

Advanced Thermodynamics and Combustion
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Module - VIII
Combustion and Flames
Lecture - 31
Droplet Evaporation and Droplet Burning

Dear learners, greetings from IIT, Guwahati. We are in the MOOCs course, Advanced Thermodynamics and Combustion, module 8, Combustion and Flames.

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So, in this module, there were 5 lectures, out of which we have covered laminar premix flame, laminar diffusion flame. Today we are going to discuss about another concept what we call as Droplet Evaporation and Droplet Burning.

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In this lecture, that is lecture number 31, Droplet Evaporation and Droplet Burning, we will touch upon the following segments, the concept of droplet evaporation through mass transfer, droplet evaporation through heat transfer, and finally, the droplet burning.

So, essentially when you look the application of this concept of droplet evaporation and burning, you may be aware that in a diesel engine combustion, we inject the fuel through a fuel injector. Fuel when it goes to the engine cylinder, this engine cylinder is already at elevated pressure and temperature that has happened during the compression stroke.

Now, at this elevated pressure temperatures, fuel is injected. Now, when the fuel comes out of the fuel injector it comes as a very tiny droplets, or the safest way to assume those droplets to be in the spherical shape and there are many or infinite number of such droplets which goes into the engine cylinders.

Now, after this droplet what we can see is that, in the engine cylinder itself there are difference due to temperatures, because already the compression temperature is at elevated pressure and temperature. So, temperature is also too high. Other aspect is that there can be possibly the effect of concentration; that means, in that cylinder there may be some pre-mixed concentration of the fuel that is one aspect.

So, when this droplet comes it sees two effects, one is the concentration difference that remains within the droplet and it is outside the droplet. Second effect is that the

temperature difference; that means, within the droplets and ambient temperatures there is also a difference.

So, there when the droplet evaporates in the engine cylinder, there can be mass transfer effect, there can be heat transfer effects. This mass transfer effect is associated with this concentration gradient and this heat transfer difference is associated with temperature difference. And side by side when the fuel ignites, so because in diesel engine there is a self ignition the fuel ignites, and there is a formation of localized flame at multiple locations.

So, in that sense, when there is a formation of flame, the two effects become predominant and this droplet starts burning. Now, when this droplet starts burning means, like the fuel already goes into combustion mode. So, when this droplet burning means initially it has fuel has come with small tiny bubbles, and finally, those bubbles disappear, combustion has completed and that we call it as a droplet burning.

And this concept of droplet burning comes into pictures when the flame is already generated within the engine cylinders. So, to get the combined effect of both mass heat transfer; that means, in a droplet burning, it leads to have a combined mass and heat transfers.

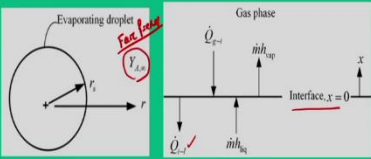
So, in our lecture today, we will touch upon some concept of mass transfer like droplets formation and evaporations, concept of heat transfer for droplet evaporation, and we will combine both of them how it gives a physical picture in the combustion mode. So, this is the essence or moral story of this lecture.

So, to start with I will talk about first on droplet evaporation by mass transfers.

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Droplet Evaporation – Mass Transfer

- The non-premixed combustion system involves the evaporation and burning of spherical liquid droplets.
- The closed form analytical solutions of governing equations allows to explore the influence of droplet size and ambient conditions of droplet evaporation/burning time.
- The knowledge of droplet gasification rates and droplet life times is important in the design and operation of practical devices.
- The evaporation of a single liquid droplet in a quiescent environment is best described in a spherically coordinate system.
- Physically, heat from ambient environment supplies the energy necessary to vaporize the liquid and the vapour diffuses from droplet surface into the ambient gas.
- The mass loss causes the droplet radius to shrink with time until the droplet is completely evaporated.



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As you can see here that when the fuel droplets can be considered as a spherically bubble, and the droplet starts and its radius keeps on changing, its radius is a variable number. I mean the size of the droplet depends on the size of the radius.

And within this spherical bubble, there is some concentration of the fuel, and outside this sphere, what we call as far field or ambient, and this concentration is something different, that is in this case I have mentioned is $Y_{A,\infty}$. So, there is a concentration difference within the sphere and the far field.

And if you look at the boundary or interface where we actually start x is equal to 0, there we can say that within the droplet it is in the liquid phase, and outside the sphere it is in the vapor phase. So, for the droplet to evaporate there must be some exchange of heat. And due to this exchange of heat, the fuel droplet diffuses into ambience. So, this is the concept of the droplet diffusion into ambience.

To summarize this droplet evaporation concept by mass transfer, I have highlighted some of the important points, and the non-premixed combustion system involves evaporation and burning of spherical liquid droplets. And for which, you need to frame the governing equations that will allow to explore the size of the droplet, ambient condition of the droplet evaporation, and burning time.

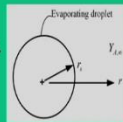
And in fact, this knowledge is required because it is very important for the design and operation of practical devices. To start with what we look at is the evaporation of a single liquid droplet in a quiescent environment and when you do that a best way to represent them is the spherical coordinate systems. So, physically the heat from the ambient environment supplies energy necessary to vaporize the liquid, and the vapour diffuses from the droplet surface to the ambient gas.

And the mass loss causes the droplet radius to shrink; that means, when it evaporates, the droplet radius shrinks to 0 size, and there we say that droplet is completely evaporated.

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Droplet Evaporation – Mass Transfer

- The determination of mass flow rate of vapour from the surface at any time instant allows to quantify the droplet radius as a function of time and the droplet lifetime.
- The mathematical model for complete process can be established with involvement of conservation laws:
 - Droplet: mass and energy conservation
 - Droplet vapour/ambient gas mixture: overall mass conservation, droplet vapour species conservation and energy conservation
- The following assumptions can be made for a simplified model:
 - The evaporation process is quasi-steady i.e. the process can be described as if it were steady state. The droplet temperature is uniform with some fixed value below the boiling point of the liquid.
 - The mass fraction of the vapour at the droplet surface is determined by the liquid-vapour equilibrium at the droplet temperature.
 - All thermo-physical properties for droplet is treated as constant.



And to do this analysis or to do this mathematical modelling, we need to involve the conservation laws for droplet where you need to recall the mass and energy conservations. We also need to recall the droplet vapor and ambient gas mixtures where we require overall mass conservations, droplet species conservation and energy conservations.

And to analyze this, we have to frame certain assumptions for our mathematical understanding. The first one is evaporation process is quasi steady. This means that process can be described as if it were in steady state. The droplet temperature is uniform with some fixed value below the boiling point of the liquid. The mass fraction of the vapor at the droplet surface is determined by the liquid vapor equilibrium at the droplet temperatures. And all the thermo-physical properties for the droplets are treated as constant.

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Droplet Evaporation – Mass Transfer

- It may be noted that the species originally in liquid phase is the species transported while the ambient fluid is stagnant. Further, the mass flow rate is constant but the mass flux follows the Fick's law of species diffusion.
- A dimensionless transfer number is defined in the expression to study the effect of vapour mass fraction on the droplet surface and far away on evaporation rate.
- When the transfer number is zero, the evaporation rate is zero and with increase in transfer number, the evaporation rate increases.

