Fundamentals of Combustion

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Lecture – 61

Combustion of carbon particle – Part 3

Two-film model and worked examples

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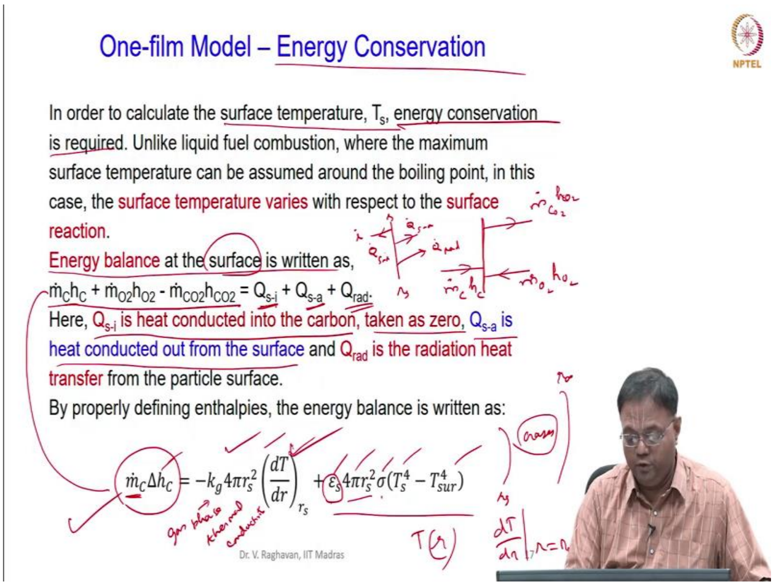

One-film Model – Energy Conservation

In order to calculate the surface temperature, T_s, energy conservation is required. Unlike liquid fuel combustion, where the maximum surface temperature can be assumed around the boiling point, in this case, the surface temperature varies with respect to the surface reaction.

Energy balance at the surface is written as,

$\dot{m}_C h_C + \dot{m}_{O2} h_{O2} - \dot{m}_{CO2} h_{CO2} = Q_{s-i} + Q_{s-a} + Q_{rad}$.

Here, Q_{s-i} is heat conducted into the carbon, taken as zero, Q_{s-a} is heat conducted out from the surface and Q_{rad} is the radiation heat transfer from the particle surface.

By properly defining enthalpies, the energy balance is written as:

$$\dot{m}_C \Delta h_C = -k_g 4\pi r_s^2 \left(\frac{dT}{dr}\right)_{r_s} + \varepsilon_s 4\pi r_s^2 \sigma (T_s^4 - T_{sur}^4)$$

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Now, to calculate surface temperature, energy conservation is required. Please understand, if you take a fuel droplet which is evaporating or burning, there is an indication for us, boiling point. When it is burning, it is nothing wrong to assume the surface temperature to be very close to boiling point, so that assumption can be made.

But here it is not possible to assume a value for the T_s. So, we have to again solve, because the T_s can be higher. So, particle can be continuously heated, and T_s can be higher also. So, there is no restriction for T_s here.

In a liquid droplet, there is a restriction that the droplet surface temperature cannot cross the steady equilibrium evaporation condition, the surface temperature cannot cross the boiling point. So, here we have to use the energy conservation to arrive at the value of T_s.

So, let us do energy balance on a surface. At this carbon surface, we will do this. So, $\dot{m}_C$ and its own enthalpy h_C. Similarly, $\dot{m}_{CO_2}$ and h_{CO2}. And here $\dot{m}_{O_2}$ and h_{O2}. So, this is the left-hand side what I am trying to do here.

So, this mix. So, this and this added together and subtracted to this. So, this this will actually go to other side basically. So, this is the chemical reaction, there will be heat released due to the chemical reaction. This can be represented by $\dot{m}_C \times \Delta h_c$, which we actually demonstrated when I did the droplet combustion.

Now, once there is a heat which is generated at the surface because here everything is completed within the surface, there is no other reaction zone. So, from the surface, there will be a heat transfer.

So, this is surface r_s, there will be a heat conduction from the surface to the interior. So, s to i is the heat conduction from the surface to the interior of the carbon particle. Then there will be a heat conduction from the surface to the ambient. So, this I will say Q_{s-a} and this will be Q_{s-i}.

Now, there will be radiation, radiation from the surface to the surrounding temperature. So, these are the two things. But in our analysis, we have made an assumption that the T_s is constant. So, at the surface, there is no temperature gradient in the particle. So, the heat conducted into the carbon can be taken as zero, because the carbon particle is assumed to be at a uniform temperature of T_s.

Now, Q_{s-a} is the heat conducted from the surface. So, we have to write a conduction equation for this, so, $-4k_g$ is the gas phase thermal conductivity. So, this $k_a dT/dr$. So, temperature decreases in the increasing radial direction, so negative sign comes for that.

And the heat is also conducted away from the surface to the ambient. So, this is positive quantity again. Now, radiative heat transfer in gray body. So, this carbon surface is assumed to be a gray body.

So, constant emissivity for the surface into the area of the surface into Stefan-Boltzmann constant σ(T_s^4 - T_{surr}^4) 4. So, this is the bulk radiative heat transfer. So, this emissivity will not change with this.

$$\dot{m}_C \Delta h_C = -k_g 4\pi r_s^2 \left(\frac{dT}{dr}\right)_{r_s} + \varepsilon_s 4\pi r_s^2 \sigma (T_s^4 - T_{sur}^4)$$

Also, one more thing here is it is not occurring in vacuum. So, please understand there is a surface, r_s, and there is a surrounding, r_∞ let us take. So, there are gases here; there are several gases present here. But we neglect the participating media here, these gases which will actually affect the radiation. Because in vacuum, we can write such a statement.

