

Fundamentals of Combustion
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Lecture - 60
Combustion of carbon particle - Part 2
One film model

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One-film Model – Mass Fluxes

Mass and species conservations: At the carbon surface, the mass flow of carbon is equal to mass flow of out going CO₂ minus the mass flow of incoming O₂.


$$\dot{m}_c = \dot{m}_{CO_2} - \dot{m}_{O_2}$$


At any other radius, r, the net mass flow is equal to mass flow of out going CO₂ minus the mass flow of incoming O₂.

$$\dot{m}_{net} = \dot{m}_{CO_2} - \dot{m}_{O_2}$$

In the steady burning with no gas-phase reactions, the mass flow rates of each species are constant: Thus the net mass flow rate is equal to the mass flow of carbon.

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So, let us do this, let us first consider the mass fluxes involved. So, this is the solid surface r_s and I can see that some mass flux comes in carbon mass flux is leaving the surface and carbon dioxide is formed and that also leaves the surface but oxygen penetrates through the surface. So, I write this.

You can see the directions also, the flux. So, $\dot{m}_c =$ (the same direction) $\dot{m}_{CO_2} - \dot{m}_{O_2}$ (in opposite direction). So, this is at the surface r_s , at any other r.

$$\dot{m}_c = \dot{m}_{CO_2} - \dot{m}_{O_2}$$

This is r_s at any other radius r, arbitrary radius you can see that there is a net flow rate which is nothing but the flow rate of CO₂ at that point and oxygen also is coming. Oxygen is always transported in this direction. So, again you can write the same thing. But please understand that there is no other consumption zone or reaction zones in the gas phase. So, when you assume steady burning of this and there are no gas phase

reactions, only one reaction is there that is heterogeneous in nature. There is no gas phase reaction.

So, the mass flow rate of the species should be constant because there is no consumption or production of any other species. So, in that case we can easily say that the net mass flow rate \dot{m}_{net} will be equal to the mass flow rate of the carbon. So, that is the steady state condition.

$$\dot{m}_{net} = \dot{m}_{CO_2} - \dot{m}_{O_2}$$

So, what we have is we have 3 species here O_2 , N_2 and CO_2 , if you try to write everything in terms of say carbon flow rate then we need to solve only one equation either taking into account of any one conservation. So, that is what gas phase species. So, we can write the flow rates of these two species basically with respect to carbon by using this equation.

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One-film Model - Reaction

NPTEL


Consider global one-step reaction at the surface, given as,
1 kg of C + s kg of $O_2 \rightarrow (1 + s)$ kg of CO_2 . ✓

It is clear that carbon burning rate (\dot{m}_C) can be used to calculate the flow rates of O_2 and CO_2 in the gas-phase:

$$\dot{m}_{CO_2} = (1 + s)\dot{m}_C; \dot{m}_{O_2} = s\dot{m}_C \quad \checkmark$$

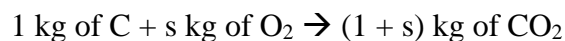
It is enough if one of the gas-phase species conservation is solved.
 Since oxygen is transported to the surface by both convection (net flow) and diffusion (noted by its participation in the reaction at the surface), and that it is in the inward direction (negative), the net mass flux of oxygen is:

$$\dot{m}_{O_2} = (\dot{m}_{CO_2} - \dot{m}_{O_2})Y_{O_2} - \rho D \left(\frac{dY_{O_2}}{dr} \right)$$



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So, the reaction what we consider is again same global single step reaction, but this is the surface reaction here 1 kg of carbon graphite plus s kg of O_2 giving 1 + s kgs of CO_2 and the carbon burning rate is indicated by \dot{m}_C .



Now, we know from this equation the mass flow rate of CO_2 will be equal to 1 + s, the magnitude of mass flow rate of CO_2 will be equal to 1 + s that of \dot{m}_C . Similarly, mass flow rate of O_2 actually please understand that the flow rate of O_2 is in the other direction but the magnitude of this mass flow rate is equal to $s(\dot{m}_C)$.