Overall mass conservation: $\dot{m}(r) = 4\pi r^2 \dot{m}''$, $\dot{m}'' = \dot{m}_A'' + \dot{m}_O'' = \dot{m}_A''$ ($\dot{m}_O'' = 0$)

Species conservation of droplet vapour: $\dot{m}_A'' = Y_A \dot{m}_A'' - \rho D_{AB} \frac{dY_A}{dr}$

Boundary conditions: $r \rightarrow \infty \Rightarrow Y_A = Y_{A,\infty}$; $r \rightarrow r_s \Rightarrow Y_A = Y_{A,s}$

Evaporation rate: $\dot{m} = 4\pi r_s \rho D_{AB} \ln \left(\frac{1 - Y_{A,\infty}}{1 - Y_{A,s}} \right) = 4\pi r_s \rho D_{AB} \ln(1 + B_Y)$

Dimensionless transfer number, $B_Y = \frac{Y_{A,s} - Y_{A,\infty}}{1 - Y_{A,s}} \Rightarrow 1 + B_Y = \frac{1 - Y_{A,\infty}}{1 - Y_{A,s}}$

r : Variable droplet radius ($r_s < r < \infty$); r_s : Liquid-vapour interface radius
 Y_A : Mass fraction of droplet vapour; D_{AB} : Binary diffusion coefficient

So, when we look at this droplet evaporation through mass transfers. What we see is that, your initial concentration which was inside the droplet was $Y_{A,s}$ which is typically maximum at the surface. r_s is nothing but the radius when it has gone to the maximum size at the surface. So, the concentration happens to be initially at this value $Y_{A,s}$, but however, ideally it should have been 1.

And when the radius keeps on increasing, when you are going along the radius, this concentration drops. That means, there is a diffusion of the droplet species into the medium. And this medium concentration was $Y_{A,\infty}$. So, here one point that I need to emphasize is the fact that we have same species which was initially in the liquid phase, and it goes to vapor phase and that species only diffuses into the medium.

So, there is no third species, only fuel, oxidizer, and product these are the 3 species. But it is only the concentration difference that happens is mainly for the fuel. I am not going to go the details into derivations. We need to recall the mass conservation. We also need to recall species conservation by invoking the Fick's law.

And important condition is the boundary conditions. Boundary conditions what we look at, $r \rightarrow \infty, Y_A \rightarrow Y_{A,\infty}$, And when, $r \rightarrow r_s, Y_A \rightarrow Y_{A,s}$ is the concentration at the surface.

So, based on this we can now find out the evaporation rate for the droplet by an expression which is the $\dot{m} = 4\pi r_s \rho D_{AB} \ln(1 + B_Y)$. So, r_s you know that it is a variable radius at

liquid vapor interface, ρ is the nothing but your density, D_{AB} is the binary diffusion coefficients.

And here we introduce one parameter what we called as B_Y , which is called in the combustion terminology as a transfer number. Basically, it is nothing but the ratio of the concentration difference at the surface and far stream. $1 + B_Y = \frac{1 - Y_{A,\infty}}{1 - Y_{A,s}}$

So, this is the transfer number. And its main significance is that the transfer number is defined with respect to mass transfer or we can say mass fraction of the droplet vapor. So, main significance is that when the transfer number is 0 evaporation rate is 0; that means, there is no droplet that gets transferred. So, that is no evaporation rate.

With increase in the transfer number the evaporation rate increases. So, this we can catch hold of from this evaporation rate expressions $\dot{m} = 4\pi r_s \rho D_{AB} \ln(1 + B_Y)$. So, here you remember the word transfer number with respect to mass transfer.

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Evaporation Rate – Mass Transfer

- The transfer number is considered as driving potential for mass transfer during droplet evaporation.
- The expression for droplet radius (or diameter) history can be found out through mass balance i.e. the rate at which the mass of the droplet decreases is equal to the rate at which the liquid is vaporized.
- In combustion terminology, transient change in square of droplet diameter is quite familiar and its time derivative is a constant quantity.

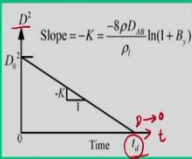
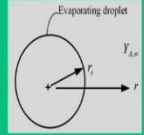
Droplet mass conservation: $\frac{dm_d}{dt} = -\dot{m}$; $m_d = \rho_l V = \rho_l \left(\frac{\pi D^3}{6} \right)$

$$\Rightarrow \frac{dD^3}{dt} = -K; \quad K = \frac{8\rho_l D_{AB}}{\rho_g} \ln(1 + B_Y)$$

$$\Rightarrow \int_{D_0}^{D^2} dD^2 = -\int_0^t K dt \quad \text{or} \quad \boxed{D^2(t) = D_0^2 - Kt} \quad (D^2 \text{ Law})$$

Droplet life time, $t_d = \frac{D_0^2}{K} \quad (D \rightarrow 0)$

m_d : Droplet mass; V : Droplet volume; $D = 2r_s$: Droplet diameter
 ρ & ρ_l : Overall density and liquid phase density; B_Y : Transfer number
 D_{AB} : Binary diffusion coefficient K : Evaporation constant

Now, once you have this transfer number, you now can see that when the droplet comes out of from the injector it has some finite diameter or size. And finally, the diameter vanishes with time. That means, when the fuel droplet evaporates; that means, the droplet vanishes, that point of time the diameter shrinks to 0 or $r_s \rightarrow 0$.

So, when that condition happens we call this as a droplet lifetime. The droplet lifetime means the droplet size which was initial diameter D_0 ; it sinks to 0 diameter at certain time span. And that time we call this as a droplet lifetime.

And so, droplet lifetime with respect to this mass transfer diffusion can be found out by considering the droplet mass conservation, which says that the rate at which the mass of the droplet decreases is equal to rate of at which the fluid is vaporized. So, $\frac{dm_d}{dt} = \dot{m}$.

So, we know that it is a spherical volume, and we also know its density and typically, we recall that the density of the droplet is in its liquid phase. So, by putting this, we can define a parameter what we call as evaporation constant and that evaporation constant is a function of this transfer number. So, $K = \frac{8\rho D_{AB}}{\rho_l} \ln(1 + B_Y)$.

Now, from this expression, we find out a relations which we normally call this as a D square law. So, square of the droplet diameter at time t is equal to its initial diameter square minus K time's t . So, with lapse of time the diameter shrinks. $D^2(t) = D_0^2 - Kt$

So, basically if you look at this particular figure, we can plot the D square versus time curve and eventually it is this equation says it is a straight line with a negative slope; that means, size of the droplet decreases with time. And what particular time t_d , this diameter goes to 0, that time we call this as a droplet lifetime.

Another point I need to emphasize is that in the combustion terminology, we use the parameter as square of droplet diameter which is more familiar rather than the droplet diameter. D square law says that it is a square of the droplet diameter which is a more appropriate term in combustion terminology.

