things. Then, just some characteristics, we will see. When a flame surrounds the droplet, this is similar to the scenario of droplet evaporating in a high ambient temperature environment.