But if there are gases, then the gases also will also absorb some heat, but we neglect that. So, it is a simplified model, only the gray body radiation is taken into account, where the emissivity is taken as constant surface area × σ(T_s^4 - T_{surr}^4) that is all. It is not affected by anything else from the surface, it radiates to the ambient that is all.

So, the gases participating media affecting radiation etcetera is not taken into account here. So, this is simple energy balance I do here. So, this is the heat of reaction Δh_C, heat of combustion into the mass rate of carbon. So, this we know. This is another equation which is generated here.

Now, somehow if I can substitute for the dT/dr at the surface for which we need the profile. So, gas phase energy conservation equation we solved and try to the get the T as a function of r, T(r) profile, then I differentiate it with respect to r, dT/dr and apply that to r = r_s and I substitute here to get the value of this.

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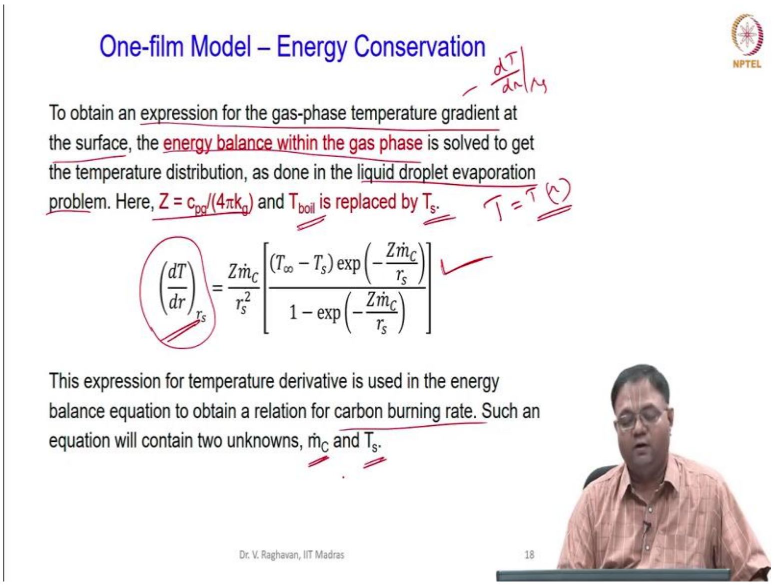

One-film Model – Energy Conservation

$- \frac{dT}{dr}\Big|_{r_s}$

To obtain an expression for the gas-phase temperature gradient at the surface, the energy balance within the gas phase is solved to get the temperature distribution, as done in the liquid droplet evaporation problem. Here, $Z = c_{pg}/(4\pi k_g)$ and T_{boil} is replaced by T_s.

$T = T(r)$

$$\left(\frac{dT}{dr}\right)_{r_s} = \frac{Z\dot{m}_C}{r_s^2}\left[\frac{(T_\infty - T_s)\exp\left(-\frac{Z\dot{m}_C}{r_s}\right)}{1-\exp\left(-\frac{Z\dot{m}_C}{r_s}\right)}\right]$$

This expression for temperature derivative is used in the energy balance equation to obtain a relation for carbon burning rate. Such an equation will contain two unknowns, $\dot{m}_C$ and T_s.

So, that is the next thing, we have already done that. So, to obtain the expression for the gas phase temperature gradient at the surface that is $(dT/dr)_{rs}$, we need to consider the energy balance within the gas phase.

It is a simple second order equation which is solved. And by using appropriate boundary conditions, we will get T as a function of r. Now, we can differentiate this and put r = r_s. We have already done it.

And whatever we have done for the droplet evaporation problem, same conservation equation and same solution is applicable here. So, by taking the Z equal to $c_{pg}/4\pi k_g$ and replacing T_{boil} by T_s here.

Then we can differentiate, the T(r) solution which is got earlier and put $r = r_s$, we get this value. So, $Z/(r_s)^2[(T_\infty - T_s)\exp(-Z\dot{m}_C/r_s)/(1-\exp(-Z\dot{m}_C/r_s)]$. So, this will be the gradient of temperature at the particle surface.

$$\left(\frac{dT}{dr}\right)_{r_s} = \frac{Z\dot{m}_C}{r_s^2}\left[\frac{(T_\infty - T_s)\exp\left(-\frac{Z\dot{m}_C}{r_s}\right)}{1-\exp\left(-\frac{Z\dot{m}_C}{r_s}\right)}\right]$$

Now, this expression is plugged into this equation here. And you get the carbon burning rate again. So, again you can see that if you write the carbon burning rate with that, you get $\dot{m}_C$ as function of T_s, again iteratively we have to solve it.

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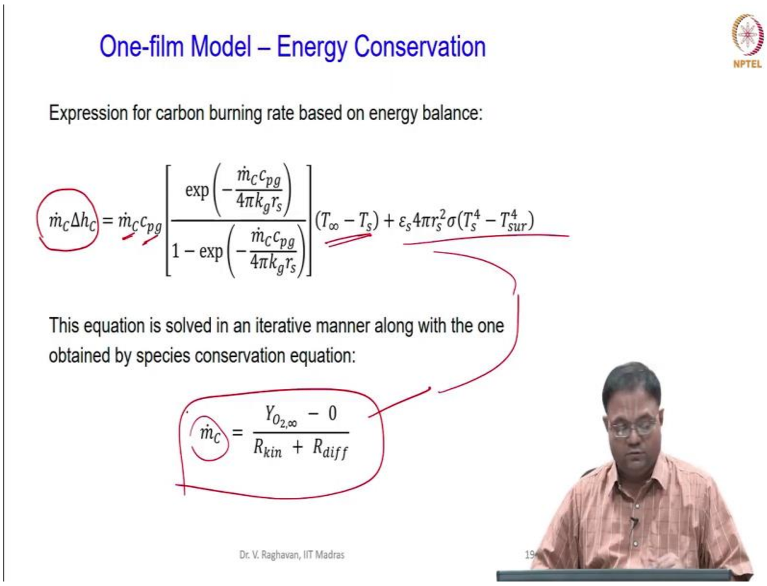