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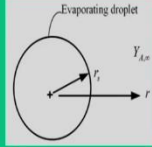
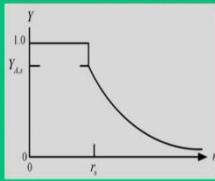
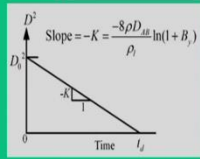
Evaporation Rate – Mass Transfer

- The transient heating of liquid does not greatly affect the droplet lifetime rather the determination of temperature at the droplet surface depends on the heat transfer to the droplet.
- The D^2 law in droplet evaporation holds good after initial transient period which says that D^2 varies linearly with time with a slope of $-K$.
- The time taken by the droplet of given initial size to evaporate completely is referred as **droplet life time**.

$D^2(t) = D_0^2 - Kt$ (D^2 law for droplet evaporation)

Droplet life time, $t_d = \frac{D_0^2}{K}$ ($D \rightarrow 0$)

D_0 : Initial droplet diameter; K : Evaporation constant

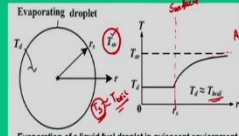
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Then moving further, it says that we define this droplet lifetime. We say that time taken by the droplet of a given initial size to evaporate completely is known as the droplet lifetime. And the D square varies linearly with time with a slope of minus K , and K stands for the evaporation constant.

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Droplet Evaporation – Heat Transfer

- The non-premixed combustion system involves the evaporation and burning of spherical liquid droplets.
- The previous discussion is dealt with a model involving mass transfer in which it is assumed that the droplet surface temperature is a known parameter.
- By introducing the fact that the evaporation rate is controlled by the heat transfer rate from ambient to surface, the droplet surface temperature may be regulated near to the droplet boiling point. It can be considered as good approximation in combustion environments where the ambient temperatures are high.
- Referring to the figure, the physical system takes heat from the ambient environment and supplies energy to vaporize the liquid fuel. It allows the fuel vapour to diffuse from the droplet surface to the ambient gas. The mass loss causes the droplet radius to shrink with time until the droplet is completely evaporated.



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Then moving further, so we now need to look into this droplet evaporation with respect to heat transfer point of view.

So, if you look at this particular figure, what it says is that same droplet it is in the conditions when it is being injected in engine cylinder, it has certain temperatures. And that temperature is T_∞ . And here we call this as a far field temperature.

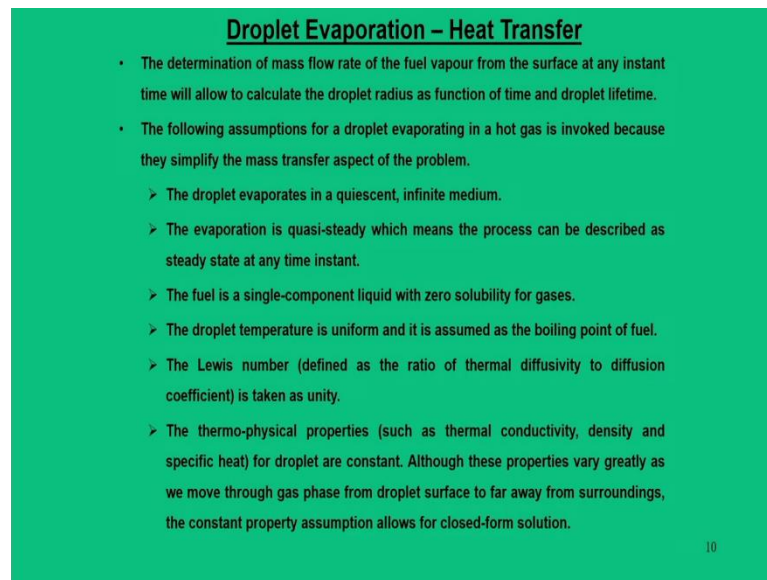
So, the droplet is seen, and ambient conditions where the temperature is T_∞ , whereas, the droplet surface temperature is T_s , and typically this T_s happens to be the boiling point which means that droplet is about to evaporate. So, at that point of time when the surface temperature is close to its boiling point, it is about to evaporate.

So, if you look at the conditions, which is at the droplet surface r_s and here we have ambient conditions, so temperature is T_∞ . So, the droplet temperature keeps on increasing. How long it will go? So, initially to start this temperature, it is at its boiling point and finally, when it goes, it can go up to maximum free stream temperatures T_∞ . So, this is the temperature distribution curve how it should look like.

So, physically what happens is that heat from the ambient environment and supplies energy to the liquid fuel. So, this energy allows the fuel vapor to diffuse from the droplet surface to the ambient gas which means the mass loss, so when this droplet evaporates there is a mass loss; this mass loss causes the droplet radius to sink with time until the droplet is completely evaporated.

So, let us see how this particular concept we are going to model. So, there in the previous study, it shows the concentration difference, in terms of mass fractions. Here it is the difference due to the temperatures.

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Droplet Evaporation – Heat Transfer

- The determination of mass flow rate of the fuel vapour from the surface at any instant time will allow to calculate the droplet radius as function of time and droplet lifetime.
- The following assumptions for a droplet evaporating in a hot gas is invoked because they simplify the mass transfer aspect of the problem.
 - The droplet evaporates in a quiescent, infinite medium.
 - The evaporation is quasi-steady which means the process can be described as steady state at any time instant.
 - The fuel is a single-component liquid with zero solubility for gases.
 - The droplet temperature is uniform and it is assumed as the boiling point of fuel.
 - The Lewis number (defined as the ratio of thermal diffusivity to diffusion coefficient) is taken as unity.
 - The thermo-physical properties (such as thermal conductivity, density and specific heat) for droplet are constant. Although these properties vary greatly as we move through gas phase from droplet surface to far away from surroundings, the constant property assumption allows for closed-form solution.

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So similar philosophy we are going to allow. So, first thing we need to determine the mass flow rate of the droplet of the fuel vapor. Second thing we must calculate the how the droplet ratio varies with time. And finally, we are going to calculate the droplet lifetime. But here the concept eventually is between the balancing the heat transfer equations.

In similar philosophy, the following assumptions were considered. The droplet evaporates in a quiescent and infinite medium. The evaporation process is quasi-study which means the process can be described as the steady state at any time instant. The fuel is considered as a single component liquid with 0 solubility for gases. The droplet temperature is uniform and it is assumed as the boiling point of the fuel.

And here also there is a parameter called as Lewis number which is defined as the ratio of thermal diffusivity to the diffusion coefficients. So, there is no mass transfer, but both the ratio is unity, Lewis number is unity means both have same effect.

The thermo physical properties such as thermal conductivity, density, specific heats for the droplet are treated as a constant. Although, they vary with respect to surroundings, but our assumption talks about the constant property situations to allow for closed form solutions.

