Course Name: Combustion of Solid Fuels and Propellants
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Lecture 33 : Combustion Times for Diffusion and Kinetic Controlled Regimes

Hello everyone. So, we are continuing our discussion on combustion of metals. And today we are starting a new module on the combustion of metals part 2. And in this modules we are going to talk about the combustion of various energetic particles, but we are going to concentrate mostly on aluminium and boron. Just to give you an idea about how the heterogeneous combustion and homogeneous combustion takes place. Because if you recall our discussion regarding the different combustion modes based on the thermodynamic point of view like the difference between the volatilization temperature of the oxides and the boiling point temperature of the metal.

Based on that we have seen that some metals can burn homogeneously in gas phase, whereas other metals may burn in heterogeneously or surface reaction can take place. Now, the boron particle can be considered to be one of the example in the heterogeneous mode of combustion, whereas aluminium can be considered as the homogeneous mode of combustion. So, we will take these two examples just to you know brush up our understanding there and how they are different. And on the other hand since these two particles are considered to be one of the major ingredients as fuel for propellant application.

So, we will just try to see various you know mechanisms involved in the ignition and combustion of boron particles as well as the issue with boron ignition, how we can enhance the ignition process of boron. Then we will just look at the same thing for aluminium particles of course, the process is different there, but we will try to understand there also. And later part of this module we will talk about the future and I mean the recent development of metal particles as ingredients or fuels for propellant application. And I will try to bring some of my you know research activities, what my research scholars have done in last 10 years. So, starting from like a droplet combustion of you know particle loaded liquid fuels, maybe slurry fuels, some spray combustion data, we may talk about you know particles can be loaded in gel fuel as well.

And of course, we can show some of the you know work done by students on the solid fuels as well, because if you look at the propellant side it can be used directly mixed the particles in the solid fuel matrix like we can bind the particles using the polymeric binder HTPB. Now oxidizer can be the solid oxidizer or if we can use it use the propellant use the solid fuel grain in the hybrid mode, then we can think of you know gaseous oxidizer. But in summary the we are going to talk about the role of the metal particles in you know aerospace application in particularly like propellant or solid fuel application. So, we will try to end up our discussion on this module by give you some give you some glimpse of the recent and future development of you know metals as fuel ingredients in the solid propellant combinations. Now, in the today's lecture we will talk the two different you know combustion times, one is for diffusion another is for kinetic control regimes, because from thermodynamic analysis we have understood that the metals can burn either heterogeneously or through surface reactions or homogeneously or through gas phase reaction.

There we have talked about the boiling point temperature of metal and compared that with the oxides volatilization or dissociation temperature. In many occasions since the oxide volatilization temperature is much higher compared to the boiling point temperature of metal, in that case homogeneous or gas phase reaction can take place for example, aluminum. Whereas, if the oxide volatilization temperature is much lower than the melting point temperature of the metal, then the surface reaction take place or heterogeneous combustion can take place. Now, once we talk about the metal particles in propellant applications, it is bringing one time scale into the problem like how the transport of mass and energy is taking place compared to the reactions. Now, in certain cases the reaction can be faster whereas, the transport of mass energy may not be that fast compared to the reaction rate.

In that case the combustion will be controlled by the transport process or the diffusion of the species and the energy transfer. So, in that case the combustion will be controlled by the diffusion mode and in that case we must need to consider the diffusion of the species there. And we cannot ignore the special non uniformity in the zone and we must need to consider the transport processes there. So, how they are going to relate with the combustion times? Of course, we have already talked about the diffusion control combustion for a single droplet. We have considered you know single droplet combustion in a quiescent media and there we have discussed about how the evaporation rate constant is found out and how we can actually calculate the you know burning time I mean sorry the evaporation time from there we got the equation.

So, we can recall those equations and we can write the same thing for you know combustion times for diffusion control case. Now, in case of kinetic control the reaction rate is comparatively slower than the transport or the chemical sorry the transport of mass and energy. So, in that case the special non uniformity can be ignored and we can actually consider that the combustion regime is kinetic control. So, we can also consider the time the combustion times for kinetic control regimes and then we can compare the diffusion control mode and kinetic control mode and try to find out one ratio of the both. And we can see what are the influencing factors for transitioning from kinetic control to diffusion control mode or diffusion control regime.