$$\dot{m}_{CO_2} = (1 + s)\dot{m}_C; \dot{m}_{O_2} = s\dot{m}_C$$

Now, I am trying to write the flow rates of O₂ and CO₂ in terms of the burning rate of the carbon itself. Obviously, based on the amount of carbon burnt that much oxygen would have diffused and that much CO₂ would have formed. So, we can easily write that by considering this reaction. While doing this the benefit what we get is one of the gas phase species is solved that is enough for us. So, let us take the carbon see oxygen transport in the gas phase. So, since oxygen is transported by both convection that is net flow and diffusion because of the participation of the oxygen in the surface reaction basically and also note that oxygen is coming towards the carbon like this, this is a carbon surface. So, it is coming in the other direction. So, the radial direction is like this. So, it is coming to the opposite direction basically. Now, the inward direction is negative that also you keep in mind. So, let us write the Fick's law for this, the net mass flow rate of oxygen, net mass flux per unit area. So, mass flux of oxygen will be equal to the net flow rate. Net flow rate is nothing but $\dot{m}_c'' \times Y_{O_2}$ minus the diffusion of oxygen.

$$\dot{m}_{O_2}'' = (\dot{m}_{CO_2}'' - \dot{m}_{O_2}'')Y_{O_2} - \rho D \left(\frac{dY_{O_2}}{dr} \right)$$

Please understand this, diffusion of oxygen we have put usual method. But diffusion is predominantly in the negative r direction that you have to understand. Because you can see that O₂, Y_{O₂} decreases in the negative r direction. Similarly, the dr also decreases in that direction. So, you have to note that the diffusion is predominantly in the negative r direction. The convection will be in the other direction, this $\dot{m}_{CO_2}'' - \dot{m}_{O_2}''$ that is the net flow which is in the other direction, in the positive r direction

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One-film Model – Oxygen Conservation

Multiplying by the surface area and writing the flow rates in terms of the carbon burning rate:


$$-\dot{m}_c'' = \frac{(1+s)\dot{m}_c'' - s\dot{m}_c''}{\dot{m}_c''} Y_{O_2} - \rho D 4\pi r^2 \left(\frac{dY_{O_2}}{dr} \right)$$


First order differential equation for mass fraction of oxygen is:

$$\dot{m}_c Y_{O_2} - \rho D 4\pi r^2 \frac{dY_{O_2}}{dr} = -s\dot{m}_c$$

Boundary conditions: At $r = r_s$, $Y_{O_2} = Y_{O_{2,s}}$ and as $r \rightarrow \infty$, $Y_{O_2} \rightarrow Y_{O_{2,\infty}}$.

Oxygen conservation equation can be integrated and using the boundary conditions, mass burning rate of carbon can be obtained.





So, now we can use this and appropriately take care of the negative and positive signs. I write the conservation equation.

Also, we can multiply the flux by the surface area of the carbon $4\pi r_s^2$ then I get the mass flow rate itself. So, we can see that negative. So, $\dot{m}_{O_2}'' = -s\dot{m}_C''$.


$$-s\dot{m}_C = ((1+s)\dot{m}_C - s\dot{m}_C)Y_{O_2} - \rho D 4\pi r^2 \left(\frac{dY_{O_2}}{dr} \right)$$

So, if you substitute it and multiply by this, I can write this net flux of the oxygen negative direction indicates that it is in the other direction so; obviously, the profile indicates that. So, that will be equal to $\dot{m}_{CO_2}'' - \dot{m}_C''$. So, this is the net flow rate basically into Y_{O_2} minus $\rho D 4\pi r^2$, you can put r_s^2 or r^2 that is not a problem. So, this is the differential equation.

$$\dot{m}_C Y_{O_2} - \rho D 4\pi r^2 \frac{dY_{O_2}}{dr} = -s\dot{m}_C$$

So, the first order differential equation for the mass fraction of oxygen can be written like this and you know that this is constant here even though unknown, it is a constant. So, we can solve this by applying the boundary conditions at the surface of the carbon which is $Y_{O_2} = Y_{O_2,s}$ that is another unknown what we have, we do not know that yet. So, then you see, you know this value $Y_{O_2,\infty}$ we know, but $Y_{O_2,s}$ we do not know. Similarly, the mass burning rate of carbon we are going to find, which is also not known. As $r \rightarrow \infty$, $Y_{O_2} \rightarrow Y_{O_2,\infty}$. So, these are the boundary conditions which we need to integrate this and solve. So, oxygen conservation equation is integrated and using the boundary condition the mass burning rate of the carbon is obtained. So, like usual procedure what we have seen previously the same thing we are trying to do here.