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Droplet Evaporation – Heat Transfer

- Based on the assumptions, it is possible to obtain the mass evaporation rate, the droplet radius history by invoking gas-phase mass conservation and gas-phase energy equation, droplet gas-phase interface energy balance and droplet liquid mass conservation equation.
- Referring to the figure, the heat is conducted to the interface from hot gas is used completely to vaporize the fuel and no heat is flowing into the droplet interior.
- The droplet temperature is uniform with boiling point of fuel ($T_d = T_{\text{boil}}$)

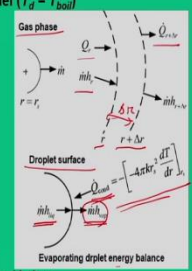
Mass conservation: $\dot{m}(r) = \dot{m}_f = \rho v_f (4\pi r^2) = \text{constant} \Rightarrow \frac{d(\rho v_f r^2)}{dr} = 0$

Energy conservation: $\frac{d}{dr} \left(r^2 \frac{dT}{dr} \right) = \left(\frac{\dot{m} c_{pg}}{4\pi k} \right) \left(\frac{dT}{dr} \right)$

Boundary conditions: $r \rightarrow \infty \Rightarrow T = T_\infty$; $r \rightarrow r_s \Rightarrow T = T_d = T_{\text{boil}}$

Evaporation rate: $\dot{m} = \frac{4\pi k_g r_s}{c_{pg}} \ln(1 + B_g)$; $B_g = \frac{c_{pg}(T_\infty - T_{\text{boil}})}{h_g}$

B_g : Dimensionless transfer number based on heat transfer
 r : Variable droplet radius ($r_s < r < \infty$); r_s : Liquid-vapour interface radius
 v_f : Bulkflow velocity; h_g : Specific enthalpy difference between gas and liquid phase
 c_{pg} : Gas phase specific heat; k_g : Gas phase thermal conductivity



Now, when you do this, we need to recall about governing equations and they are gas-phase, mass conservation, gas-phase energy equations, droplet gas-phase interface energy balance and droplet liquid mass conservation equations. I am not deriving it. It is available in the books. But what I am trying to say is that how the energy balance takes place at the droplet surface and in the gas-phase.

So, what we look at? In the gas-phase so, in the gas-phase means already the droplet has vaporized. So, prior to that on the droplet surface, there is a heat or enthalpy which is the mass flow rate into h liquid, means enthalpy at the liquid state and that goes to the vapor. So, it is a latent heat.

So, that goes and that things at the same time along this droplet surface there is a Q conduction that happens. So that means, this energy is going to balance with this Q conduction that comes from this spherical bubble. And again in the gas-phase, we are looking at the certain layers after different r.

So, one is r, other is $r + dr$. So, there the difference between these two radius is δr . So, along this δr , we can find out the energy balance. Now, when you do this we can write this energy conservation equations and the boundary conditions what we look at already have mentioned $r \rightarrow \infty, T \rightarrow T_\infty$, when r is equal to r_s at the surface. We say that it is at the boiling temperatures.

So, ultimately in the end, what we are going to recall is that evaporation rate we need to find out. And if you look at this expression closely this resembles similar to that of heat transfer analysis study. But only difference that we have here the parameters involving thermo physical properties, such as thermal conductivity in the gas-phase, specific heat of the gas-phase.

Of course, radius of the droplet already was there in the previous expression what other difference that we have is the transfer number. But here the transfer number B_q is defined with respect to heat transfer. So, $B_q = C_{pg}(T_\infty - T_{boil})/h_{fg}$. So, this transfer number is defined with respect to this.

So, in other words what we say, we are able to express evaporation rate as a function of transfer number.

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Droplet Evaporation – Heat Transfer

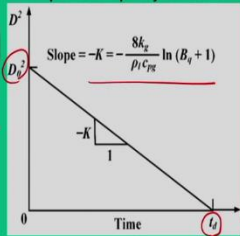
- The expression for droplet radius (or diameter) history can be found out through mass balance i.e. the rate at which the mass of the droplet decreases is equal to the rate at which the liquid is vaporized.
- The D^2 law in droplet evaporation is holds good after initial transient period which says that D^2 varies linearly with time with a slope of $-K_q$.
- The time taken by the droplet of given initial size to evaporate completely is referred as **droplet life time**.

Droplet mass conservation: $\frac{dm_d}{dt} = -\dot{m}$; $m_d = \rho_l V = \rho_l \left(\frac{\pi D^3}{6} \right)$

$$\Rightarrow \frac{dD^3}{dt} = -K_q; \quad K_q = \frac{8k_g}{\rho_l c_{pg}} \ln(1+B_q) \quad \& \quad B_q = \frac{c_{pg}(T_\infty - T_{sat})}{h_{fg}}$$

$$\Rightarrow \int_{D_0}^0 dD^3 = - \int_0^{t_d} K_q dt \quad \text{or} \quad D^3(t) = D_0^3 - K_q t \quad (D^3 \text{ Law})$$

Droplet life time, $t_d = \frac{D_0^3}{K_q} \quad (D \rightarrow 0)$



m_d : Droplet mass; V : Droplet volume; $D = 2r$: Droplet diameter; D_0 : Initial droplet diameter
 ρ_l : Liquid phase density; c_{pg} : Gas phase specific heat; k_g : Gas phase thermal conductivity
 h_{fg} : Specific enthalpy difference between gas and liquid phase
 K_q : Evaporation constant based on heat transfer; B_q : Dimensionless transfer number based on heat transfer

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Now, when you do this then we are now able to frame how a certain initial size of droplet shrinks to 0 diameter or when it completely evaporates.

So, based on this, we are now able to find the droplet lifetime t_d and by which the initial size of the droplet D_0 , its size drops after certain time, with a negative slope $-K$. And this negative slope is a function of the thermo physical properties and the transfer number. And this K here we call this as evaporation constant based on the heat transfer. And B_q is the dimensionless transfer number based on heat transfer.

So, based on this we are now in a position to express the evaporation constant K_q and the transfer number B_q . From this we can recall the mass balance expressions in a transient study. We say that rate at which mass of the droplet decreases is equal to the rate at which the fuel is vaporized so, taking into these things.

So, we can start with $\frac{dm}{dt} = \dot{m}$. By putting its geometrical parameters and putting the expressions for the $\dot{m}$ we can arrive at the D square law, $D^2(t) = D_0^2 - K_q t$. And this is also a linear relation.

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Droplet Burning

- The extension of mass transfer and heat transfer of droplet evaporation leads to subsequent development that includes a spherically symmetric diffusion flame that surrounds the droplet.
- The uniform temperature on the droplet surface is relaxed which requires species conservation in the gas phase.
- The following assumptions would lead to a simplified model of droplet combustion that preserves flow physics and agrees well with experimental results.
 - The burning droplet is surrounded by a spherical symmetric flame and it exists in a quiescent, infinite medium. There is no interaction with any other droplets so that convection effects are ignored.
 - The droplet burning process is treated as quasi-steady.
 - The fuel is a single component liquid with zero solubility for gases.
 - The phase equilibrium prevails at the liquid-vapour interface.
 - The pressure is uniform and constant.
 - The radiation heat transfer is negligible.

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So, having said the droplet evaporation by mass transfer and heat transfer, we are now in a position that we can think of that situations where the droplet has already evaporated and flame has been generated, when the flame has been generated, so droplet is within the flame.

So, in a situation that within certain flame range, there may be multiple number of such droplets possible. And in this case the both temperature as well as concentrations becomes significant parameters. So, we are now going to study the combined effect of temperatures and concentration with respect to droplet evaporation and subsequently we are going to calculate the droplet lifetime.