So, let us look at what we did in the previous module. I will just try to give you a glimpse of the equations what we already wrote. So, for a diffusion for diffusion control case and if we say that the Lewis number is unity Lewis number is going to tell us like thermal diffusivity versus the mass diffusivity. So, if we consider the Lewis number to be unity. So, this is defined is the thermal diffusivity by the mass diffusivity.

In this case the mass consumption rate what we have said the mass consumption rate per unit surface area what you have written? We have written the equation as m dot by 4 pi r p square I am writing the particle diameter particle radius here earlier we have used the general radius r, but now since we are concerning our discussion to metal particles. So, I am writing this as m dot by 4 pi r p square where r p is the particle radius and that we got the equation something like rho D by r p ln 1 plus B and we have defined this that B is the like mass transfer number or transport number rho is the gas density. So, in case of fuel droplet evaporation we have said that rho is the density of the media consisting of fuel vapour and oxidizer vapour. So, we have considered that one. So, similarly it is like the gas density D is the gas mass diffusivity alpha is the gas thermal diffusivity if you wish to write thermal diffusivity of course, r p is the particle radius ok

$$\frac{m^{\cdot}}{4\pi r^2} = \frac{\rho D}{r}\ln(1+B)$$

Now, we have also told ourselves that if it is the vaporizing particle in case of vaporizing particle we can have the B transport number based on the coupling function between the energy and oxidizer and we wrote the equation something like B O Q in terms of like mixture ratio stoichiometric into Y o infinity into delta H r f plus C p T infinity minus T s divided by the latent heat of vaporization. I think in the previous lecture we had seen this one where you know heat of reaction of the fuel per unit mass is given by delta H r f Y infinity Y o infinity is the mass fraction of oxidizer at the far from the particle surface, C p is the specific heat, T infinity is the gas temperature far from the surface, T s is the surface temperature, L V a p is latent heat of vaporization. Now, also we have said that particle with heterogeneous surface reaction we can obtain the coupling function of the fuel of oxidizer species equation. So, for particle with heterogeneous surface reaction this transport number can be obtained from the coupling function of fuel oxidizer species equation. So, we have already written that this is going to be B O F oxidizer and fuel species equation and this was given as mixture ratio stoichiometric into Y o infinity plus Y f s divided by 1 minus f s this was the definition given there.

$$Bo,q\ = \frac{\left(\frac{F}{O}\right) st\ Yo\infty\ \Delta hrf\ + cp\ (T\infty - Ts)}{Lvap}$$

$$Bof\ = \frac{\left(\frac{F}{O}\right) st\ Yo\infty\ \ + Yfs}{1 - Yfs}$$

Now, if there is no volatility of the fuel if there is no volatility of the fuel we can write that Y f s is going to be 0 mass fraction of the fuel at the surface is going to be equal to 0. So, we can write B O F as simply f by o stoichiometry into Y o infinity that I think we have written. And if you look at this equation for the mass consumption rate per unit particle surface area this equation a. So, from equation a we can simply write the mass consumption rate per unit surface area will now become rho D by R p ln 1 plus f by o stoichiometry Y o infinity this is the equation. Now, if you recall we had got the diffusion time for evaporation if you recall the evaporation time for the droplet which has the initial diameter D 0 we already got in the previous discussion same thing if we apply and if you try to write the combustion times for the diffusion control case we can simply write the burning time for diffusion is going to be equal to density of the particle initial diameter of the particle divided by 8 into rho D ln 1 plus B.

$$Bof \ = \left(\frac{F}{O}\right) st \, Yo\infty$$

$$\frac{m^{\cdot}}{4\pi r^2} = \frac{\rho D}{r} \ln\left(1 + \left(\frac{F}{O}\right) st \, Yo\infty\right)$$