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One-film Model – Carbon Burning Rate


Separating the variables, integrating and using the boundary conditions, one by one:

$$\dot{m}_C \frac{dr}{\rho D 4\pi r^2} = \frac{dY_{O_2}}{s + Y_{O_2}}$$

$$-\frac{\dot{m}_C}{\rho 4\pi D r} = \ln \left[\frac{s + Y_{O_2}}{s + Y_{O_{2,\infty}}} \right]$$

$$\dot{m}_C = 4\pi r_s \rho D \ln \left[\frac{s + Y_{O_{2,\infty}}}{s + Y_{O_{2,s}}} \right] \quad (A)$$

Unknown in the above equation is mass fraction of O₂ at the surface.



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So, by separating the variables and integrating I get the equation and boundary condition one by one you have to apply. First you apply the boundary condition for the infinity and next you apply the boundary condition for the surface.

So, you get the final equation like this. So, you can see this, separate the variable, \dot{m}_C'' is taken as constant. So, dr by the term involving the radius is present. Also, you see $4\pi\rho D$ are constants here. Similarly, the oxygen mass fractions taken other side and this is integrated to get an expression like this.

$$\dot{m}_C \frac{dr}{\rho D 4\pi r^2} = \frac{dY_{O_2}}{s + Y_{O_2}}$$

$$-\frac{\dot{m}_C}{\rho 4\pi D r} = \ln \left[\frac{s + Y_{O_2}}{s + Y_{O_{2,\infty}}} \right]$$

$$\dot{m}_C = 4\pi r_s \rho D \ln \left[\frac{s + Y_{O_{2,\infty}}}{s + Y_{O_{2,s}}} \right] \quad (A)$$

Now, apply the boundary conditions and you get the final equation for \dot{m}_C'' involving the Y_{O_2} at the infinity and Y_{O_2} at the surface. So, again a similar expression, where $4\pi r_s$ and a driving parameter ρD because it is species consideration. The driving parameter for the mass is ρD and natural logarithm of some term. So, this obviously can be written as $1 + B$ which we will do later.

Again, similar to what we got for the droplet combustion we get an equation for this, but these are the unknown here, r_c maybe known, Y_{O_2} infinity is known, s is known s is got by, see 1 kg of carbon + s kg of $O_2 \rightarrow (1 + s)$ kg CO_2 from that we can calculate the s value.

So, the unknown here is surface what is the value at the surface? Similarly, what in the left-hand side we have to find. So, these are the two. The unknown has to be found.

So, how to do this? Again, you can see the procedure is not very complicated, it is exactly similar to what we have done for the droplet combustion and we have got this again, unknowns are there, non-linear equations, profiles are non-linear we may have to include one more equation and solve it iteratively.

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One-film Model – Surface Kinetics

The surface reaction, $C + O_2 \rightarrow CO_2$ is assumed to be of **first order**.
Its rate (kg/m^2s) depends upon the oxygen concentration:


$$\dot{m}_{C,s} = k_c M_C [O_2]_s$$


Here, $k_c = A \exp[-E_a/R_u T_s]$. Writing $[O_2]$ in terms of mass fraction:

$$\dot{m}_{C,s} = k_c \frac{M_C M_{mix}}{M_{O_2}} \frac{p}{R_u T_s} Y_{O_2,s}$$

Relating the burning rate to the carbon mass flux at the surface:

$$\dot{m}_C = 4\pi r_s^2 k_c \frac{M_C M_{mix}}{M_{O_2}} \frac{p}{R_u T_s} Y_{O_2,s} = K_{kin} Y_{O_2,s} \quad (B)$$





Now, let us consider the surface kinetics, I have to produce one more equation. So, for doing that I have to consider surface kinetics here. Because we have already discussed that Y_{O_2} at the surface is dependent on surface reaction. So, I need to consider something on surface kinetics.

So, what we assume here is this equation, surface reaction $C + O_2 \rightarrow CO_2$ is assumed to be first order. When you say its first order then it depends upon the oxygen concentration.

So, the mass flow rate of the carbon, that is the burning rate. So, this is kg/m^2s . This is mass flow rate of carbon kg/m^2s , that will be written as some rate constant $k_c \times$ molecular weight of carbon.

$$\dot{m}_{C,s} = k_c M_C [O_2]_s$$

And this is the concentration of oxygen at the surface. So, this is $kmol/m^3$, concentration of carbon. Now, molecular weight is $kg/kmol$ and this left-hand side is kg/m^2s . So, this means the unit of k_c should be what.