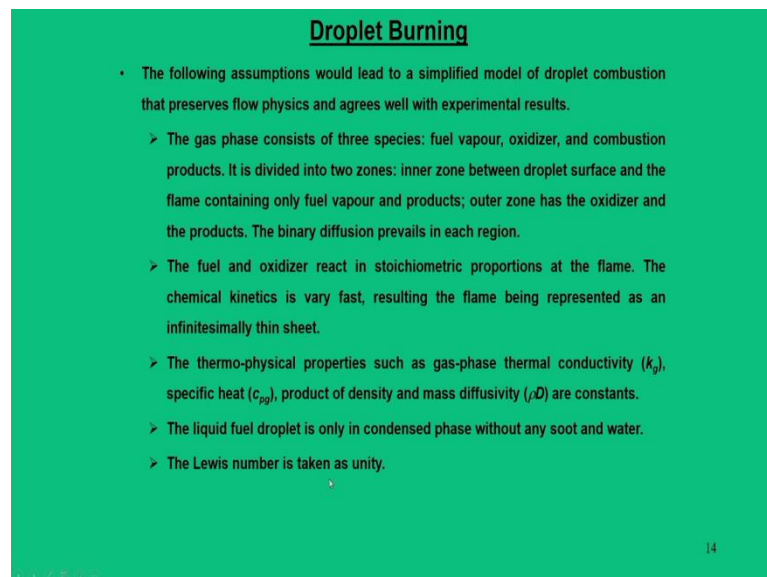
So, the extension of mass and heat transfer of droplet evaporation leads to the subsequent development that includes a spherically symmetric diffusion flame that surrounds a

droplet. Now, in this case, the uniform temperature which we assume to be at boiling temperature is now relaxed; that means, analysis becomes more complicated. But, however, there are certain assumptions that has to be considered to frame these governing equations and finding it solutions.

The burning assumptions are as follows. The burning droplet is surrounded by a spherical symmetric flame and it exists in a quiescent, infinite medium. And there is no interaction with any other droplets, so that convection effects can be ignored.

The droplet burning process is treated as a quasi-steady. The fuel is a single component liquid with 0 solubility for gases. The phase equilibrium prevails at the liquid vapor interface. Pressure is uniform and constant. Radiation heat transfer is negligible.

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Droplet Burning

- The following assumptions would lead to a simplified model of droplet combustion that preserves flow physics and agrees well with experimental results.
 - The gas phase consists of three species: fuel vapour, oxidizer, and combustion products. It is divided into two zones: inner zone between droplet surface and the flame containing only fuel vapour and products; outer zone has the oxidizer and the products. The binary diffusion prevails in each region.
 - The fuel and oxidizer react in stoichiometric proportions at the flame. The chemical kinetics is very fast, resulting the flame being represented as an infinitesimally thin sheet.
 - The thermo-physical properties such as gas-phase thermal conductivity (k_g), specific heat (c_{pg}), product of density and mass diffusivity (ρD) are constants.
 - The liquid fuel droplet is only in condensed phase without any soot and water.
 - The Lewis number is taken as unity.

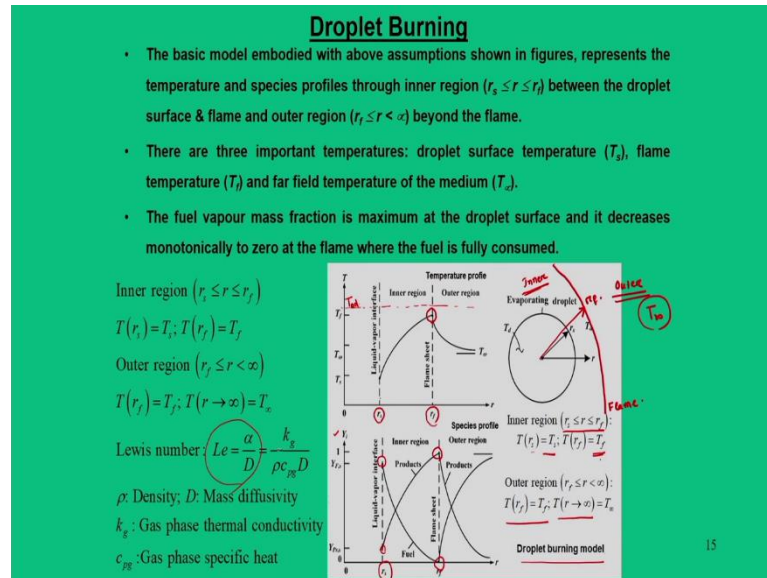
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Then, the gas-phase consists of 3 species, fuel vapor, oxidizer, and combustion products. And it is divided into two zones; one is inner zone between the droplet surface and the flame containing the fuel. That fuel containing only fuel vapor and products, outer zone contains the oxidizer and the products. And the binary diffusion prevails in each regions.

Now, when you deal with reactions, the fuel and oxidizer react in a stoichiometric proportion at the flame, the chemical kinetics is very fast, so that the flame can be treated as a very thin regions or very infinitesimally small sheet. The thermo-physical properties such as gas-phase thermal conductivity, specific heat, product density and mass diffusivity

are constants. The liquid fuel droplet is only in condensed phase without any soot and water. The Lewis number is taken as unity. So, these are the assumptions that we have for the droplet burning.

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And I need to emphasize more on this particular diagram, to emphasize what is this inner region and what is the outer regions. First to recall that this is your droplet, spherical that size changes with time. At one particular point this droplet has certain surface. And from this viewpoints, we can say that somewhere we can define a flame which are of certain radius r_f .

So, we say it is a flame which has certain radius r_f , and within this there are two zones one is inner, other is outer. And this inner range stands $r_s \leq r \leq r_f; T(r_s) = T_s, T(r_f) = T_f$.

And when you go to the outer regions; that means, when $r_f \leq r \leq \infty; T(r_f) = T_f, T(r \rightarrow \infty) = T_\infty$. Now, if you look at the temperatures things; so, this is where we have liquid surface interface at radius r_s , and this is where we see this the flame sheet at radius r_f . And within the inner regions we can see that; obviously, there will be an increase in the temperatures. How long it can increase? It can go up to the flame temperature T_f .

And typically one way to assume that maximum flame temperature could be T_{af} . So, somewhere in this domain we can drop another fixed line which we can call this as T adiabatic. So, adiabatic flame temperature may be above this line which is a fixed line. But

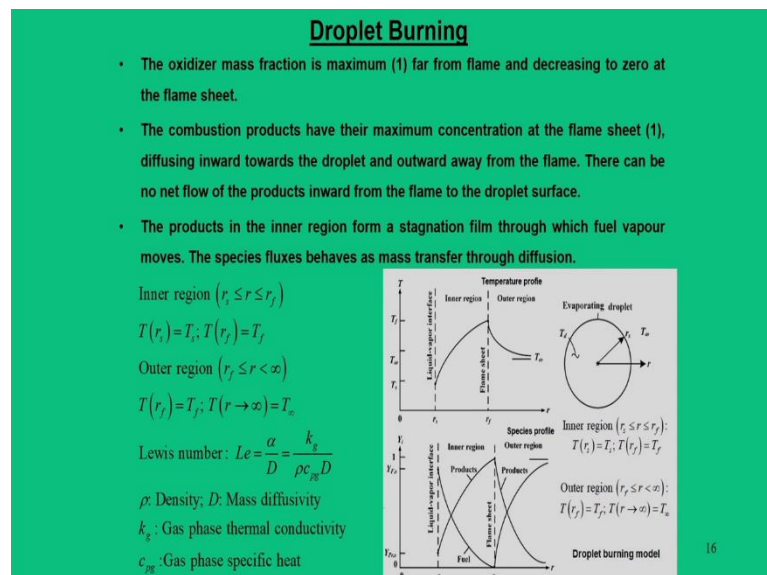
after this flame sheet this temperature again falls down. So, this is how the temperature curve and irrespective whether we have fuel, oxidizer or lean or rich. So, this is the temperature distribution.