One-film Model – Energy Conservation

Expression for carbon burning rate based on energy balance:

$$\boxed{\dot{m}_C\Delta h_C} = \dot{m}_C c_{pg}\left[\frac{\exp\left(-\frac{\dot{m}_C c_{pg}}{4\pi k_g r_s}\right)}{1-\exp\left(-\frac{\dot{m}_C c_{pg}}{4\pi k_g r_s}\right)}\right](T_\infty - T_s) + \varepsilon_s 4\pi r_s^2\sigma(T_s^4 - T_{sur}^4)$$

This equation is solved in an iterative manner along with the one obtained by species conservation equation:

$$\boxed{\boxed{\dot{m}_C} = \frac{Y_{O_{2,\infty}} - 0}{R_{kin} + R_{diff}}}$$

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So, that is the equation we get. So, I just substitute that $\dot{m}_C \Delta h_C$ this equation, Δh_C equal to, now I have substituted this $(dT/dr)_{rs}$ to this here and I got this equation here. So, $\dot{m}_C c_{pg}$ into some exponential terms into $T_\infty - T_s$ plus the radiation term.

So, this is what I get. And I can see that this equation will be iteratively solved, because $\dot{m}_C$ and T_s both are unknown here. So, when you want to solve for $\dot{m}_C$ etcetera, again you have to use this. So, couple this equation plus this equation to solve for the mass burning rate of the carbon, so that is the way you solve for the one-film model.

$$\dot{m}_C \Delta h_C = \dot{m}_C c_{pg} \left[\frac{\exp\left(-\frac{\dot{m}_C c_{pg}}{4\pi k_g r_s}\right)}{1 - \exp\left(-\frac{\dot{m}_C c_{pg}}{4\pi k_g r_s}\right)} \right] (T_\infty - T_s) + \varepsilon_s 4\pi r_s^2 \sigma (T_s^4 - T_{sur}^4)$$

$$\dot{m}_C = \frac{Y_{O_{2,\infty}} - 0}{R_{kin} + R_{diff}}$$

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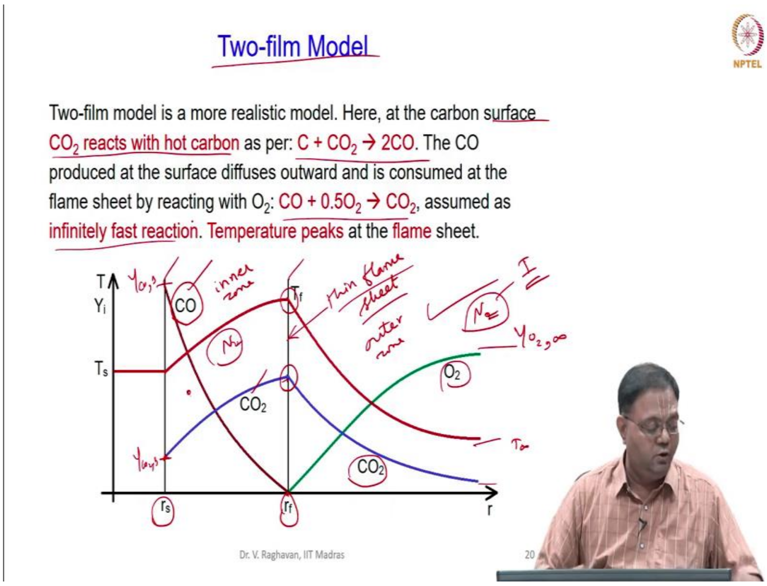

Two-film Model

Two-film model is a more realistic model. Here, at the carbon surface CO_2 reacts with hot carbon as per: $C + CO_2 \rightarrow 2CO$. The CO produced at the surface diffuses outward and is consumed at the flame sheet by reacting with O_2: $CO + 0.5O_2 \rightarrow CO_2$, assumed as infinitely fast reaction. Temperature peaks at the flame sheet.

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Next is two-film model, as I told you in this predominantly CO_2 and C reacts at the surface r_s to form CO. And CO diffuses towards the flame which is at a particular radius say r_f from the interior, then you say the gaseous reaction between the O_2 and CO occurs and CO_2 is formed there producing a peak temperature at that location, thin flame sheet.

This is a thin flame sheet. Now, the temperature diffuses towards the surface say T_f and T_s. So, that is profile here. And in the ambient it decays to the ambient temperature. So, this will be the T_∞ here. Now, carbon dioxide goes to ambient as well as it reaches surface. So, this will be the CO_2 at the surface, and this is Y_{CO} at surface. So, this is T_s what I have put here.

Now, it goes to a low value here, CO_2 goes to a low value. Oxygen from the $Y_{O2,\infty}$ goes to a 0 value at the flame. So, at the flame both CO and O_2 are assumed to be completely consumed. And this is the reaction C + CO_2 occurs at this sheet, that is a carbon surface.

So, CO_2 reacts with the hot carbon particle surface as a surface reaction and produces CO, and a homogenous reaction occurs and this is infinity fast reaction producing a thin flame sheet. So, this is the two-film model.

Why this model has been developed? Because when you measure something here near to the surface, there was actually very little oxygen or no oxygen at all measured here, so that means, that oxygen diffusion through a surface is not possible. That was one indication. And the CO_2 was higher than CO, that is another indication that CO is predominantly formed at the surface. So, based upon that this two-film model was constituted.