This I am simply writing from the analysis we have done for the droplet evaporation case where we have written the evaporation time as the rho L D 0 square divided by 8 rho ln sorry D into ln 1 plus B. I think in the previous lecture we have seen this one for the fuel droplet evaporating in oxidizing environment of course, in a cohesion media surrounding by the oxidizer and there we find out that. So, same thing we have applied here. So, for the diffusion control regime case the combustion time can be given by this equation. So, let us give a name as B.

$$t\, b,\ diff \ = \ \frac{\rho do^2}{8\rho D \ln(1+B)} \ - (B)$$

So, for a particle with surface reactions this is just for the diffusion with evaporation case, but if we have the surface reaction we can modify this one by using the transport number for that particular case where we have the surface reaction and we have already modified that by this one. So, we can simply update that equation by putting the value of B. So, let us say for a particle with surface reactions, what will be the reaction time scale? This T b diffusion is going to be rho p D 0 square divided by 8 into rho into D into ln. I am simply replacing the B with 1 plus F by O stoichiometric Y O infinity. This I think we already had in the previous equation.

You see for the particle with heterogeneous surface reactions we can write this BoF coupling function between the oxidizer and fuel species reactions and we have said that for no volatility of the fuel we can consider Y f s we can assume Y f s to be 0. So, BoF finally, becomes F by O stoichiometry Y O infinity and this one we have replaced in the equation A and from there actually basically we can replace with this equation this is the time commotion time for diffusion case. So, T b diffusion is simply going to be this we just simply replace B with this. So, if you look at here we have simply replaced B with this one. So, this is the equation for the combustion time for diffusion control case where rho p is we have not said it earlier.

$$t\, b,\ diff \ = \ \frac{\rho do^2}{[8\rho D \ln \quad]\left[1 + \left(\frac{F}{O}\right) st \, . \ Yo\infty\right]} \ - (C)$$

So, rho p here is the particle density and D 0 is the initial diameter initial particle diameter or initial diameter of the particle of the particle ok. So, for diffusion control regime we can actually get the time for the combustion T b diffusion by this equation. Now, for kinetic control case what we said for kinetic control case we had assumed that diffusion rate of the oxidizer to the surface is much faster compared to the reaction rate at the particle surface. So, the spatial non uniformity can be ignored and we can approximate the oxidizer mole fraction at the surface. So, what we are saying is like no spatial non uniformity exist in case of kinetic control combustion.

So, if the oxidizer mole fraction at the surface is X o infinity the same thing will be there sorry this is at the surface. If these are the surface the same mole fraction will be there at the far field or far from the particle just because we had considered the spatial non uniformity does not exist in this case. So, we can say approximately this X o s is approximately equal to X o infinity and for this case the mass consumption rate. So, this is like oxidizer mole fraction. So, the mass consumption rate per unit area was given at the molecular rate of the product into K into pressure P into X o

$$\frac{m^{\cdot}}{4\pi r^2} \approx MWp \times PXow$$

Here K is the rate of surface reaction X o is of course, the oxidizer mole fractions we have already written. So, if we just find out the time for combustion time for time for kinetic control regime, T b kinetic is given by rho p d 0 by 2 m dot a molecular weight into K into P into X o infinity. For this one I think one can refer to the chemical kinetics part for diffusion control and kinetic control reaction rate for any combustion book one can refer to it and just look at these equations for reaction rate just to brush up the things. So, what we are going to do is we are going to compare the kinetic control case and diffusion control case for the two time scale what we got for diffusion control and kinetic control. If we look at carefully for the diffusion control case the T b is actually proportional to d 0 square or the diameter square.

$$t\, b, x\, in = \frac{\rho do}{2MWp \times PXo\infty}$$

Whereas, in case of kinetic control regime the time scale the time T b is proportional to d 0 or just you can say only diameter not diameter square. Another important consideration we can look at in case of kinetic control regime the T b is found out to be inversely proportional to the pressure. You see there is no pressure equation in case of divisional control combustion time. So, we can say that it was independent of pressure under the diffusion control case, whereas, the here is actually inversely proportional. Now, if we compare these two time combustion time like for diffusion control and kinetic control the dominant combustion mechanism can be found out if we compare the two time scale and one number is defined is called the Dam kohler number.