Now, when you look at the effect with respect to concentrations, we see that in the vertical line if you talk about mass fractions and one is at r_s , at this particular surface there is no product formed, but the fuel has highest mass fractions on the surface, or close to 0 products at the r_s location.

So, with time or with increase in the radius, what happens the fuel mass fraction drops. How long it drops? It goes to 0 at the flame radius, and the same flame radius your product concentration goes up, shoots up, and it goes to close to 1. Then, that happens in the regions. In the outer regions, if you look at the product value that drops down, and whereas, on the flame sheet, again we have this concentration, this fuel concentration goes up.

So, this is what we call as a droplet burning model. And in this case, one important segment or point to be noted is the Lewis number which gives the combined effect of mass diffusivity and thermal diffusivity. So, that is the ratio means, $Le = \frac{\alpha}{D} = \frac{k_g}{\rho c_{pg} D}$.

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Droplet Burning

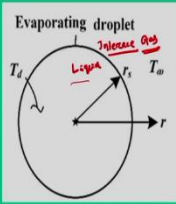
- One of the assumption involves the phase equilibrium at the liquid-vapour interface.
- The Clausius – Clapeyron equation can be invoked for equilibrium between liquid and vapour phase of the fuel at the interface.
- The partial pressure of the fuel vapour is expressed in exponential form for which the constants (A & B) are obtained from Clausius – Clapeyron equation. Subsequently, the fuel partial pressure can be related to fuel mole fraction/mass fraction.

Partial pressure of fuel vapour: $p_{F,s} = A \exp(-B/T_s)$; Fuel vapour mole fraction: $\chi_{F,s} = \frac{p_{F,s}}{p}$

Fuel vapour mass fraction: $Y_{F,s} = \chi_{F,s} \left[\frac{MW_F}{\chi_{F,s}(MW_F) + (1 - \chi_{F,s})MW_{pr}} \right]$

$$\Rightarrow Y_{F,s} = \frac{A \exp(-B/T_s) (MW_F)}{A \exp(-B/T_s) (MW_F) + [p - A \exp(-B/T_s)] MW_{pr}}$$

p : mixture pressure
 MW : Molecular weights (Subscripts F: Fuel; pr: products)
 A & B : Constants to be obtained from Clausius-Clapeyron equation



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So, based on this I have explained this, then we are now moving on to the another aspect what happens at the liquid surface or gas interface.

So, this is the interface location. So, interface location means this is a liquid and this is the gas-phase, and at interface liquid region, we define the partial pressure of the fuel vapor in an exponential manner. So, partial pressure of fuel vapor $p_{F,s} = A \exp(-B/T_s)$, T_s is nothing but the surface temperature of the droplet. And typically, one simplest way to use the value of the boiling point.

And then, at these things we can recall our earlier equations Clausius-Clapeyron equations for a two-phase system. So, this we derived when we were discussing about the thermodynamic property relations for a two-phase situation. And you can see its utility at the locations where we are seeing liquid and gas-phase, and we are looking some kind of relations which can fit to solve the fundamental concept of droplet burning.

So, here we need to recall the Clausius-Clapeyron equations. And by considering this, it is possible to find the fuel mole fractions; it is possible to find the A and B. So, all these things that has to be taken into account while solving this droplet burning equations.

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Droplet Burning

- The problem statement involves one of the objective is to determine the droplet mass burning rate for a given initial droplet size and the conditions far from the droplet.
- The other objective is to obtain expressions describing temperature and species profiles, along with the relationship to calculate flame radius, flame temperature, droplet surface temperature and fuel vapour mass fraction at the droplet surface.
- Finally, by knowing the instantaneous burning rate, droplet lifetimes can be calculated and D^2 law for burning droplets can be established.
- There are five relationship needed to solve the five unknown quantities:
 - Energy balance at the droplet surface
 - Energy balance at the flame sheet
 - Oxidizer distribution in the outer region
 - Fuel vapour distribution in the inner region
 - Phase equilibrium at the liquid-vapour interface

The diagram illustrates the energy and mass balances at two key locations in a droplet burning system:

- Flame sheet, $r = r_f$:** This diagram shows the energy balance at the flame sheet. It includes the heat flux $Q_{r=f} = -k(4\pi r_f^2) \left(\frac{dT}{dr} \right)_{r_f}$ and the mass flow rates $\dot{m}_f h_f$ and $\dot{m}_o h_o$. The text "Surface energy balance at the flame sheet" is present.
- Interface, $r = r_i$:** This diagram shows the energy balance at the liquid-vapour interface. It includes the heat flux $Q_{r=i} = -k(4\pi r_i^2) \left(\frac{dT}{dr} \right)_{r_i}$ and the mass flow rates $\dot{m}_l$ and $\dot{m}_v$. The text "Surface energy balance at liquid-vapour interface" is present.

Additional labels in the diagram include "Mass flow relationship at flame sheet" and "Phase equilibrium at the liquid-vapour interface".

So, ultimately by considering all these aspects, we need to study two things. First thing we need to determine the similar way which we call as droplet burning rate for a given droplet size, and the conditions which is far from the droplets. So, we also need to calculate the lifetime for the droplet.

So, for that droplet lifetimes needs to be calculated. D square law has to be found out. So, this is the very basic concept that we need to do. Now, to get all these things through this process what we also have to find out is the expressions for describing temperature and species profile, along with the relationship with the flame radius, flame temperatures, droplet surface temperature and fuel mass fractions.

So, this quantity needs to be found out first to arrive at D square law and other subsequent analysis with respect to droplet size and the droplet lifetime.

So, basically there are 5 equations that needs to be invoked. One is energy balance at the droplet surface, energy balance at the flame sheet, oxidizer distribution at the outer regions, fuel vapor distribution at the inner regions, phase equilibrium at the liquid phase vapor interface that we did it that in the last slide we talk about recalling Clausius-Clapeyron equations.

So, this particular picture shows the surface energy balance at the flame sheet, at the liquid vapor interface. This particular expression shows the mass flow relationship at the flame

sheet. So, basically, along this flame sheet there are two parameters which is $\dot{m}h_f$ and that is for the fuel. The other side is you have oxidizer, and we have products.

And at the interface of liquid and vapour, there is a balance of heat; that means, a specific enthalpy at the liquid state and specific enthalpy at the vapor state. There is a difference, and the difference in both the thing is nothing but your latent heat.

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Droplet Burning

- The problem statement involves one of the objective is to determine the droplet mass burning rate for a given initial droplet size and the conditions far from the droplet.