So, this kmol cancels, kg/m³. So, it should be kg/m²s. So, this will be m/s. Now, it becomes a kg, this cancels, kg/m²s. So, the unit of k_C will be m/s.

Now, as done for other rate coefficients, k_C also can be expressed in an Arrhenius form where there is a pre-exponential factor A, then the activation energy E_a, universal gas constant and the surface temperature.

$$k_C = A \exp[-E_a/R_u T_s]$$

So, we can do this. Let us assume that the parameters A and E are known. Anyway, we have to do experiments to determine the rate constant for the char oxidation.

We have to again do experiments, isothermal experiments varying the temperatures in a range and tried to extract the values of A and E_a and now let us assume that is known to me. So, again now if you involve this, T_s becomes unknown again. To calculate T_s we have to invoke one more equation.

$$\dot{m}_{C,s}'' = k_C \frac{M_C M_{mix}}{M_{O_2}} \frac{p}{R_u T_s} Y_{O_{2s}}$$

Now, k_C I substitute here $\dot{m}_c'' = k_C$ into concentration I try to write in the different way here that is concentration is nothing, but O₂ at the surface is equal to molecular weight of the see p/R_uT_s.

So, R_u divided by molecular weight of the mixture and I am dividing by molecular weight of O₂ also. See actually concentration is what, pv = nR_uT. Now, we can see that concentration will be p = cR_uT. So, using this we can find the concentration basically.

So, for getting concentration I have to get the mass fraction. So, I have to multiply by molecular weight of mixture by molecular weight of O₂. So, p/R_uT will give you the concentration. So, concentration is written, but I want mass fraction.

So, when I want to convert the mass fraction, I have to involve mole fraction. So, when I convert that I have to multiply by molecular weight of mixture by molecular weight of O₂. So, when I do this, I get this equation. It is again using this equation plus the mole fraction to mass fraction conversion I get this.

Now, this is known now I try to write this \dot{m}_c , mass burning rate of the carbon will be equal to $4\pi(r_s)^2 \times \dot{m}_c''$. So, $4\pi(r_s)^2$ into this term I multiply I get this now. I call this as K_c × Y_{O_{2,s}} some kinetic parameter into Y_{O_{2,s}}. This is the kinetic parameter I am talking about and Y_{O_{2,s}}

So, this let us take as equation B equation A already is solved by oxygen conservation equation. Then by taking into account of surface kinetics I have created the equation B

which is like this where the kinetic parameter k_c is involved. So, that is K kinetics, some coefficient involving kinetics into $Y_{O_2,s}$.

$$\dot{m}_c = 4\pi r_s^2 k_c \frac{M_c M_{mix}}{M_{O_2}} \frac{p}{R_u T_s} Y_{O_{2s}} = K_{kin} Y_{O_{2s}} \quad (B)$$

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One-film Model – Electrical Analogy

The kinetics parameter K_{kin} depends on pressure, temperature and particle radius.

Equation (B) is solved to get the value of mass fraction of oxygen at the particle surface and this is substituted in equation (A).
An electrical analogy is done as follows for Equation (B):

$$\dot{m}_c = K_{kin} Y_{O_{2s}} = \frac{(Y_{O_{2s}} - 0)}{\frac{1}{K_{kin}}} = \frac{\Delta Y}{R_{kin}} \quad (C)$$

$\frac{1}{K_{kin}} = R_{kin}$

Equation (A) is written as:

$$\dot{m}_c = 4\pi r_s \rho D \ln \left[1 + \frac{Y_{O_{2,\infty}} - Y_{O_{2,s}}}{s + Y_{O_{2,s}}} \right]; B = \frac{Y_{O_{2,\infty}} - Y_{O_{2,s}}}{s + Y_{O_{2,s}}}$$

R_{diff}

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Now, under steady state condition A and B should be the same. So, the kinetic parameter depends upon pressure, temperature and particle radius. That is also known to me anyway it will invoke another unknown which is T_s . So, that we have to solve again, but anyway at the time being let us assume T_s is known to me then you will proceed.

