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

Lecture – 56

Droplet evaporation and combustion - Part 3 Droplet combustion (simplified analysis)

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Scenario is same thing here. So, the surface temperature will be very close to boiling point because now; obviously, the flame temperature is much higher than the T_{∞} , T_{∞} will be now equivalent to flame temperature, which is much higher than the boiling point. So, you will see that the surface temperature here will reach a closer value to the boiling point, but it cannot exceed the boiling point again.

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Droplet Combustion

In general, the transport processes, and more specifically the evaporation process in this heterogeneous case, are much slower than the chemical kinetics. Therefore, this problem may be analysed by considering only the transport processes involved in mass and energy conservation equations, as done in SCRS. Further, when a flame surrounds the droplet, it is similar to a droplet evaporating in a very high ambient temperature environment. However, in the case of droplet evaporation, the ambient fluid (oxidizer) reaches the droplet surface due to diffusion. In the case of droplet combustion, in contrast, oxygen is consumed in the flame zone and the products of combustion, formed in the flame zone, diffuse towards the droplet surface. In the steady burning regime, even when a flame surrounds the droplet, the surface temperature is a few degrees less than the boiling point of the liquid. Dr. V. Raghavan, IIT Madras

So, the problem in hand is nothing but, it is similar to the droplet evaporating in a high ambient temperature environment; there is a difference yet. What is that? If you have a droplet evaporation alone, then you can see that the oxidizer will come to the droplet surface. The ambient fluid which is the oxidizer reaches the droplet surface because there is no reaction; so, it reaches droplet surface.

However, when there is a droplet combustion and the flame zone prevails it actually separates the gas phase into two regions. So, oxygen or oxidizer cannot now penetrate into the droplet. So, nitrogen can penetrate, but oxygen cannot penetrate across the flame to the surface; in the region between the surface and the flame there will be no oxygen.

So, oxygen is consumed in the flame zone and the products are formed, products of combustion are formed in the flame zone. So that means, that oxygen cannot come to this. Similarly, fuel can reach the ∞; $Y_{F,\infty}$ at a larger radius; here there is none like that, you have to see that the fuel is consumed in the flame zone.

So, outside the flame there will be no fuel left. So, these are the two differences. But, other than that you can see that when you see the inner zone it is pretty much the evaporation problem where, instead of oxidizer products actually diffuse into this zone.

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So, if you see here the inner zone alone for example, you have a surface and a flame and this flame is going to provide heat to the surface. Products are formed at the flame; so, that diffuses here. So, that is the gas which is diffusing here and the vapors are generated from the droplet surface diffuse towards the flame that is it; so, that scenario prevails here.

So, in steady burning regime when a flame surrounds the droplet as I told you the T_f will be much higher than the boiling point in general. So, in that case surface temperature is still few degrees less than the boiling point, it cannot exceed the boiling point; so, this very important. So, and T_{∞} does not have any influence here because, it is now away from the flame zone itself. So, flame temperature will have the influence plus we can say that the equilibrium burning, if it prevails due to steady burning then you can say that the surface temperature T_s will be less than the boiling point, few degrees less than the boiling point. So, this is the characteristic of droplet combustion.

So, you can see that we are assuming a one-dimensional flame which is spherical, spherically which is adhering to the droplet surface at a distance say r_f from the center of the droplet. And, this as the droplet regresses basically you can see that the steady evaporation range is formed. Now, what happens is say diameter of droplet is going to decrease and it going to 0 value, then the flame will reduce to a 0 value. So, till that some vapors will be there. So, first the droplet diameter will shrink to a 0 value. So, that is the lifetime, then the flame or the whatever fuel which is left over, the flame radius which is higher than the droplet radius that will reduce to 0 value.

So, that is the way we will see this, but everything happens in steady state. So, at any particular diameter if you want to see the rate at which it burns, that will be the same at all the diameters. (Refer Slide Time: 04:15)

Now, let us do some simplified analysis of droplet combustion, simplified analysis in which the assumptions are made. So, lot of assumptions we are going to make, as I told you spherically symmetric flame exist over a spherical droplet.

So, again this assumption will make us to go only for a one-dimensional analysis; radial coordinate. Then the burning process is quasi steady; that means, even when there is a regression of the droplet surface, at every time instant the burning rate is the same. So, burning rate is constant. Next is phase equilibrium prevails at the interface; that means, there is a definite value of T_s and Y_{FS} . Pressure is uniform and constant.