Again, when you increase the complexity, your problem also will be more complex. We are not going to solve everything, but we will give the procedure to solve as well as the final equation.

So, we can see that again like in the droplet combustion, there is an inner zone here where you can see that the CO_2 formed diffuses towards the surface and participates in surface reaction and CO forms there, and that diffuses towards the flame and gets consumed there.

So, oxygen is not present here. So, if you see here CO and CO_2 are the two species what we have. Go to the ambient. Ambient you have this. One more thing is nitrogen also is present. Nitrogen will be everywhere that is another complexity in this.

When you use air nitrogen will be there. Nitrogen will not be consumed here. So, nitrogen will be here and also here. So, due to the presence of nitrogen, we can see that there will be some mass fraction of oxygen, CO and nitrogen will be there, but nitrogen is inert. So, it will not participate in any reaction, but it will be there in both the zones.

So, if you do not consider nitrogen, the other species are only two species here. In the outer zone here you have O_2 and CO_2 and inert species. So, I say this is inert species, CO_2, O_2 and inert species. In the inner zone, CO, CO_2 and inert species, these are the three species what we have in the zones.

So, again what we have seen in the droplet combustion thing. But there will be only one reaction zone which is at the flame, but here there is the reaction zone at the flame which is homogenous in nature, gas phase reaction and there is a surface reaction at the surface. So, these are the two things which you differentiate between the carbon particle combustion and the droplet.

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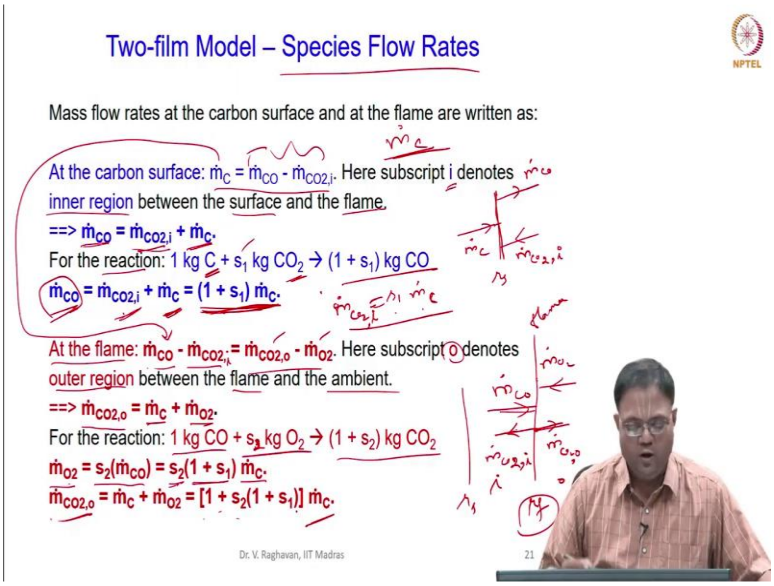

Two-film Model – Species Flow Rates

Mass flow rates at the carbon surface and at the flame are written as:

At the carbon surface: $\dot{m}_C = \dot{m}_{CO} - \dot{m}_{CO2,i}$. Here subscript i denotes inner region between the surface and the flame.

==> $\dot{m}_{CO} = \dot{m}_{CO2,i} + \dot{m}_C$.

For the reaction: 1 kg C + s_1 kg CO_2 → $(1 + s_1)$ kg CO

$\dot{m}_{CO} = \dot{m}_{CO2,i} + \dot{m}_C = (1 + s_1)\,\dot{m}_C$.

At the flame: $\dot{m}_{CO} - \dot{m}_{CO2,i} = \dot{m}_{CO2,o} - \dot{m}_{O2}$. Here subscript o denotes outer region between the flame and the ambient.

==> $\dot{m}_{CO2,o} = \dot{m}_C + \dot{m}_{O2}$.

For the reaction: 1 kg CO + s_2 kg O_2 → $(1 + s_2)$ kg CO_2

$\dot{m}_{O2} = s_2(\dot{m}_{CO}) = s_2(1 + s_1)\,\dot{m}_C$.

$\dot{m}_{CO2,o} = \dot{m}_C + \dot{m}_{O2} = [1 + s_2(1 + s_1)]\,\dot{m}_C$.

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Now, let us see the species flow rates. Now, carbon surface, so r_s, CO is formed and that goes away like this $\dot{m}_{CO}$. CO_2 which is formed from the flame that comes in.

So, I will say this is the mass flow rate of CO_2 in the inner surface, 'i' represent the inner surface. So, this is the conservation here, so that is the conservation of this. Now, i denotes the inner region as I told inner region between the carbon surface and the flame.

$$\dot{m}_{CO} = \dot{m}_{CO2,i} + \dot{m}_C.$$

For the reaction: 1 kg C + s_1 kg CO_2 → $(1 + s_1)$ kg CO

$$\dot{m}_{CO} = \dot{m}_{CO2,i} + \dot{m}_C = (1 + s_1)\,\dot{m}_C.$$

Now, from this we can write $\dot{m}_{CO}$ will be equal to $\dot{m}_{CO2,i} + \dot{m}_C$. Now, what is happening at the surface is the surface reaction. So, this is the surface reaction here, 1 kg of carbon, s_1 kg of CO_2 is because there are two reaction, the stoichiometric coefficients are designated as s_1 and s_2 here. For the surface reaction, I am designating the stoichiometric coefficient as s_1 kg of CO_2 giving 1 + s_1 kg of CO.

Now, mass balance $\dot{m}_{CO} = \dot{m}_{CO2,i}$, at the inner plus $\dot{m}_C$ which is written as 1 + s_1 times. So, from this equation, I can write 1 plus s_1 times mass balance of C will be equal to that of CO_2.

