


Fundamentals of Combustion for Propulsion
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Lecture – 33
Tutorial

Hello everyone, hope you are enjoying the lectures of Fundamentals of Combustion for Propulsion. There were some requests for a problem solving session, I have put together some material for I will; I have put together a few simple problems that will reinforce some of the ideas that we have discussed so far in the course. So, in this short video, we will go through a few worked examples and see how it goes from there, ok.

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Fundamentals of Combustion for propulsion

(1) Stoichiometry $C_8H_{18} + 12.5 \left(O_2 + \frac{7.9}{21} N_2 \right) \rightarrow 8CO_2 + 9H_2O + \frac{7.9}{21} \times 12.5 N_2$


$\begin{matrix} \text{n-octane} & & \uparrow & & \\ & 21\% \text{ by Vol } O_2 & & & \\ & 79\% \text{ by Vol } N_2 & & & \end{matrix}$

Mass basis $\left(\frac{O}{F} \right)_{Stoic} = \left(\frac{A}{F} \right)_{Stoic} = \frac{12.5 \times \left[32 + \frac{7.9}{21} \times 28 \right]}{12 \times 8 + 1 \times 18} = 15.1$

(2) Formation enthalpy $C_8H_{18} + 12.5 \left(O_2 + \frac{7.9}{21} N_2 \right) \rightarrow 8CO_2 + 9H_2O + \frac{7.9}{21} \times 12.5 N_2$

Elements in naturally occurring form are taken to have $\Delta_f^\circ = 0$

$8C_{(gr)} + 9H_{2(g)} \rightarrow C_8H_{18(l)} \quad \Delta_{f, C_8H_{18}}^\circ = -250 \frac{kJ}{mol}$



I will start with the idea of will start with the so, this is. Let us start with the idea of stoichiometry; let us a take for simplicity the fuel as a normal octane and the oxidizer as air.

Remember that air has 21, approximately 21 percent by volume of oxygen and 79 percent by volume of nitrogen, ok. This 3.76 is nothing, but maybe I will explicitly write it as 79 by 21, ok.

For every 21 percentage of oxygen, there is 79 percentage of nitrogen. This is what we will treat approximately as air; there are some traces of argon, carbon dioxide and so on which we will ignore for the purposes of the current discussion. A stoichiometrically balanced reaction for octane would should result in 8 moles of carbon dioxide and 9 moles of water vapor or water plus whatever nitrogen has left, ok. To balance this reaction we need 8 moles of diatomic oxygen and 4 and a half moles of diatomic oxygen for the steam part. So, the total number of diatomic oxygen moles that will balance this equation is 12.5.

So, 12.5 is, 12.5 moles of oxygen is required for stoichiometrically balanced reaction of octane. And since 21 percent of oxygen comes with 79 percent of nitrogen in air, we also have that $79 \text{ by } 21 \text{ times } 12.5$, ok. So, this is the stoichiometrically balanced reaction for octane.

With this now we can calculate the oxidizer to fuel ratio; the oxidizer here being air, this is also the air to fuel ratio for stoichiometry, will be the amount of this is on mass basis. This is just the amount of oxidizer which in this case is 12.5 times the molecular weight of oxygen which is 32 plus $79 \text{ by } 21 \text{ times the molecular weight of nitrogen}$. This is the mass of the oxidizer divided by the mass of the fuel; the fuel has 8 carbon atoms each 12 grams per mole plus 18 hydrogen atoms which is 1 gram per mole, ok.

So, this will give you an air to fuel ratio of about 15.1 which is a number that is more or less for all hydrocarbon fuels, the oxidizer to fuel ratio or the air fuel, stoichiometry air to fuel ratio will be about 15 to 20. So, that is as far as stoichiometry is concerned. Let us move on to the idea of formation enthalpy.


This is also something that we discussed in class and I will take the same example to motivate the idea of formation enthalpy. Recall that formation enthalpy is defined as the enthalpy of reaction in which component is formed from its naturally from the component elements


which are occurring in the elemental natural form, let me repeat that, ok. Let me first give these elements in naturally occurring form are taken to have 0 formation enthalpy, ok.