Fuel droplet mass burning rate, $\dot{m}_f = \frac{4\pi k_g r_f \ln(1+B_{fg})}{c_{pg}}$

Transfer number for droplet burning, $B_{fg} = \frac{(\Delta h_c/v) + c_{pg}(T_\infty - T_f)}{q_{c,i} + h_g}$

Fuel mass fraction at the droplet surface, $Y_{F,s} = \frac{B_{fg} - (1/v)}{B_{fg} + 1}$

Droplet surface temperature, $T_f = \frac{-B}{\ln \left[\frac{Y_{F,s} p MW_p}{A(Y_{F,s} MW_F - Y_{F,s} MW_p - MW_F)} \right]}$

Flame temperature, $T_f = \frac{q_{c,i} + h_g}{c_{pg}(1+v)} (v B_{fg} - 1) + T_i$; Flame radius, $r_f = r_i \frac{\ln(1+B_{fg})}{\ln[(v+1)/v]}$

$q_{c,i}$: Heat conducted into droplet interior per unit mass of fuel droplet
 k_g, c_{pg} : Thermal conductivity and specific heat in gas phase
 h_g : Specific enthalpy difference between gas and liquid phase
 p : mixture pressure; MW : Molecular weights (Subscripts F : Fuel; p : products)
 A & B : Constants to be obtained from Clausius-Clapeyron equation; T_∞ : Temperature at far field
 Δh_c : Specific enthalpy of combustion; r_i : Radius of droplet surface; v : Stoichiometric air-fuel ratio

Flame sheet, $r = r_f$

Interface, $r = r_i$

Liquid phase | Gas phase

Mass flow relationship at flame sheet

So, by considering this we are now framing the following relations. First one is fuel droplet mass burning rate. So, this is again with respect to thermo physical parameter k_g, c_{pg} . And one more number we recall B_{fg} and this is nothing but your transfer number for droplet burning.

And if you see this expression, this expression is different than that of other two situations like mass transfer and heat transfer. Because this analysis was done with respect to flame as well as the droplet simultaneously, so it involves the specific enthalpy of combustion.

Then, stoichiometric air fuel ratio, and this specific heat in the gas-phase and enthalpy difference between liquid and gas-phase, far field temperature and T_s . T_s stands for surface temperature. And far field temperature can be up to the T_∞ , we can have two approximations, one is this T_∞ can be at flame temperature or T_∞ can be at adiabatic flame temperatures.

So, with this one can see that what is the role of this droplet burning. And accordingly, this has a net effect in calculating the droplet lifetime. Then, we can find out the fuel mass fraction of the droplet, droplet surface temperatures, then flame temperature, flame radius. All these numbers can be calculated by knowing these thermo physical properties. And of course, we also require to know the molecular weight of fuel products and partial pressures, total pressures, fuel mass fractions and so on. So, this will give you the value of all these numbers.

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Droplet Burning

- The droplet mass burning rate in terms of transfer number is identical expression described earlier. The burning rate constant can be defined after a steady-state temperature is reached.
- Assuming transient heat-up period small, in comparison to droplet life time, the D^2 law for droplet burning can be established and droplet life time can be found.

Droplet burning rate constant, $K = \frac{8k_g}{\rho_l c_m} \ln(1 + B_{m,s})$

Transfer number for droplet burning, $B_{m,s} = \frac{(\Delta h_c / \nu) + c_m (T_s - T_\infty)}{q_{c,l} + h_g}$

D^2 law : $D^2(t) = D_0^2 - Kt$

Droplet life time : $D^2(t_d) = 0 \Rightarrow t_d = \frac{D_0^2}{K}$

Δh_c : Specific enthalpy of combustion
 D_0 : Initial droplet diameter; D : Droplet diameter; t : time
 h_g : Specific enthalpy difference between gas and liquid phase
 k_g, c_m : Thermal conductivity and specific heat in gas phase
 T_s : Droplet surface temperature; T_∞ : Temperature at far field
 ρ_l : Density in liquid phase; ν : Stoichiometric air-fuel ratio
 $q_{c,l}$: Heat conducted into droplet interior per unit mass of fuel droplet

Interface, $r = r_f$

Liquid phase	Gas phase
$\dot{m}_l h_{l,s}$	$\dot{m}_g h_{g,\infty}$
$\dot{Q}_{c,l}$	$\dot{Q}_{f,s} = -k(4\pi r_f^2) \left(\frac{dT}{dr} \right)_{r_f}$

Surface energy balance at liquid-vapour interface

Flame sheet, $r = r_f$

$\dot{Q}_{f,s} = -k(4\pi r_f^2) \left(\frac{dT}{dr} \right)_{r_f}$	$\dot{Q}_{f,s} = -k(4\pi r_f^2) \left(\frac{dT}{dr} \right)_{r_f}$
$\dot{m}_g h_{g,\infty}$	$\dot{m}_p h_{p,\infty}$

Surface energy balance at the flame sheet

Flame sheet

$\dot{m}_g = \nu \dot{m}_f$	$\dot{m}_p = (\nu + 1) \dot{m}_f$
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Mass flow relationship at flame sheet

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Now, after knowing all these things, we will be now able to find a parameter, and here the parameter we call this as a droplet burning rate constant. This number is similar to the the previous value of K. And here what is the difference that changes is nothing but your transfer number expression that is a different number.

And this transfer number is we have to get it with the combined effect of flame as well as the droplet. So, based on this rate constant we can be able to frame the D square law and with this D square law we can find out the droplet lifetime D square by K. So, we can find out the droplet lifetime. So, this is all about the droplet burning, which talks about the combined role of heat and mass transfer during the burning of the droplet.

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Numerical Problems

Q1. Consider the combustion of n-heptane droplet with its diameter is 100 μm . Determine, the mass burning rate, flame temperature, ratio of flame radius to droplet radius at atmospheric condition. Assume quiescent surroundings and the droplet is at its boiling point.

Given: C_7H_{16} (n-heptane), $D_0 = 100 \mu\text{m}$, $T_b = 371 \text{ K}$, $T_\infty = 300 \text{ K}$, $\rho_f = 684 \text{ kg/m}^3$, $\rho_a = 1.2 \text{ kg/m}^3$, $\mu_a = 1.8 \times 10^{-4} \text{ Pa}\cdot\text{s}$, $k_a = 0.026 \text{ W/m}\cdot\text{K}$, $c_{pg} = 1.8 \text{ kJ/kg}\cdot\text{K}$, $\Delta h_c = 44926 \text{ kJ/kg}$, $\gamma = 16$, $\eta = 0.6$.

Solution:

(a) Mass burning rate, $\dot{m}_f$:

$$\dot{m}_f = \frac{4\pi D_0^2 \rho_f \eta \Delta h_c}{c_{pg} (T_b - T_\infty)} = \frac{4\pi (100 \times 10^{-6})^2 \times 684 \times 0.6 \times 44926}{1.8 \times (371 - 300)} = 3.1 \times 10^{-8} \text{ kg/s}$$

(b) Flame temperature, T_f :

$$T_f = \frac{(\rho_f D_0^2 \eta \Delta h_c) / (c_{pg} (1 + \gamma))}{[\gamma B_{op} - 1] + T_b} = 962 \text{ K}$$

(c) Ratio of flame radius to droplet radius, r_f/r_d :

$$r_f/r_d = \left(\frac{\rho_f}{\rho_a} \right)^{1/3} = 35$$

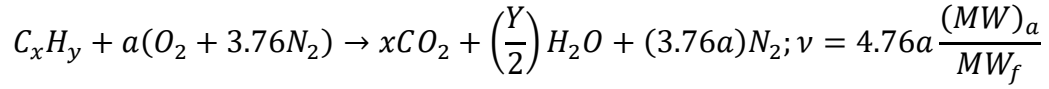
So, this concludes the lecture part for this module. And of course, towards the end we are now going to discuss one simple numerical problems based on the understanding of mainly droplet burning. So, we are going to consider the combustion of n-heptane droplet. So, the word n-heptane normally we use in the diesel engine combustions. While calculating the cetane number n takes a very crucial role, that means, it is an ideal fluid for diesel engines.