These assumptions are very important. Then, the reaction is represented by the global single step that is 1 kg of fuel react with the s kg of oxidizer to form $1 + s$ kgs of products So, you use an assumption what we make for diffusion flames. Then as I told you the gas phase is now having two zones here. The inner zone corresponding to the region between the droplet surface and the flame and this contains only fuel vapor and the products.

At outer zone, which is after the flame r_f , $r = r_f$ will consist of only the products and the oxidizer. There is no fuel present there.

And, since only two species are present in any zone, inner zone fuel and product, outer zone oxygen and products. Only two species are present in these zones, binary diffusion can be invoked. For example, in inner zone I can say D_{FP} as a binary diffusivity.

In outer zone I will say D_{OP} oxidizer and products that is it. So, this binary diffusion can be invoked. So, that there is no need of creating any diffusion coefficient or anything. Then, in order to get rid of them

Now so, these are the typical profiles what I want is try I assume that the flame is very thin and the chemical reaction or the kinetics is very fast, infinitely fast.

And, I do not take into account of radiation, which is negligible. In fact, actually the heat addition to the droplet is predominant through conduction only. So, we can neglect the radiation Then, what I have not done in the previous case, I have tried to do here; that is I am invoking Lewis number = 1 here because I have coupled this species and the energy transport.

So, in order to do that I assume that the transport coefficient, see for example, we can say the $\alpha = D$. So, actually this we can write basically as $\lambda/c_p = \rho D$. So, this is the driving force for the heat transfer and this is the driving force of mass transfer; I will say the driving forces are the same. Then finally, I also assume that all the properties are constant. So, this also I assume.

So, these are the set of assumptions which are made to simplify the complex problem of droplet combustion. Its a heterogeneous problem, please understand that here there is a liquid and there is a gas phase here and you can see that the vapors come out here.

So, that we have to understand see we do not need to solve for the liquid phase, but we have to couple the condition from the gas phase to the interface. So, the interface actually the droplet surface or what I called interface there we need some balancing conditions in order to get the value.

So, as we got for the burning rate, we use the condition of the interface m dot into h_{fg} equal to the conduction from the gas phase to the interface.

So, similar conditions for coupling the interface and the gas phase is required. Since, we are assuming that there is no flow within the liquid or the uniform temperature prevails in the liquid which is fine after the wet bulb condition is reached, then liquid phase need not be solved

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Now, these are the typical profiles what I want to generate by solving the equations. So, you can see this I have clearly divided the regime of the into two, a thin flame at rf, a thin flame. So, that is at r_f , then you can see that there is a temperature decrease towards the ambient. So, this will asymptotically reach the ambient temperature after a long time.

Then, you can see that there is a definite temperature here T_f , flame temperature and there is a definite temperature T_s which under steady condition is constant. So, you can see that this decrease is there in this. So, exponentially non-linear decrease will be there in this. So, this is the profile for the temperature in the inner and outer zone. If you take the profile for the fuel, there is a definite mass fraction of fuel.

So, once this is definite, this is also fixed. These are connected basically T_s and Y_{FS} are connected. So, there is a definite value for Y_{FS} and you can see that the Y_{FS} decreases to a 0 value at the flame. So, this is flame radius, at the flame radius it decreases to 0. Similarly, ambient oxidizer has a mass fraction of 1, this is mass fraction 1; ambient oxidizer which consists of oxygen plus nitrogen etcetera has a mass fraction of 1.

Basically, I say oxidizer and I am normalizing the mass fraction to 1. So, that asymptotically comes in and diffuses towards the flame. And, it will be consumed at the flame surface where the fuel and oxidizers are consumed you can see that products are formed. So, mass fraction of product is 1, P is product basically and the product diffuses towards this zone.

This is very important to understand because, there is only one flux here, the product cannot dissolve into the liquid phase. So, product cannot dissolve into the liquid phase. So, it can only diffuse towards this, but if you see it can be convected also in this direction. So, it has a flux in this direction. So, you can see the product can be convected also. So, in this we can say Y_F + $Y_P = 1$ and in this zone, you can say $Y_O + Y_P = 1$.

So, these are the structure, basically these profiles I want to calculate. So, I am interested in calculating 5 unknowns here. They are surface mass fraction of the fuel, surface temperature, flame radius; the location of flame for a given r_s . For a given r_s at the surface, radius I need to find, what is r_f, then the flame temperature. And, the final thing which is very important is the mass burning rate of the fuel at a particular r_s . So, r_s is fixed here.

So, for a particular r_s I am trying to do this because whatever be the r_s value, if the steady combustion occurs then at all r_s mass burning constant will be the same. Like evaporation constant there will be a burning constant, the burning constant will be the same. But, the burning rate will depend upon the radius that we can see later. So, these are the 5 unknowns; the surface quantities Y_{FS} and T_s , the flame quantities r_f and T_f and the mass burning rate.