Others which are not naturally occurring formed from these elements and the enthalpy of that reaction is called the enthalpy of formation, I will give you a simple example. Let us take for example, octane itself; octane is made up of elemental carbon in graphite form which is a naturally occurring form plus 9 H₂ which is the naturally occurring form of hydrogen element which is diatomic hydrogen gas will form C₈H₁₈ which is a liquid under normal conditions of temperature and pressure.

And the enthalpy change of this reaction is the enthalpy of formation of octane, which as it turns out to be is negative 250 kilo Joules per mole, turns out to be negative 250 kilo Joules per mole.

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$$\left(\frac{\dot{F}}{\dot{F}} \right)_{\text{Stoic}} - \left(\frac{\dot{F}}{\dot{F}} \right)_{\text{Stoic}} = \frac{12 \times 8 + 1 \times 18}{21} = 15.1$$

(2) Formation enthalpy $\text{C}_8\text{H}_{18} + 12.5 \left(\text{O}_2 + \frac{7.94}{21} \text{N}_2 \right) \rightarrow 8\text{CO}_2 + 9\text{H}_2\text{O} + \frac{7.94 \times 8}{21} \text{N}_2$

Elements in naturally occurring form are taken to have $h_f^\circ = 0$

$R_1: 8\text{C}_{(gr)} + 9\text{H}_{2(g)} \rightarrow \text{C}_8\text{H}_{18(l)} \quad h_{f, \text{C}_8\text{H}_{18}}^\circ = -250 \frac{\text{kJ}}{\text{mol}}$

$R_2: \text{C}_{(gr)} + \text{O}_{2(g)} \rightarrow \text{CO}_{2(g)} \quad h_{f, \text{CO}_2}^\circ = -393.5 \frac{\text{kJ}}{\text{mol}}$

$R_3: \text{H}_{2(g)} + \frac{1}{2} \text{O}_{2(g)} \rightarrow \text{H}_2\text{O}_{(l)} \quad h_{f, \text{H}_2\text{O}_{(l)}}^\circ = -285.8 \frac{\text{kJ}}{\text{mol}}$

$\text{H}_{2(g)} + \frac{1}{2} \text{O}_{2(g)} \rightarrow \text{H}_2\text{O}_{(g)} \quad h_{f, \text{H}_2\text{O}_{(g)}}^\circ = -241.8 \frac{\text{kJ}}{\text{mol}}$

$R = 8R_2 + 9R_3 - R_1 \Rightarrow \Delta H = 8h_{f, \text{CO}_2}^\circ + 9h_{f, \text{H}_2\text{O}_{(l)}}^\circ - h_{f, \text{C}_8\text{H}_{18(l)}}^\circ$

Let us call this reaction 1, let us call this reaction just reaction R. And if you take C O_2 , to form C O_2 carbon and oxygen by the way the naturally occurring form of oxygen is gaseous oxygen in diatomic form; forms carbon dioxide gaseous form. The enthalpy of this reaction is the formation enthalpy of carbon dioxide, ok. And, the other one that we will need for this discussion is the formation reaction for water.

Hydrogen gaseous hydrogen combines with gaseous oxygen to form liquid water and the formation reaction; this is a formation reaction for liquid water and this has an enthalpy of negative 285.8 kilo Joules per mole. Keep this other reaction also in mind. It is a reaction for steam formation which is same H_2O , but in gaseous form; the enthalpy a formation of this reaction where the final product which is water is in steam form is negative 241.8 kilo Joules per mole.

Now, if you observe we can write reaction R, you can write reaction R as equal to 8 times reaction 2 plus 9 times reaction 3 minus reaction 1. Excuse me, notice that in reaction R 12.5 times 79 by 21 nitrogen is on both the sides; therefore, for the purposes of stoichiometry, for the purposes of enthalpy calculation it is the effects will cancel out, so it need not be explicitly included.

Therefore, the enthalpy change or the enthalpy of combustion or octane, which is the enthalpy change of reaction R, when octane plus stoichiometric amount of air gets converted into carbon dioxide and water vapor; I am sorry carbon dioxide and water. And the reactants and the products are at the same temperature and pressure; that is you have burnt octane and air it has gone to a higher temperature, you have extracted all the heat from the product gases and brought the product gases back to 300 Kelvin's.