And it is denoted as (Da) it is basically the ratio between the diffusion time by kinetic control time. So, you just put the equation there we can end up getting molecular weight into K into P into X o infinity of course, one d 0 will be there because there is a d 0 square. So, one d 0 will be there in the numerator divided by 2 here there is a 8. So, it will become 4 into rho into d ln 1 plus f by o stoichiometry into mass fraction of oxidizer infinity. So, what does it tell us that this is the ratio of the diffusion control versus the kinetic control case.

$$\frac{tb\ diff}{tb\ xin} = \frac{MWp \times PXo,\infty do}{4\rho \ln\left[1+\left(\frac{F}{O}\right)st\ .\ Yo\infty\right]}$$

So, it can actually gives us that if d A is equal to 1 that is going to defines the transition you know between diffusion control and kinetic control regime sorry kinetic control regimes. So, what we can say here is that this is you know if we say that for a large particle if you look at for the large particle. So, it is kind of a some inverse relationship exist between the particle diameter and the pressure you see pressure is here particle diameter is here. So, what we can say that for a large particle with high pressure it is expected that the combustion will be more likely to be the diffusion control because you see the Dam kohler number is going to be greater than 1. So, it will be expected to have like diffusion control combustion regime if we have if we consider the large particle with the high system pressure whereas, in case of small particles with low pressure that may lead to like kinetic control combustion.

So, this is very important consideration like particles with larger diameter and high pressure. So, from this Dam kohler number equation you can show that the large particle large particles with you know high combustion pressure or yeah high combustion pressure basically we are talking about the combustion pressure in the system this is you know most likely towards the diffusion control regime diffusion control combustion whereas, small particles at low combustion pressure it is you know expected to have like kinetic control regimes kinetic control combustion. And this way actually we can define the burning of various you know size of particles and we can observe the they are burning mechanisms and we can find out how they are behaving several you know experimental studies and numerical studies are available in literature for boron as well as you know other metal particles and they can actually define how the burning is taking place whether it is a diffusion control or kinetic control case based on the particle sizes. But you know at the advance of nanotechnology once the particle sizes are coming towards the nano scales then there is one more time scale sorry one more length scale is becoming very important because of you know the if the size of the particles is very small of the order of like 100 nanometer or so, then we can actually compare the length scale with the length scale of the metal with the mean free path. Now a comparison with the length scale of the particle or the metal particles with that of the mean free path of the ambient gas we can get to know whether continuum condition exists like whether the particles can be distinguished separately from the gas molecules or not.

So, this is a this is an another length scale consideration we have to consider if we compare the Knudsen number. So, what is telling by definition is Knudsen number is defined as mean free path of the gas molecules divided by the particle diameter 2 into or basically the mean free path by particle radius you can say. So, this is a dimensionless parameter here it is telling that if the particle diameter is becoming very small and if it is comparable to the mean free path of the ambient gas then the combustion scenario or combustion mode may be different because in that case the macroscopic particles consideration may not exist because we cannot consider the macroscopic particles in the continuum gas. So, we have to see that if the diameter of the particle is becoming so small how we can characterize that length scale by considering the Knudsen number. So, I think we can briefly talk about this part in the following lecture just to you know know that this is another I mean another length scale considerations coming out due to the advancement of the nanotechnology because in many occasions the part it is has been said that the nanoparticles are behaving much better than the micron size counterpart.

$$Kn = \frac{2\lambda}{dp}$$

So, if the particle size are becoming 100 nanometer or even smaller then we must need to compare that with the mean free path of the ambient gas and just to see that whether the continuum is existing or not in that case it may so happen that the particles cannot be you know separately treat as the macroscopic particles in the continuum gas. So, just we want to just you know look at little further before we close the discussion and then I think we can talk about the two different particles like boron particles and aluminum particles and their combustion mechanism and we will move ahead ok. So, let us stop here today we will continue in the next lecture. Thank you.