These are the things which we need and I have clearly designated zones as the inner zone where the radius is say $r_s \le r \le r_f$, that is this inner zone. And, the outer zone is basically r_f is the flame radius is less than equal to r is less than infinity. So, you can go to any far distance.

Then, please understand as I explained here; since the products cannot dissolve into the liquid phase, you can say that the product can reach droplet surface only by diffusion. And, no net flow of products inward at the inner region is possible. So, product cannot have a flux in the inner region, net flux, so; that means, to say $\rho_p v_p = 0$, net flux of this product will be 0.

So, that we have already seen in the Stefan problem also, we have seen that the gas B only comes into the column by the diffusion, same way because only flux present there. Because, it cannot go into this liquid phase only flux is present from the surface to the ambient. So, that is the flux what we have basically here. But, in this case after this there can be a convection also. Actually, there is a flux for this to go towards the infinity because this flux basically will be added up from the convective flux is nothing but the flux which is actually convecting the product. That convective flux will be imparted to the product also; so, that will be shown here.

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Now, let us see the conservation equations, mass conservation says that I have the surface of the droplet. So, this is droplet. Now, there is a mass flux which is coming for the fuel which is nothing, but the $\rho_f v_f$ at the surface basically into area of the surface. Now, this is actually constant. So, when I say steady evaporation this is at the given r_s this is constant.

$\dot{m}(r) = \dot{m}_F = constant$

Now, this is known to me known to be constant so; that means, that at any radius, at any radial location the mass flow rate; this is the only mass rate. So, mass should be conserved. So, at any radius the mass flow rate should be same as the mass flow rate of the vapors from the droplet surface. So, mass flow rate at any radius is equal to the fuel flow rate or I say fuel vapor flow rate from the droplet surface. So, that is the conservation of mass.

So, this basically if say for example, the ambient fuel also can go into the liquid and condense and go into liquid phase, then I cannot say this. Because, then there will be a opposite direction transport also where the ambient gas also goes into the liquid. But, here since gas cannot dissolve in the liquid, we can easily say that the only convection is due to the evaporation; Stefan's velocity will induce this. This is Stefan velocity. So, ρ into that velocity in the area of cross section will give you the mass flow rate.

So, this is the conservation of the mass, the entire mixture mass. Then species conservation, as I told you let us take the inner region first; in the inner region only fuel and the product are present.

So, F and P exist and net flux of P is zero; that means, we can say that this is the equation written for fuel correct. For the product what I will write I will put $0 = (\dot{m}^{\prime\prime})_F Y_P - \rho D(dY_P/dr)$; that is all, that will be the consideration of product in the inner zone.

$$
(\dot{m}^{\prime\prime})_F=(\dot{m}^{\prime\prime})_FY_F-\rho D(dY_F/dr)
$$

So, we can see that the mass flux which is actually written as $\rho_F v_F$ at the surface. So, this is the mass flux. So, this is actually the total mass flux. So, this is the total mass flux which is actually equal to the mass of the fuel alone in this case.

So, this Fick's law, for the product I can say that the net flux of the product, this is $(\dot{m}^{\prime\prime})_P = 0$. So, that will be equal to the convective flux plus diffusion flux. So, the convective flux basically is contributed by the fuel alone.

So, this is the equation for the product. So, that anyway in the absence of that I could find this and using this I can write this equation, here I want to find this. So, multiply this by the $4\pi r^2$. So, we get this equation for the mass flow rate of the fuel. So, this is the equation what I get, but it cannot be solved easily.

So, I need to know Y_F profile and whatever we did for the evaporation problem you have to do this. So, this gradient has to be calculated and so on. But anyway, I can solve this now first order equation in $Y_F I$ get. So, first order equation in Y_F , I can solve this. So, this is constant. So, using this I can solve the Y_F profile.

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How? Now, boundary condition for the first order differential equation in Y_F what we have written here; m_F equal to minus $4\pi r^2 \rho D/(1-Y_F) \times dY_F/dr$. This first order differential equation can be solved by using two boundary condition

When $r = r_s$, $Y_F = Y_{FS}$ but Y_{FS} is the function of T_s that you have to just to keep in mind. Now, let us assume that T_f is known.

$$
\dot{m_F} = -4\pi r^2 \frac{\rho D}{1 - Y_F} \frac{dY_F}{dr}
$$

So, we will not worry about that now, we know that there are 5 unknowns. So, we have to somehow create 5 equations to solve this. So, what are the unknowns? Again we will see, Y_{FS} , Ts, the interface quantities and the flame quantities, radius and temperature of the flame and the mass burning rate. These are the 5 quantities which we are interested in.