That amount of heat is the enthalpy of combustion of octane, which from the definition of formation enthalpy now is 8 times the formation enthalpy of C O_2 plus 9 times the formation enthalpy of H_2O liquid minus the formation enthalpy of octane sorry C_8H_{18} liquid.

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$$\begin{aligned} \text{HCV}_{\text{C}_8\text{H}_{18}} &= -5470 \frac{\text{kJ}}{\text{mol}} = -48 \frac{\text{kJ}}{\text{g}} \\ \uparrow & \quad \uparrow \\ \text{H}_2\text{O}(\text{l}) & \quad \text{exothermic} \end{aligned}$$
$$\begin{aligned} \text{LCV}_{\text{C}_8\text{H}_{18}} &= -5074 \frac{\text{kJ}}{\text{mol}} = -44.5 \frac{\text{kJ}}{\text{g}} \\ \uparrow & \\ \text{H}_2\text{O}(\text{g}) & \end{aligned}$$

(3) Adiabatic flame temperature



You can plug in the numbers, I have given you the formation enthalpies earlier and then you will get what is called the higher calorific value of octane as negative 5470 kilo Joules per mole which meant divided by the molecular weight of octane will give you the calorific value ok, sorry this is per gram. I have explicitly retained the negative sign, because this is an exothermic reaction, ok.

And, it is HCV when the final product, the final water is in liquid form. But, in reality the combustion products are usually at a temperature that is much higher than the boiling point of water, and water usually exists as steam in real applications. Under such conditions, the heat or the energy that can be extracted by combustion of this fuel when the water is in water vapor form is you should use the formation enthalpy for steam instead of liquid water. If you

plug in that number in the equation that I showed in the previous page, you will get 5074 slightly lower energy.

Because the energy that is required for converting liquid water and the steam has been taken from the fuel itself, this will give you negative 44.5 kilo Joules per gram. This is the lower calorific value and the relevant number for the enthalpy of combustion of octane. And this is another feature of all hydrocarbon fuels; on a mass basis more or less all the hydrocarbons have the same calorific value of about between 45 and 50 kilo Joules per gram. So, with this background, let us move on to the third idea which is the idea of adiabatic flame temperature, idea of adiabatic flame temperature.

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(3) Adiabatic flame temperature

$$C_8H_{18} + 12.5 \left(O_2 + \frac{7.9}{21} N_2 \right) \rightarrow 8CO_2 + 9H_2O + 12.5 \times \frac{7.9}{21} N_2$$

$$5047 = \left(8 \times \underset{\substack{\uparrow \\ 42 \text{ J/mol-K}}}{\bar{C}_{p,CO_2}} + 9 \times \underset{\substack{\uparrow \\ 32.4 \text{ J/mol-K}}}{\bar{C}_{p,H_2O}} + 12.5 \times \frac{7.9}{21} \times \underset{\substack{\uparrow \\ 39 \text{ J/mol-K}}}{\bar{C}_{p,N_2}} \right) (T_f - T_0)$$

$$T_f = 300 \text{ K} + \frac{5047}{8 \times 42 + 9 \times 32.4 + 12.5 \times \frac{7.9}{21} \times 39} = 2351 \text{ K}$$



And let us take the same reaction and calculate, try and calculate the adiabatic flame temperature of the products. We will assume as a first approximation that the products are only carbon dioxide, water vapor and nitrogen.

Now, it is very easy to calculate the adiabatic flame temperature. We saw just a few moments ago that, the enthalpy of combustion lower calorific value of octane is 5074 kilo Joules per mole that is exothermic. And, when you burn octane what happens is that, this 50 for every mole of octane that you burn, 5074 kilo Joules of energy is of chemical energy is converted into heat and that heat is used to raise the temperature of the product gases from raise the temperature of the product gases.