Now, equation B is solved to get the value of mass fraction of oxygen at a particle surface and substitute in equation A. And again, this is not very easy to do, when you try to solve these non-linear things are there and you will get a very complicated equation when you try to solve it, but anyway that is the only way to go about that or another method is to follow an electrical analogy.

$$\dot{m}_c = K_{kin} Y_{O_{2s}} = \frac{(Y_{O_{2s}} - 0)}{\frac{1}{K_{kin}}} = \frac{\Delta Y}{R_{kin}} \quad (C)$$

So, equation B is written like this. So, \dot{m}_c equal to some coefficient of kinetics, K kinetics into $Y_{O_{2,s}}$ which we write as some difference. So, $Y_{O_2}/(1/K_{kin})$. So, this is the resistance R_{kin} . So, this $1/K_{kin}$ is called R_{kin} that is the resistance offered to the kinetics at the surface.

So, what is driving the combustion reaction is the gradient of this. So, how fast this is consumed, there is oxygen which is coming to the surface how fast it is consumed. So, this 0, I am just putting to indicate that if the kinetics is higher it will consume fast. So, this is like a ΔY gradient divided by the resistance to that will be inverse of the coefficient of kinetics. So, I can write this as equation C and this is like one surface.

See for example, this is surface R_s and there is one. So, this mass of carbon flows here and here oxygen comes in and this I call R_{kin} , the rate at which the surface reaction takes place. So, that this mass of carbon is burnt. So this is one of the analogy what I make.

See, here surely $Y_{O_2} = 0$ at this point, interior of the carbon Y_{O_2} is 0 but here at the surface it is $Y_{O_2,s}$. So, the difference between these two is $Y_{O_2,s} - 0$ that is like a potential and the resistance which is offered is this R_{kin} and this is nothing, but like a current flow the mass of the carbon flows out.

So, this is electrical analogy which we make normally in heat transfer problems also we make this same analogy, temperature difference taken as a voltage difference and what are the factors affecting this heat transfer that will be taken as resistance and the heat flow itself will be taken as current.

So, similar to that analogy we are taking the difference in the mass fraction of the O_2 as a driving force and the resistance offered is nothing but the it will be inversely proportional to the reaction rate. So, K_{kin} here you can see that that is K_{kin} is proportional to the reaction rate.

So, one by that it will be inversely proportional so that will be resistance of the chemical kinetics. So, that is one way to do. So, I get one equation.

Similarly, I can also work with the equation A which we have got here by using the oxygen mass fraction conservation. Here, you can see that some term here in the natural logarithm can be written in terms of $1 + B$ and we can define a B number, that is what I am trying to do here. So, when I write that as $1 + B$, the B number comes to be like this. Y_{O_2} infinity minus Y_{O_2} surface again that is the difference which is occurring in the gas phase now.

Now, this occurs at the surface and we are concentrating on the surface to the interior to get this equation where the surface kinetics is important. Now, when I say diffusion of gases, that is the oxygen basically in the gas phase. Now, I have to take the condition in the gas phase. So, what are the resistance there to the gas phase or what is the driving force in the gas phase diffusion for oxygen etcetera.

Obviously, this difference is called ΔY here and that will be the driving force for me, for the oxygen to penetrate from the gas phase to the surface. Then the rate at which it is consumed at the surface is what we have described here.

So, that resistance is R_{kin} , the resistance offered to the diffusion I have to find now in the gas phase that will be called $R_{diffuse}$. So, you have to write this equation in a different way to get that.

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One-film Model – Electrical Analogy

Expanded in a Taylor series
B² and higher order terms are dropped.

The term $\ln[1 + B]$ is approximately equal to B, when B is small. Thus,


$$\dot{m}_c = 4\pi r_s \rho D \frac{Y_{O_2,\infty} - Y_{O_2,s}}{s + Y_{O_2,s}}$$


$$\dot{m}_c = \frac{(Y_{O_2,\infty} - Y_{O_2,s})}{(s + Y_{O_2,s}) / (4\pi r_s \rho D)} = \frac{\Delta Y}{R_{diff}} = -\frac{\dot{m}_{O_2}}{s} \quad (D)$$

This is like carbon flowing from interior to the surface and oxygen being consumed from its surface value to zero at the interior. Here, the resistance is R_{kin} . Oxygen transported from ambient to the surface has a resistance of R_{diff} . This is like two resistors in series:

$$\dot{m}_c = \frac{Y_{O_2,\infty} - 0}{R_{kin} + R_{diff}}$$

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Now, if I want to do this, I want to eliminate the natural logarithm. So, I have written this $\ln(1 + B)$ and if B is very small what I can do. So, when I have $\ln(1 + B)$ this can be expanded in a say Taylor series and when B is small, the B^2 and higher order terms are dropped.