So, now, I put this s_1 times oxygen, $s_1 \times \dot{m}_C$. So, CO_2 is $\dot{m}_{CO2}$ that is oxidized here will be equal to s_1 times $\dot{m}_C$. So, when I put that, I get this equation $1 + s_1 \times \dot{m}_C$. The mass rate of CO_2 is written as $s_1 \times \dot{m}_C$, this I will say, due to this plus $\dot{m}_C$ so $1 + s_1 \times m_C$, so that we can write. So, this you keep in mind. So, these are the fluxes or the flow rates in the carbon surface.

Now, at the flame surface, this is the flame here, flame r_f and this r_s. Now, what happens at the flame? CO which is formed that goes here. Now, CO_2 which is formed at the flame will come here like this to the inner zone. And it also get away to the outer zone $\dot{m}_{CO2,o}$. And oxygen from the ambient comes in here, so $\dot{m}_{O2}$. So, these are the mass balances in the flame r_f.

$$\dot{m}_{CO} - \dot{m}_{CO2} = \dot{m}_{CO2,o} - \dot{m}_{O2}.$$

Here subscript o denotes outer region between the flame and the ambient.

$$\dot{m}_{CO2,o} = \dot{m}_C + \dot{m}_{O2}.$$

For the reaction: 1 kg CO + s_2 kg O_2 → $(1 + s_2)$ kg CO_2

$$\dot{m}_{O2} = s_2(\dot{m}_{CO}) = s_2(1 + s_1)\,\dot{m}_C.$$

$$\dot{m}_{CO2,o} = \dot{m}_C + \dot{m}_{O2} = [1 + s_2(1 + s_1)]\,\dot{m}_C.$$

So, $\dot{m}_{CO} - \dot{m}_{CO2}$ this is actually inner zone, will be equal to, so, $\dot{m}_{CO}$ and this in the inner, see this is going away and this is coming in. So, that equal to $\dot{m}_{CO2,o}$ which is going out $\dot{m}_{O2}$ coming in, so this is the balance. So, subscript o is the outer region between the flame and the ambient. So, this is inner region and this is outer region.

Now, what is the reaction taking place at the flame zone? This is the flame, what is the reaction gas phase. So, 1 kg of CO + s_2 kg of O_2 → 1 + s_2 kg of CO_2. Now, what we did there? We will do the same thing here $\dot{m}_{CO}$ will be equal to $s_2 \times \dot{m}_{CO}$ or $s_2(1 + s_1)\dot{m}_C$. Combining this, we can write.

So, here also we can see that when we combine this $\dot{m}_{CO2,o}$ outer will be equal to $\dot{m}_C$ + $\dot{m}_{O2}$ that is it. So, you know this equation here. So, $\dot{m}_{CO}$ - $m_{CO2,i}$, this is $\dot{m}_C$. So, this is substituted here as $\dot{m}_C$. Now, I can write $\dot{m}_{CO2} = \dot{m}_C + \dot{m}_{O2}$.

And I also use this equation to write every flow rate in terms of $\dot{m}_C$. So, the main purpose of this is to write all the flow rates as the carbon flow rate from the surface. So, I have already written for the flow rate of CO using the surface reaction of coefficient $1+s_1\dot{m}_C$ For O_2, it is $s_2(1 + s_1) \times \dot{m}_C$; for CO_2 going out, it will be $(1 + s_2)(1 + s_1)\dot{m}_C$ that is it.

So, when I do this for all the flow rates, I need to only solve for one species CO_2 that is enough for me, then we can write everything in terms of this. So, let us take CO_2, and I can solve the CO_2 in the inner region and outer region and formulate the problem.

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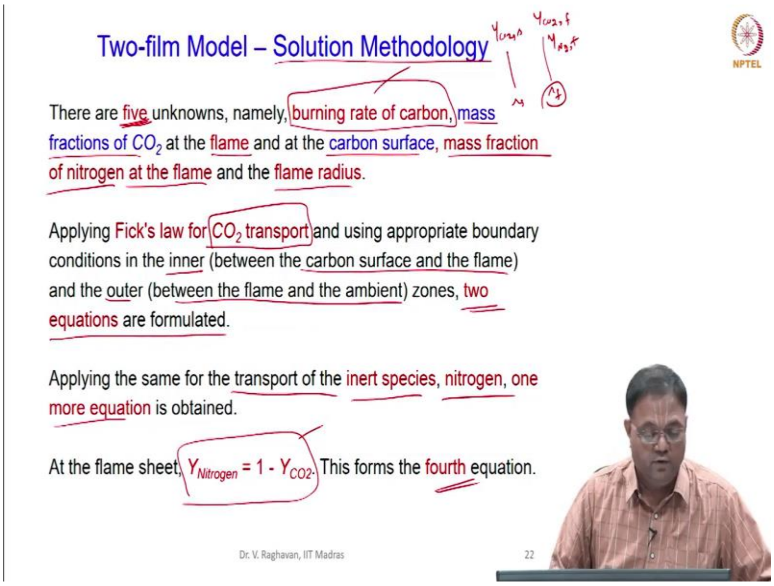

Two-film Model – Solution Methodology

There are five unknowns, namely, burning rate of carbon, mass fractions of CO_2 at the flame and at the carbon surface, mass fraction of nitrogen at the flame and the flame radius.

Applying Fick's law for CO_2 transport and using appropriate boundary conditions in the inner (between the carbon surface and the flame) and the outer (between the flame and the ambient) zones, two equations are formulated.

Applying the same for the transport of the inert species, nitrogen, one more equation is obtained.

At the flame sheet, $Y_{Nitrogen} = 1 - Y_{CO2}$. This forms the fourth equation.

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So, I am not going to solve it. So, the procedure for solving, the solution methodology is outlined here which is as follows. So, I am interested in solving five unknowns, when I am interested in mainly solving the burning rate of carbon, so that will additionally involve four more unknowns.