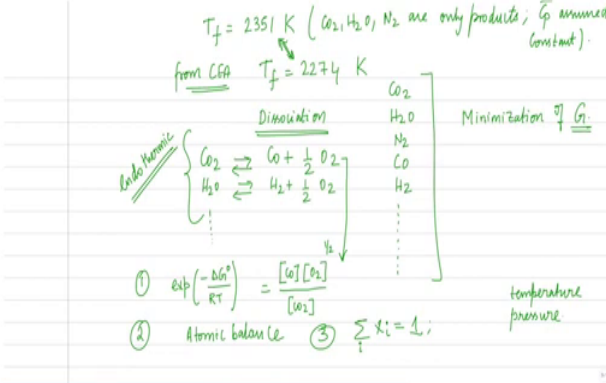
So, if we start with an initial temperature of 300 Kelvin's and supply 5047 kilo Joules of heat to these product gases; whatever temperature the product gases go to, is the adiabatic flame temperature. Therefore, the adiabatic flame temperature can be simply calculated by saying that, by burning 1 mole of C_8H_{18} 5047 kilo Joules of energy is liberated and that simply raises the temperature of 8 moles of CO_2 9 moles of H_2O , plus 12.5 times 79 by 21 moles of nitrogen, times R_f minus T_0 .

So, this simple formula, we know the molar specific heats of nitrogen water vapor and carbon dioxide, it is of course, C_p is C_p for multi atomic molecules or a function of temperature. But, approximate values for these quantities are 42 Joules per mole Kelvin for CO_2 , 32.4 Joules per mole Kelvin for a water vapor, and for nitrogen it is 39 Joules per mole Kelvin.

So, if you plug in these numbers you can get a value for T_f which is T_0 , which is the initial temperature is 300 Kelvin plus 5047 divided by. Well, I did not calculate that number 8 times 42 excuse me, 9 times 32.4 plus 12.5 times 79 by 21 times 39 we will get a number of 2351 Kelvin's. So, an adiabatic combustion at constant pressure of octane with stoichiometric amount of oxidizer, which is stoichiometric amount of air producing only 8 moles of CO_2 , 9 moles of water vapor and rest nitrogen.

Assuming these specific heat values, the adiabatic flame temperature is 2351 Kelvin's. This is a simple estimate for the adiabatic flame temperature of octane. Remember this value.

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Handwritten slide content showing chemical equilibrium analysis for octane combustion:

- Top left: NPTEL logo
- Top center: $T_f = 2351 \text{ K}$ (from CEA), $T_f = 2274 \text{ K}$ (from CEA)
- Top right: $(\text{CO}_2, \text{H}_2\text{O}, \text{N}_2 \text{ are only products; } T_p \text{ assumed constant})$
- Center: Chemical reactions:

$$\begin{aligned} \text{CO}_2 &\rightleftharpoons \text{CO} + \frac{1}{2} \text{O}_2 \\ \text{H}_2\text{O} &\rightleftharpoons \text{H}_2 + \frac{1}{2} \text{O}_2 \end{aligned}$$
- Right side: List of species: $\text{CO}_2, \text{H}_2\text{O}, \text{N}_2, \text{CO}, \text{H}_2$
- Bottom left: Equilibrium equation: $\exp\left(-\frac{\Delta G^\circ}{RT}\right) = \frac{[\text{CO}][\text{O}_2]}{[\text{CO}_2]}$
- Bottom center: Atomic balance: $\sum_i x_i = 1$
- Bottom right: Minimization of G
- Bottom right: Temperature pressure

T_f is 2351; assumptions are $\text{CO}_2, \text{H}_2\text{O}$ and N_2 are the only products and C_p bar assume constant. Now, I gave a demonstration of how to calculate the adiabatic flame temperature using the chemical equilibrium and analysis code. And, if you use that code and calculate from CEA, if you calculate; you will get an adiabatic flame temperature of 2274 Kelvin's for the same reaction octane with stoichiometric amount of air.

Why is there a difference? Here is a difference of about 80 Kelvin's, ok. Why is there a difference? So, if you look at the product concentrations that CEA gives, product concentrations that CEA gives; in addition to $\text{CO}_2, \text{H}_2\text{O}$ and nitrogen, you will also find CO, H_2 and traces of several other species, ok. So, one of the reasons or one of the primary

reasons why the estimate of the adiabatic temperature from the simple calculation differs from the actual numbers is; because of the phenomenon of dissociation. What I mean by that is that CO_2 at 2351 Kelvin's will not remain CO_2 , it will dissociate into CO and O_2 .