Then, I can say $\ln(1 + B)$ will be approximately equal to B. That means that I will just put B here instead of $1 + B$ this simplification what I am trying to do.

So, B is defined here. So, $\ln(1 + B)$ is just written as B here and now I can write, so keeping this as ΔY , I can keep other terms here. So, that is what I am trying to do here. So, \dot{m}_c is some ΔY here divided by other terms. So, $s + Y_{O_2,s} / 4\pi r_s \rho D$.

$$\dot{m}_c = 4\pi r_s \rho D \frac{Y_{O_2,\infty} - Y_{O_2,s}}{s + Y_{O_2,s}}$$

$$\dot{m}_c = \frac{(Y_{O_2,\infty} - Y_{O_2,s})}{(s + Y_{O_2,s}) / (4\pi r_s \rho D)} = \frac{\Delta Y}{R_{diff}}$$

$$= -\frac{\dot{m}_{O_2}}{s} \quad (D)$$

So, this term I call it the resistance offered to the diffusion; obviously, because the diffusion coefficient comes to the bottom here. So, this is the resistance which is offered. So, diffusion is directly proportional to ρD , now in this term $(s + Y_{O_2,s})/4\pi r_s \rho D$. The diffusion term ρD comes in the denominator. So, this is taken as resistance offered to the diffusion.

So, to these surface r_s , from the infinity oxygen diffuses here. Now, second, that is the resistance for this. So, here it will be $O_{2,\infty}$. So, this is again $Y_{O_2,s}$. So, this is the potential difference and this is R_{diff} , this resistance is R_{diff} .

So, the amount of mass of O_2 coming from the gas phase to the surface is restricted by this R_{diff} term. R_{diff} is the resistance. So, we can write like this. So, this is going to restrict this. So, when I write this mass flow rate of carbon, we can write $\Delta Y/R_{diff}$.

So, the equation D is written for the gas phase diffusion where the driving force is this ΔY . $Y_{O_2,\infty} - Y_{O_2,s}$ divided by the resistance which is offered. So, that is written by $(s + Y_{O_2,s})/4\pi r_s \rho D$.

So, we have this circuit now. So, you can see r_s and there is one resistance which I call R_{kin} resistance. So, this will be the mass flow rate and there is another resistance here which is called R_{diff} , diffusion resistance for the mass flow rate of oxygen from the ambient towards this and we can see this is the value of $Y_{O_2,s}$.


Here, in this point $Y_{O_2} = 0$ and when you go to infinity Y_{O_2} will reach a value of Y_{O_2} infinity. So, this is the electrical circuit we have. So, mass transport of oxygen, put negative sign indicating that it is opposite direction to the radial coordinate or the mass flow of the carbon.

$$\dot{m}_C = \frac{Y_{O_2,\infty} - 0}{R_{kin} + R_{diff}}$$

Now, what is this? Starting from $Y_{O_2,\infty}$ the mass fraction of oxygen goes to 0. So, that is the total ΔY . So, $Y_{O_2,\infty} - 0$ divided by there are two resistance connected in series. Here one is the resistance offered to the diffusion in the gas phase, another one is the resistance offered to the chemical kinetics at the surface of the solid.

So, when you add, then they are in series. So, the net effective resistance offered is addition of these two R_{Kin} plus R_{diff} . So, this will be the total mass flow rate. This is the easiest way to do.

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One-film Model – Resistances

Values of the kinetic and diffusion resistances are:

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

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:

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

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Now, I have the values of R kinetics defined, I have the value of R diffusion. So, once you know this I can solve, anyway you can see that if you want to calculate R_{diff} again you need the value of $Y_{O_{2,s}}$. So, you have to have iterative solution only.

See, R kinetics on the other hand, R kinetics is written with the kinetics parameters here. So, you can see this k_c $1/k_c$. So, $4\pi(r_s)^2 k_c$ and molecular weights $\times p/R_u T_s$, again T_s is unknown here. Anyway, T_s is assumed to be known in this analysis. Again, we have to use energy equation to solve T_s that would be done later.

$$R_{kin} = \frac{sR_u T_s}{4\pi r_s^2 M_{mix} k_c p}$$

So, if we keep this, k_c is known, everything is known, T_s is assumed to be known. So, K kinetics. So, R_{kin} can be got but R_{diff} will involve $Y_{O_{2,s}}$ and that should be again iteratively got.