First is the mass fractions of CO_2 at the flame and at the carbon surface. So, at the flame there will be CO_2, at the surface r_s we will have Y_{CO2},s. So, these are the two unknowns I additionally have. Similarly, mass fraction of nitrogen at the flame, please understand nitrogen is inert species that will also penetrate everywhere. So, what is the value of nitrogen at the flame? Y_{N2} at the flame, I want this. So, these two I want then the flame radius itself is unknown.

So, these are the five unknowns I want to solve basically in order to just solve the primary variable, that is mass burning rate of carbon that is what I am interested in. So, I will take CO_2 transport in both inner which is between the carbon surface and the flame, and the outer which is between the flame and the ambient. So, appropriate boundary conditions will be used.

What are the boundary conditions? You know that already we have discussed. So, at the surface $Y_{CO2,}$r= r_s, $Y_{CO2} = Y_{CO2,s}$; at the flame $Y_{CO2} = Y_{CO2,f}$; at infinity, it will be $Y_{CO2,\infty}$. So, using boundary conditions we can solve.

Similarly, these are the boundary conditions we can solve this. So, two equations will be got when you solve, one for inner zone and one for outer zone. When you solve this, CO_2 transport is taken into account, we will take two equations. I want five equations.

Then the second is transport equation of nitrogen has to be solved. So, inert species say nitrogen I will get one more equation. Here again we will consider the outer zone and try to solve the nitrogen. I will get one more equation for nitrogen. So, three equations are got now.

At the flame sheet, oxygen is consumed, CO is consumed, only two species are there. What are they? The inert species and the CO_2 which is formed. So, this identity applies $Y_{N2} + Y_{CO2} = 1$. So, I use this. That is the fourth equation I get.

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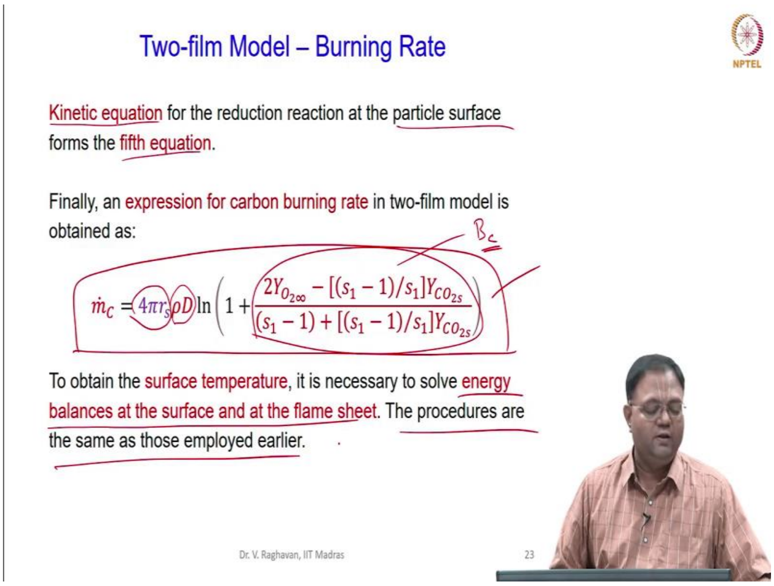

Two-film Model – Burning Rate

Kinetic equation for the reduction reaction at the particle surface forms the fifth equation.

Finally, an expression for carbon burning rate in two-film model is obtained as:

B_c

$$\dot{m}_C = 4\pi r_s \rho D \ln\left(1 + \frac{2Y_{O_{2\infty}} - [(s_1 - 1)/s_1]Y_{CO_{2s}}}{(s_1 - 1) + [(s_1 - 1)/s_1]Y_{CO_{2s}}}\right)$$

To obtain the surface temperature, it is necessary to solve energy balances at the surface and at the flame sheet. The procedures are the same as those employed earlier.

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The fifth equation will be the kinetic equation. Let us take the kinetic equation at the particle surface that will be the fifth equation. I am not going into details of that you can refer the Turns book again, there also limited details are given. So, you can check them. So, you can see that again some complexity is there we have to form five equations and solve them.

Finally, you get a expression like this for the mass burning rate of carbon which is very similar to the droplet combustion $4\pi r_s$, driving force $\rho D \ln(1+B)$. The B number is written in different way. So, this is a B number here. So, I will say the B for carbon.

$$\dot{m}_C = 4\pi r_s \rho D \ln\left(1 + \frac{2Y_{O_{2\infty}} - [(s_1 - 1)/s_1]Y_{CO_{2s}}}{(s_1 - 1) + [(s_1 - 1)/s_1]Y_{CO_{2s}}}\right)$$

Now, again you can see that there is an unknown here. For solving this, we need surface temperature. A surface temperature is determined by energy balance which we have illustrated for the one-film model. Similar energy balance you have to make both at the surface of the carbon particle as well as at the flame sheet to get the surface temperature.

So, you have to solve this along with those energy balances, and iteratively you have to follow the procedures what are illustrated earlier to solve this. So, two-film model finally, you will get profiles like this and a burning rate for this which will be slightly accurate than the one-film model. So, these illustrate the methodology which is involved.

But please understand that in reality, any carbon combustion is not so easy. So, one-film or two-film model is much complicated. So, we need lot of assumptions to make, and like simplification what we have done here such simplifications have to be made at any point in time.