So, we will take the equation. So, we will try to build 5 equations out of the conservation equations what we have. So, first we have taken the conservation equation of the fuel from which we have generated a first order differential equation; using the boundary conditions for the fuel at $r = r_s$ as $Y_F = Y_{FS}$ and as at the flame $r = r_f$, $Y_F = 0$. So, by using these two boundary conditions I can solve this.

Now, again conveniently the properties term I write as Z. And, the suffix f is given because I am saying that I am trying to put the constant for the fuel conservation equation. So, Z_f fuel conservation equation will be equal to $1/4\pi\rho D$. So now, if you use this and integrate the fuel conservation you get the profile with one unknown constant here.

$$
Y_F(r) = 1 + C_1 \exp\left(-\frac{Z_F \dot{m}_F}{r}\right)
$$

So, this is profile. So, how will you calculate the constant? Then you use this one of the boundary conditions; that is at the surface $r = r_s$, $Y_F = Y_{FS}$. Then you substitute here to get the value, then get the value of C_1 and update the value of the profile. So, when only one constant is there, one of the boundary condition is enough for me to use. So, use this to evaluate the constant.

So, when I say $r = r_s$, I put this $r = r_s$ here and Y_{FS} in the left-hand side I will put as $Y_F(r)$ will be Y_{FS}. So, once I put this the only unknown is C_1 , I calculate C_1 and substitute back to the profile I get this $Y_F(r)$. Y_F at any radius will be equal to $(1 - Y_{FS}) \exp(-Z_F m_F/r) / \exp(-Z_F m_F/r_s)$. So, this will be the profile.

$$
Y_F(r) = 1 - \frac{(1 - Y_{FS}) \exp\left(-\frac{Z_F \dot{m}_F}{r}\right)}{\exp\left(-\frac{Z_F \dot{m}_F}{r_S}\right)}
$$

So, you can verify the boundary conditions again what we have done earlier, when you put $r =$ r_s here; this will be Y_{FS} So, this will be Y_{FS}, I am putting $r = r_s$. So, if I put $r = r_s$ this exponential term will cancel out each other. So, we will get $1 - 1 - Y_{FS}$ which will be equal to Y_{FS} , so, that is correct. So, when you go to other condition where you put $r = r_f$, Y_F should be equal to 0. Now, from that actually I do not need that boundary condition at all to solve because only one constant. But, actually I can use this boundary condition to solve for m_F which is also unknown.

So, actually speaking based upon these conditions, for example, Y_{FS} goes to 0 like this, this is the flame zone. So, from Y_{FS} value Y_F value goes to 0 value here, this is 0.

So, based upon these two values see for example, based upon T_s , this is a function of T_s . So, based upon T_s there will be a Y_{FS} value and that will be this profile basically. Now, the mass burning rate basically can be an eigenvalue between the r_f and this. At r_f this is $r = r_f$, this is r_s and this is the function of r coordinate. So, this is Y_F .

Now, please understand that based upon the Y_{FS} value and the r_f value, m_F can be an eigenvalue. So, if you vary Y_{FS} then r_f also will vary, then m_F also will vary. So, this m_F can be got as eigenvalue between these two. So, first boundary condition $r = r_s$, $Y_F = Y_{FS}$, I have used to create a profile for this. Now, if I substitute $r = r_f$ in this, I know $Y_F = 0$; then I can find the value of m dot F.

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So, applying the boundary condition at $r = r_f$, $Y_F = 0$; then I will not get Y, I can get this as eigenvalue. But anyway, I will not keep that as the value there; either you can calculate m_F using this or in this case what I have done is I have calculated Y_{FS} itself.

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See please understand that if you go back in this equation unknowns are Y_{FS} , if you want to calculate Y_F as a function of radius what are the unknowns I have? I have this and m_F, these are the two unknowns I have; because Z_F is constant and r_s is also fixed already. So, at any r if I want to calculate the value of Y_F , I need these two quantities.

So, either I can use this equation to calculate m_F or we can use the equation to calculate Y_F . Basically, I am not going to use this to calculate any one quantity, this is one of the equations I want to generate one of the equations to calculate one of the unknowns. So, there should be 5 equations. So, I do not have I have not created any equation till now, there are 5 unknowns here, 5 variables to be solved. So, let us find one by one.

So, the first variable is Y_{FS} . So, write this equation in terms which have two unknowns here, Y_{FS} and \dot{m}_F . So, I can use this to find any one and put the equation ready for us. So, that is what I am trying to do, but I am actually putting the Y_{FS} in the left-hand side; I can also do the other one m_F also could be put in the left-hand side.