So, I have put the value of the diffusion resistances here, you can see that the kinetic resistance and the diffusion resistance is $sR_u T_s / 4\pi(r_s)^2 M_{mix}$. This is the rate coefficient for the surface reaction into pressure.

As I told you surface temperature, reaction rate, surface radius and the pressure everything dictates the resistance here and it is inversely proportional see when the k_c is higher reaction rate is higher, resistance is low, pressure is higher resistance is low and so on.

Here diffusion again, when the ρD is higher then the diffusion resistance will be low and so on. So, this is the scenario here. So, as I told you R_{diff} involves the surface mass fraction of the oxygen, this term.

$$R_{diff} = \frac{s + Y_{O_2,s}}{\rho D 4\pi r_s}$$

So, iteratively you have to solve it. So, guess the value or combine the equation and do it as this. So, a quadratic equation can be generated and solved or iterative procedure also can be used to solve. So, there are techniques to solve this.

Now, before doing that we can also try to eliminate one of the resistances, if one is very low in value compared to this.

So, $Y_{O_2,\infty}$ divided by the net effective resistance which is the sum of these two, if one is very much higher than the other then I can neglect the other value.

So, to analyze that let us take the ratio of resistances, the kinetics resistance to diffusion resistance is written like this. I have to just factorize this. So, $s + Y_{O_2,s}$, then $R_u T_s /$ molecular weight of mixture $\times p \times D$. So, $\rho D / k_c$, rate of this and the surface radius itself.

$$\frac{R_{kin}}{R_{diff}} = \left(\frac{s}{s + Y_{O_2,s}} \right) \left(\frac{R_u T_s}{M_{mix} p} \right) \left(\frac{\rho D}{k_c} \right) \left(\frac{1}{r_s} \right)$$

So, if I write like this basically it is actually this. So, if we take this into account, there are the scenarios. Let us say this ratio is much greater than 1, ratio is much less than 1 or it is almost equal to 1. Now, you will get the modes of the combustion.


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One-film Model – Combustion Modes

✓ If $R_{kin} \ll R_{diff}$, the combustion is diffusion controlled. This happens when r_s is large, T_s and p are high.
Here, $\dot{m}_C = Y_{O_2,\infty} (R_{diff} + r_s)$

If $R_{kin} \gg R_{diff}$, the combustion is kinetically controlled. This happens when r_s is small, T_s and p are low.
Here, $\dot{m}_C = Y_{O_2,\infty} / R_{kin}$

If $R_{kin} \approx R_{diff}$, the combustion is controlled by both kinetics and diffusion.
Here, $\dot{m}_C = Y_{O_2,\infty} / (R_{diff} + R_{kin})$





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So, the combustion modes of carbon will be classified into 3 when the kinetic resistance is much lesser than the diffusion resistance then it is diffusion control because kinetic resistance is very less. So, kinetic is very fast.

So, what is controlling is the amount of oxygen which is reaching the surface that is controlled by the diffusion, so that is going to control the entire process. So, the process will be diffusion controlled.

$$\dot{m}_C = Y_{O_2,\infty}/R_{Diff}$$

So, when the kinetic resistance is small that indicates that the surface reactivity is very high, reactions are very high. So, it will be finished and it is just waiting for oxygen to come to the surface and once the oxygen comes here the reaction is completed instantaneously.

So, the diffusion of the oxygen towards the surface will control the combustion process. So, this will occur when the r_s is large, this particle diameter or T_s and p being high you will get the diffusion control.

On the other hand, the resistance due to this is neglected and you can write this without involving the resistance to the kinetics. The other extreme case is when the kinetic resistance is much higher than the diffusion resistance then obviously the diffusion is faster here.

$$\dot{m}_C = Y_{O_2,\infty}/R_{Kin}$$

So, the process is kinetically controlled. Oxygen is available readily. Once the oxygen comes in it is instantaneously provided to the surface but the chemical reaction takes some time to finish. So, it is kinetically controlled. So, this is the other extreme.

When very small, the oxygen is present everywhere, very small particle the reaction takes some time to finish. The oxygen immediately will diffuse into this and wait till reaction is complete and so on.

So, low T_s , low p and small r_s this situation will be there, again only the kinetic resistance is included in the equation but in other cases the resistances are not much different and the ratio is 1, then it is controlled by both kinetic and diffusion. We have to use the entire equation like this. So, these are the mode. So, as I told you T_s is unknown here.

$$\dot{m}_C = Y_{O_2,\infty}/(R_{Diff} + R_{Kin})$$