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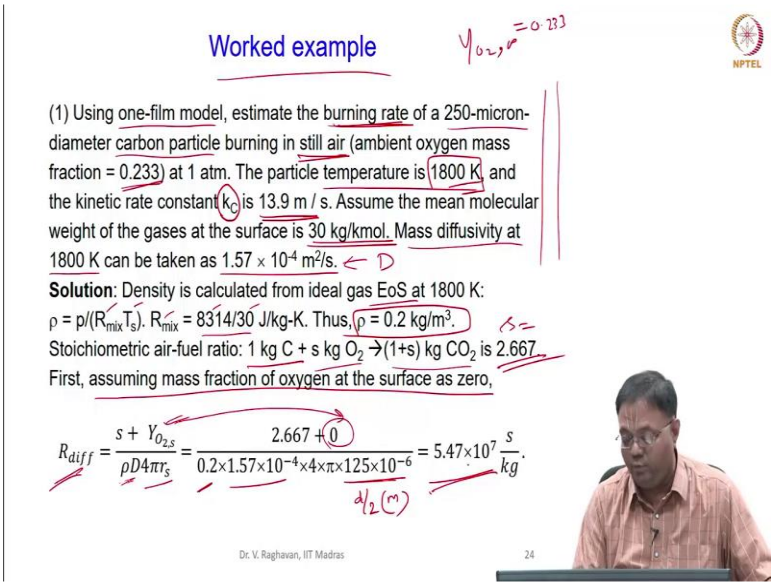

Worked example

$Y_{O_2,\infty} = 0.233$

(1) Using one-film model, estimate the burning rate of a 250-micron-diameter carbon particle burning in still air (ambient oxygen mass fraction = 0.233) at 1 atm. The particle temperature is 1800 K, and the kinetic rate constant k_C is 13.9 m / s. Assume the mean molecular weight of the gases at the surface is 30 kg/kmol. Mass diffusivity at 1800 K can be taken as 1.57×10^{-4} m²/s. ← D

Solution: Density is calculated from ideal gas EoS at 1800 K: $\rho = p/(R_{mix}T_s)$. R_{mix} = 8314/30 J/kg-K. Thus, $\rho = 0.2$ kg/m³.

s =

Stoichiometric air-fuel ratio: 1 kg C + s kg $O_2 \rightarrow (1+s)$ kg CO_2 is 2.667.

First, assuming mass fraction of oxygen at the surface as zero,

$$R_{diff} = \frac{s + Y_{O_2,s}}{\rho D 4\pi r_s} = \frac{2.667 + 0}{0.2\times1.57\times10^{-4}\times4\times\pi\times125\times10^{-6}} = 5.47\times10^{7}\,\frac{s}{kg}.$$

d/2 (m)

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So, let us see one worked example on this. Let us consider one-film model and try to estimate the burning rate of a carbon particle which has a diameter of 250 microns. So, 250 micron carbon particle is burning in an oxygen environment a still air environment, stagnant air environment. The entire particle is at same temperature of 1800 K. The mass fraction of the oxygen in the ambient air (standard air) is 0.233. So, $Y_{O2,\infty}$ is 0.233. Now, there is the kinetic rate constant k_c is given as 13.9 m/s, as I told that the unit is m/s.

Now, one more thing what is given is, since the gas phase species are CO_2, O_2 and N_2, we can take the average molecular weight or a mean molecular weight of the gases is equal to 30 kg/kmol.

And mass diffusivity has to be calculated at the temperature here, 1800 K, surface temperature, because we are interested in surface reactions there. So, that is equal to

1.57×10^{-4} m^2/s. We can also estimate this from tables. So, these are the values. So, this is the value of D.

Now, how to calculate the mass burning rate of the carbon? So, density is calculated from the ideal gas equation of state $\rho = p/RT$, but this R is the R_{mix}.

So, mixture R is estimated by R_u/MW, so that is got. So, then if you substitute here, T_s is 1800 K, you get the ρ as 0.2 kg/m^3 that is the density of the gas mixture. Now, density of the gas mixture is known; D is also known. So, the product ρD can be calculated.

Now, this reaction takes place at a surface, which is heterogeneous reaction 1 kg of carbon + s kg of O_2 → (1 + s) kg of CO_2. The s is stoichiometric air fuel ratio. So, s = 2.667. So, we can get the value of s. Now, I calculate the resistances, the diffusion resistance is nothing but $(s + Y_{O2,s})/\rho D \times 4\pi r_s$.

Now, as a first step, I will assume the mass fraction of oxygen at the surface to be 0, and calculate the resistance for the diffusion as 5.47×10^7 s/kg, this is what I get s/kg. So, ρ is 0.2, diffusion coefficient is 1.57×10^{-4} which is given.

So, $4\pi r$, this r is see diameter is given, so it is d/2, and converted into m. So, d is 250 microns. So, 125 microns of radius. So, 125×10^{-6} meters, so that is the radius here. So, substitute it, I get the R value, it is 5.47×10^{-7}.

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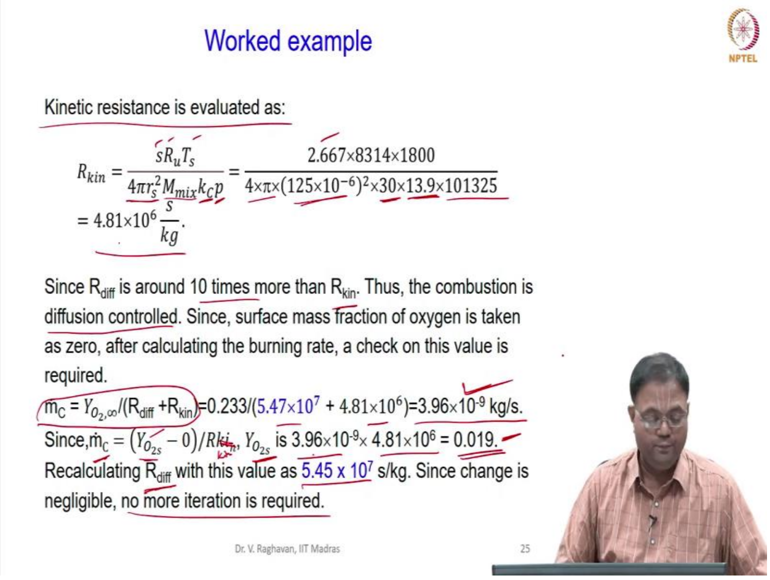