Similarly, water vapor at 2351 Kelvin's will not remain as water vapor, but it can dissociate into hydrogen and oxygen and several other reactions can happen of decreasing importance. And these dissociation reactions are endothermic, these reactions are endothermic; and therefore, they take up heat and bring down the flame temperature, ok. And the way NASA, CEA calculates the equilibrium temperature is by minimization of Gibbs free energy, standard thermodynamic procedure for calculating equilibrium states in minimization of Gibbs free energy. I will not go into the details, but I leave it as an exercise for you to try and calculate the equilibrium composition.

For I assume that you have pure CO_2 at 2351 Kelvin's or some high temperature 2000 Kelvin's. And, if the temperature is held constant at 2000 Kelvin's and the pressure is held constant at 1 bar and you can consider a few cases 1 bar, 10 bar, and 13 bar. Calculate, try and calculate the equilibrium composition of CO_2 dissociation; that is if you allow for sufficiently large time, at the end of it how much of the CO_2 would have dissociated into CO and half O_2 .

As a simple example of that, you can look at the problem for example, of dissociation of pure carbon dioxide into carbon monoxide and oxygen; you can calculate the equilibrium composition by simple relation which connects the equilibrium constant to the Gibbs free energy change of this reaction which is exponential minus ΔG^0 by $R T$, ok. This is the Gibbs free energy change for this reaction. This is one equation, you have three unknowns; the two other equations come, this is one equation; the other equation is conservation of number of atoms called atomic balance.


If you start with 1 mole of CO_2 ; then at the end of the process, once equilibrium state is reached you will still have Avogadro number of carbon atoms and twice the Avogadro number of oxygen atoms. So, that is at atomic convert atomic balance; that will give you one additional equation to solve. The third equation is a simple relation that the sum of the mole

fractions must be equal to 1, ok. If you put these three equations together, you can solve for the equilibrium composition of C O_2 dissociation, steam dissociation, water gas shift reaction and so on and so forth.

And, combine this with the calculation of the adiabatic flame temperature, you will get from starting estimate of 2351, you account for more and more dissociation; you will slowly approach the number that you get from CEA. In fact, CEA is essentially does the same thing by minimising the Gibbs free energy and you can use the tool to calculate. A one advantage of doing this calculation is, you can check the effect of initial temperature; we know that as the temperature becomes higher and higher the dissociation the extent of dissociation goes up.

You can see the effect of temperature, I will not say initial temperature; I just say temperature and you can also see the effect of pressure. At a given temperature, as the pressure increases the extent, you will see that the extent of dissociation decreases; the famous a Shockley is principal, fine. That brings us to the end of the discussion on adiabatic flame temperature.

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Propellant burn rate calculation

AP / HTPB 86% AP and 14% HTPB

43% \swarrow 43%
 400 μ m 20 μ m
 (coarse) (fine)

$\rho_{AP} = 1950 \text{ kg/m}^3$
 $\rho_{HTPB} = 930 \text{ kg/m}^3$

1 kg propellant
 430g \rightarrow 400 μ m
 430g \rightarrow 20 μ m
 140g \rightarrow HTPB

(i) Binder thickness (coated over all AP particles with uniform thickness)

(a) Volume of binder (HTPB) = $\frac{m_{HTPB}}{\rho_{HTPB}} = \frac{0.140}{930}$

is to be coated over 430g of 400 μ m AP and 430g of 20 μ m AP with uniform thickness (t_b)

Let us move on to the next topic which is some basic calculations required for propellant burn rate prediction. This is a topic that was discussed in some detail during the lectures. So, I will show you the basics, I probably went through the equations a little bit faster during the lecture.

What we will do, what you will do now is take a simple propellant composition and try to go through the steps of propellant burn rate calculation, ok. So, the example I have chosen today is an ammonium perchlorate, HTPB propellant; remember that ammonium perchlorate is the oxidizer, and HTPB is the fuel. The propellant I have chosen today has 86 percent ammonium perchlorate and rest is HTPB 14 percent HTPB, ok. Remember that the you may recall that the stoichiometric AP HTPB proportion is close to about 90 percent AP and 10 percent HTPB.