Now, I designate this equation as E. So, this has two unknowns again one of the unknown is evaluated as a function of other unknown. Now, if \dot{m}_F is known then Y_{FS} can be evaluated. So, this is the equation E, I am keeping this. So, one of the equations is generated correct. So, please understand that out of the 5 unknowns, what I want?

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

I need to generate 5 equations, now I have created one equation; equation E is the first equation I have created. Now, let us do the inner zone alone, inner zones the conservation equation of the species in which the Y_F has been taken into account. Now, at the flame sheet you know the mass conservation is what?

$$
\dot{m}_F + \dot{m}_O = \dot{m}_P
$$

See at the flame sheet what happens, fuel comes here, mass conservation, fuel comes in, then oxidizer comes in and products leave. So, this is a conservation. So, m_F and m_O , they are added and m_P goes out.

Now, I know that from the equation 1 kg fuel, 1 kg fuel + s kg oxidizer \rightarrow 1 + s kg of products; I can write this equation as $\dot{m}_F + s \times \dot{m}_F$ that is nothing, but $(1 + s) \dot{m}_F$. This is the \dot{m}_P .

So, this you can write. Now, please understand the fluxes. So, when I say these are fluxes, you can see that when I say (\dot{m}_0) ", this is in the opposite direction, it is a vector; it is in opposite direction. So, ρv. So, that vector comes in. So, in the other direction that is negative r direction and that will be equal to $-(s \times m_F")$.

Do you understand know, if you take the magnitudes here I am trying to take the magnitude of the entire mass balance; what is the mass of the fuel entering the flame in the flame zone. So, when I say mass of the fuel entering the flame, mass of the oxidizer entering the flame, mass of the products produced at the flame. So, that is the conservation, but when you see in the flux way you can see you have to see the direction.

Now, we can see that fuel is entering in the radial direction which is positive, oxidizer is entering in the other direction. So, I have to put s times the mass flux of fuel, but that should be given a negative sign because these are entering in the other direction. When I say flux, when I say the mass flow rate there please understand that I am only taking the magnitudes to conserve the mass. But when I say flux, I need to take direction properly. So, you can see that the (\dot{m}_O) " will be equal to $-(\sin F)$. For the products, fuel is going in this direction, products are also going in this direction by flux; please understand why products are going in this direction? Product has no flux in the inner side; this is flame, this is inner region and this outer region.

Since, the product only diffuses through the inner region, it cannot have a flux in the inner region; because if it has a flux at this then it should go into the liquid also. So, it has no flux in the inner region.

So, this is not there for the products. So, the products actually can have a flux in the outer region; so, you can see that (\dot{m}_P) " which is in the same direction as (\dot{m}_F) ", you can write the flux as $(1 + s(m_F)") = (m_P)$.

So, these two you should understand and also this identity is there $Y_P + Y_O = 1$. So, using this the oxidizer conservation can be written like this. So, \dot{m}_F , now you see the positive sign because, the oxygen is coming from the other direction. So, negative of negative becomes positive here. So, again you can see this I am putting this $s + Y_0$ here to get this, you can write this.

So, you take the conservation equation and substitute this value, you will get this. These are the conservation equation for Y_0 . So, first order differential equation for Y_0 , please understand that ρ D is constant, \dot{m}_F is constant here, s is also known. Now, you can solve this problem, separate the variables and integrate and solve the problem, but boundary condition have to be seen.

So, please understand that the overall mass conservation is the mass of fuel plus mass of oxidizer entering the flame zone will be converted into products, the flow rates are defined like this. So, when you take into consideration of this reaction, mass flow rate of fuel $+ s \times$ mass flow rate of fuel, that is mass flow of oxidizer will be this. But I am saying mass flow rate, then I only take the magnitude.

If I want to write in the flux terms, when you write the governing equation, I should take into account fluxes; see actually this. So, this is total flux of mass, I need to know this total flux into Y_O - ρD, that is constant; so, dY_O/dr. So, this is the equation I have from Fick's law, but I do not know m dot double dash here.

$$
\dot{m}_F = +4\pi r^2 \frac{\rho D}{s + Y_0} \frac{dY_0}{dr}
$$

So, in order to write this I am trying to do these assumptions and draw the conclusion. Once I know (\dot{m}_F) ", when I write (\dot{m}_O) " in terms of (\dot{m}_F) ", I know the value of that; so, I can write this equation. So, that is what I am trying to do here. So, once I do this then I get this first order equation which can be solved now.