Worked example

Kinetic resistance is evaluated as:

$$R_{kin} = \frac{sR_uT_s}{4\pi r_s^2 M_{mix} k_C p} = \frac{2.667\times8314\times1800}{4\times\pi\times(125\times10^{-6})^2\times30\times13.9\times101325}$$
$$= 4.81\times10^6\,\frac{s}{kg}.$$

Since R_{diff} is around 10 times more than R_{kin}. Thus, the combustion is diffusion controlled. Since, surface mass fraction of oxygen is taken as zero, after calculating the burning rate, a check on this value is required.

$\dot{m}_C = Y_{O_2,\infty}/(R_{diff} + R_{kin}) = 0.233/(5.47\times10^7 + 4.81\times10^6) = 3.96\times10^{-9}$ kg/s.

Since, $\dot{m}_C = (Y_{O_{2s}} - 0)/R_{kin}$, $Y_{O_{2s}}$ is $3.96\times10^{-9}\times 4.81\times10^6 = 0.019$.

Recalculating R_{diff} with this value as 5.45×10^7 s/kg. Since change is negligible, no more iteration is required.

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Now, kinetic resistance is evaluated. In this you can see that $sR_uT_s/(4\pi r_s)^2MW_{mix}\times k_c\times p$.

$$
\begin{aligned}
R_{kin} &= \frac{sR_uT_s}{4\pi r_s^2 M_{mix} k_C p} \\
&= \frac{2.667\times 8314\times 1800}{4\times\pi\times(125'10^{-6})^2\times 30\times 13.9\times 101325} \\
&= 4.81\times 10^6\,\frac{s}{kg}
\end{aligned}
$$

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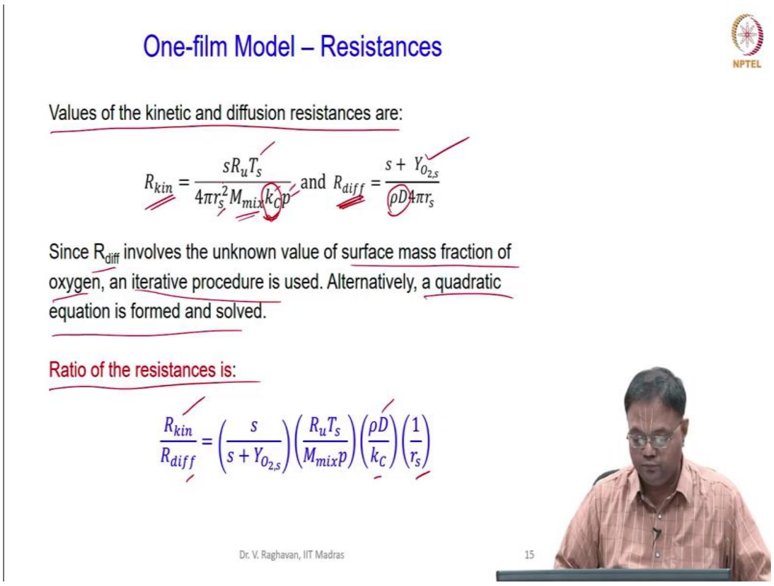

One-film Model – Resistances

Values of the kinetic and diffusion resistances are:

$$R_{kin} = \frac{sR_uT_s}{4\pi r_s^2 M_{mix} k_C p} \text{ and } R_{diff} = \frac{s + Y_{O_{2,s}}}{\rho D 4\pi r_s}$$

Since R_{diff} involves the unknown value of surface mass fraction of oxygen, an iterative procedure is used. Alternatively, a quadratic equation is formed and solved.

Ratio of the resistances is:

$$\frac{R_{kin}}{R_{diff}} = \left(\frac{s}{s + Y_{O_{2,s}}}\right)\left(\frac{R_uT_s}{M_{mix}p}\right)\left(\frac{\rho D}{k_C}\right)\left(\frac{1}{r_s}\right)$$

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So, if you go here you can see that this pressure is 1 atmosphere, substitute here, k_c value is 13.9 m/s, molecular weight of mixture is 30 and r_s is 125 microns, so $4\pi(r_s)^2$ square.

So, s is given. So, if you substitute all these, you get this 4.81×10^6. The previous was 5.47×10^7. So, you can see this, this resistance is one order of magnitude less or 10 times times more than, approximately 10 times more than R_{kin}. So, this means that the combustion is diffusion controlled.

But anyway, we will use both resistances to calculate the mass burning rate of carbon. As 0.233 is $Y_{O2,\infty}$ divided by this plus this, I get the mass flow rate of carbon as 3.96×10^{-9}. But I will try to verify now, I try to find the mass flow rate of carbon as Y_{O2}, by just using the kinetic resistance this is R_{kin}. So, $Y_{O2,s}/R_{kin}$.

Now, I try to estimate Y_{O2} from this with the known value of $\dot{m}_C$ now. I get $Y_{O2,s}$ as this $\dot{m}_C R_{kin}$. So, R_{kin} is this into m_C is this. So, when I substitute and multiply, I get $Y_{O2,s}$ is very low value 0.019. Now, I recalculate with this value of $Y_{O2,s}$ the diffusion resistance that is 5.45×10^7; previously I got 5.47×10^7, there is only a little change.

So, since the change is negligible, no more iterations required. So, we can just leave the burning rate as this, that is enough. So, this completes the exercise, worked example.