But there are processing issues associated with mixing a lot of solids solid ammonium perchlorate into liquid monomer of hydroxy terminated poly butadiene. Therefore, in practical applications typically the total amount of solid substances; including ammonium perchlorate, aluminium catalyst, etcetera does not exceed 86, 87 percentage. So, the example I have chosen is 86 percent AP and 14 percent HTPB. In this particular example, we will take this 86 percent AP to be composed of two different particles sizes; one is 400 micrometre and the other is 20 micrometre. Usually in practice this is referred to as coarse AP, this is referred to as fine AP, ok.


We will assume that of the 86 percent 43 percent is 400 micron and another 43 percent is 20 microns and the rest is HTPB. Some numbers that we will need for calculation is the density of AP which is 1950 kilograms per meter cube and density of HTPB is approximately 930 kilograms per meter cube. Let us start the calculation. Recall that the first step is to calculate binder thickness; the binder is HTPB and it is assumed to be coated over all AP particles 400 micron and to 220 micron with uniform thickness.

So, the first step in the calculation of propelling burn rate is a calculation of binder thickness, ok. So, first step in that is, calculate how much binder is there to begin with, so volume of binder or volume of HTPB is ok. For simplicity we will assume, we have 1 kilogram of this propellant, ok. So, for this particular example, we will take 1 kg propellant 86 percent is AP therefore, 860 grams is AP; out of that 430 grams is 400 microns assume that you are making a 1 kilogram batch.

To make 1 kilogram batch of this particular composition; you should take 430 grams of 400 micron AP, another 430 grams of 20 micron AP and 140 grams of HTPB plus HTPB plus other curing agents and other additives which are added to HTPB, but I'll simply refer to that entire mix as HTPB, ok. Therefore, the volume of the binder is the mass of the binder by the density of the binder, ok. Let me refer to just to avoid confusion and refer to both, I will refer to be refer to in to a simply HTPB; mass of the binder is 0.140 kilograms, we just saw it is one forty grams divided by the density of HTPB is 930, ok.

So, this is the volume of the binder and this volume is to be coated over 430 grams of 400 micron AP and 430 grams of 200 micron AP, I am sorry 20 micron AP with uniform thickness; which will assume is uniform thickness which will denote as t_b .

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430g → 400 μm
 430g → 20 μm
 430g → HTPB

(i) Binder thickness (coated over all AP particles with uniform thickness)

(a) Volume of binder (HTPB) = $\frac{m_{HTPB}}{\rho_{HTPB}} = \frac{0.140}{950}$

is to be coated over 430g of 400 μm AP and 430g of 20 μm AP with uniform thickness (t_b);


 $\text{Volume}_{400} = \frac{\pi}{6} \left[(400 + 2t_b)^3 - 400^3 \right] \times N_{400}$
 $N_{400} = \frac{0.43 \text{ Kg}}{1950 \times \frac{\pi}{6} \left(\frac{400}{10^6} \right)^3} = \dots$


 $\text{Volume}_{20} = \frac{\pi}{6} \left[(20 + 2t_b)^3 - 20^3 \right] \times N_{20}$
 $N_{20} = \dots$


Now, it is very simple, you have considered one 400 micron AP particle; if one 400 micron AP particle is surrounded by or coated by binder, the thickness of the binder is t_b and therefore, when you coat the 400 micron particle with thickness t_b , diameter will increase to 400 plus 2 times t_b , right. So, the volume of this binder, this volume I am referring to this coated volume is assuming the particles to be spherical is $\frac{\pi}{6} (400 + 2t_b)^3$ minus 400 cube, ok.

It is simply the volume of the AP plus the binder minus the volume of the AP is what is left which is the binder. This is for one AP particle; therefore, the total volume is this multiplied

by number of 400 micron AP particles. So, number of 400 micron AP particles is simply, the mass of 400 micron AP particles which is 430 grams, so 0.43 kilograms divided by the mass of one AP particle. Mass of one AP particle is the density of AP multiplied by the volume of one AP particle which is $\pi \times 400^3 \times 10^{-6}$ raised to 6 cube, ok.

So, this will be a very large number, but this and multiplied with the volume of binder coating one particle, we will get all the binder coated over 400 micron particle. Similarly 20 micron and same thickness ok; this is a 20 micron particle, 20 micron AP particle. So, this is 20, this diameter is 20 the whole diameter is 20 plus 2 t b micrometre, ok. Similarly this volume 400, volume over 400 is this much; volume over 20 will be 20 plus 2 t b cube minus 20 cube times N 20. And, N 20 would be same 0.43, ok.