So, we are looking at the droplet of n-heptane fuel and its initial size is supposed to be 100 micrometer. We need to find out the mass burning rate, flame temperature, ratio of flame radius to droplet radius at atmospheric conditions. Assume quiescent surroundings and the droplet is at boiling point. For the solutions please refer the expressions for droplet burning. So, you have to recall the expressions for the droplet burning.

Apart from this we also need to find the data. That data refers for a fuel which is n-heptane. So, n-heptane fuel has a molecular formula C_7H_{16} and it has molecular weight 100. So, of course, molecular weight for air is 29. Then, other parameters we are looking at the quiescent surrounding, surroundings in this case we say it is T_∞ as 300 K. Surface temperature of the droplet is nothing but boiling point temperature.

And for this fuel that is n-heptane this number is 371 K. We also require $c_{pg} = 1.8 \text{ kJ/kg}\cdot\text{K}$, that is for n-heptane. Then Δh_c , that is enthalpy of combustion is 44926 kJ/kg . Other parameter require thermal conductivity $K_g = 0.026 \text{ W/m}\cdot\text{K}$. And our initial diameter is D_0 is 100 micron. So, r_s is 50 microns.

Then, what we do not know is ν which is stoichiometric air fuel ratio. To do that we have to recall this fundamental combustion equation



$$a = x + \frac{y}{4} = 7 + \frac{16}{4} = 11; \nu = 15.2$$

$$\dot{m}_f = \frac{4\pi K_g r_s}{C_{pg}} \ln(1 + B_{o,q}); B_{o,q} = \frac{\left(\frac{\Delta h}{\nu}\right) + C_{pg}(T_\infty - T_s)}{q_{il} + h_{fg}}$$

For the time being let us take this number q_{il} as 0, because at the interface both the heat balance.

So, by putting this we can find out this $B_{o,q} = 8.5$ and $\dot{m}_f = 3.1 \times 10^{-8} kg/s$. So, mass burning rate or droplet evaporation rate is $3.1 \times 10^{-8} kg/s$. Second part is flame red temperature $T_f = \frac{q_{il} + h_{fg}}{C_{pg}(1+\nu)} [\nu B_{o,q} - 1] + T_s$. Now, all the numbers is known from the data.

So, flame temperature is 962 K.

Third parameter is radius $r_f = r_s \left[\frac{\ln(1+B_{o,q})}{\ln\left(\frac{1+\nu}{\nu}\right)} \right]$. So, this will implies rf by rs which is ratio of flame radius to droplet radius. That number is 35. So, we can say droplet radius is 35 times smaller than the flame radius.

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Numerical Problems

Q2. Consider the combustion of n-heptane droplet with its diameter is 100 μm . Determine, the lifetime of the droplet. How does it compare with pure vaporization with far field temperature of 1927°C and 689°C.

Burning $B_{0,q}$ Pure Vaporization B_q

$T_\infty = 1927^\circ\text{C} \approx 2200\text{ K}$ (T_{Ad})
 $689^\circ\text{C} \approx T_\infty$ (flame temp)

$\rho_l = 684\text{ kg/m}^3$
 $\rho_g = 1.05\text{ kg/m}^3$
 $D_{0,q} = 8.5$
 $u_g = 0.6926\text{ m/s}$
 $C_{p,g} = 4.22\text{ kJ/kg}\cdot\text{K}$

(i) Burning
 $K = \frac{8K_g}{\rho_l C_{p,g}} \ln(1 + B_{0,q})$
 $K = 5.8 \times 10^{-7}\text{ m}^2/\text{s}$
 $t_d = \frac{D_0^2}{K} = 0.018\text{ s}$

(ii) Pure Vaporization
 $B_q = \frac{C_{p,g}(T_\infty - T_{\text{sat}})}{h_{fg}}$
 $T_\infty = 2200\text{ K}$
 $T_{\text{sat}} = 373\text{ K}$
 $B_q = 24.42$
 $K = 8.3 \times 10^{-7}\text{ m}^2/\text{s}$
 $t_d = \frac{D_0^2}{K} = 0.020\text{ s}$

$T_\infty \rightarrow T_f = 942\text{ K}$
 $B_q = 8.4$
 $K = 5 \times 10^{-7}\text{ m}^2/\text{s}$
 $t_d = 0.020\text{ s}$

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Now, second part of this problem, we need to find out the lifetime of the droplet, and how does it compare with pure vaporization with far field temperature of this.

So, basically we are going to compare burning versus pure vaporization. So, in this case, the difference will be the transfer number. So, we need to find out the transfer number for burning which is $B_{0,q}$ and for pure vaporization this transfer number is B_q . So, with that difference we need to compare.

Second thing, two far field temperatures that I was mentioning, one is 1927 C, this is close to 2200 K. So, typically we are calling this as a adiabatic flame temperature for hydrocarbon fuel. Other is 689 C, which refers to flame temperature in our previous question one. So, this is flame temperature.

So, if this is the situation, we are going to find what is the lifetime for this droplet. So, the problem is very simple. So, to do this, we need to find out rate constant for the droplet burning which is $K = \frac{8K_g}{\rho_l C_{p,g}} \ln(1 + B_{0,q}) = 5.8 \times 10^{-7}\text{ m}^2/\text{s}$; $\rho_l = 684\text{ kg/m}^3$

Then, subsequently we will find out droplet lifetime $t_d = \frac{D_0^2}{K} = 0.018\text{ s}$, Second thing, pure vaporization this is the part we say burning.

When you say pure vaporization, so $B_q = \frac{c_{pg}(T_\infty - T_{boil})}{h_{fg}}$. Now, T infinity can have two numbers, one is 2200 K other could be 962 K, and this is nothing but your flame temperatures as derived in the question number 1.

$$@T_\infty = 2200K, B_q = 24.42; K = 8.3 \times 10^{-7} m^2/s; t_d = 0.012s$$

So, you can see that in this case when you call about pure vaporization, we expect droplet lifetime is 0.12 seconds for which we can say there is a large difference. So, the idea of talking about $T_\infty = 2200K$ is not a realistic, rather we should see this T infinity close to the flame temperatures.

So, instead of that this particular things if you say

$$@T_\infty = T_f = 962K, B_q = 8.6; K = 5 \times 10^{-7} m^2/s; t_d = 0.02s$$

So, we can say that when our ambient condition is approximated at the flame temperatures, the pure burning model and pure vaporization model, they give a close resemblance.

So, this gives the fact that pure vaporization model with very good approximations can also lead to the concept of droplet burning. So, this is all about this lecture for today.

Thank you for your attention. Once again, thank you. So, let us close this session.