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Handwritten calculations and a table for binder volume calculation.

For 400 μm AP: $\text{Volume}_{400} = N_{400} \frac{\pi}{6} [(400 + 2t_b)^3 - 400^3]$, $N_{400} = \frac{0.43}{1950 \frac{\pi}{6} (\frac{400}{10^4})^3}$

For 20 μm AP: $\text{Volume}_{20} = N_{20} \frac{\pi}{6} [(20 + 2t_b)^3 - 20^3]$, $N_{20} = \frac{0.43}{1950 \frac{\pi}{6} (\frac{20}{10^4})^3}$

for every 400 μm there will be 8000 20 μm particles

$\text{Volume binder} = \frac{0.14}{930} = \text{Volume}_{400} + \text{Volume}_{20}$

$t_b = 1.8 \mu\text{m}$

$t_b (\mu\text{m})$	$d_{AP} (\mu\text{m})$	ρ_{AP}	$T_f (K)$	L_i	$\eta_i (\frac{\text{kg}}{\text{m} \cdot \text{s}})$	at 20 μm
1.8	400	987	1706	0.46	4.75	
1.8	20	987	1960	0.54	7.37	


So, we were looking at volume 400 is N_{400} multiplied by π by 6×400^3 plus $2 \times t_b$ the whole cube minus 400^3 . And volume 20 is N_{20} π by 6×20^3 plus $2 \times t_b$ of whole cube minus 20^3 . N_{400} is 0.43 by 1950 π 6×400^3 by 10^6 raised to 6, because you are converting microns to meters, ok. And, N_{20} will similarly be 0.43 over 1950 which is a density of AP π by 6×20^3 by 10^6 raised to 6 cube.

As you can immediately see N_{400} itself will be a large number and N_{20} will be 8000 times more, ok. So, 400 micron surrounded by binder, 20 micron surrounded by binder; even visually you can appreciate the fact that 400 micron is AP rich and 20 micron is fuel rich. And for every 400 micron particle, since 400 micron and 20 micron are in equal mass proportion; for every 400 micron particle, there will be 8000 20 micron.

And this is a major source of heterogeneity of these composite solid propellants and that is the reason why the statistical approach is required for calculating its burn rates. So, we have calculated the volume. Now all we need to do is, recall that we calculated the volume of the binder or volume of the HTPB is 0.14 by 930. And this will be the volume, if it is coated with thickness t_b over 400 micron and 20 micron particles. So, by equating this to volume 400 plus volume 20; you can see that the only unknown in this equation is a binder thickness which you can calculate; I already calculated it, turns out to be around 1.8 micrometre.

So, a 400 micron particle is coated with 1.8 micron thickness binder and a 20 micron particle is also coated with 1.8 micrometre thickness. And that is the reason why the 400 micron particle has lot more AP than proportionally; I mean the fraction of the AP of the large particle is much higher than smaller particles. and that is in fact the next thing that we will calculate. With this thickness, we know this is 400 microns, we know the thickness of the binder; we can calculate the percentage AP. So, the percentage AP for this particle is as I said very high, this is mostly AP 97.6 percent AP and this is 76.2 percent AP.

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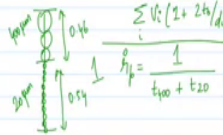
Overall AP = 86%

Volume binder = $\frac{0.14}{930} = \text{Volume}_{400} + \text{Volume}_{20}$

$t_b = 1.8 \mu\text{m}$

$t_b (\mu\text{m})$	$d_{AP} (\mu\text{m})$	% AP	$T_f (K)$	L_i	$\dot{m}_i \left(\frac{t_b}{s} \right)$	at 20 atm
1.8 ✓	400	98.7 ✓	1706 ✓	0.46 ✓	4.75 ✓	
1.8 ✓	20	76.2 ✓	1960 ✓	0.54 ✓	7.27 ✓	

$L_i = V_i \left(1 + \frac{2t_b}{d_i} \right)$; $L_{400} = \frac{0.43}{1950} \left(1 + \frac{2 \times 1.8}{400} \right)$
 $\sum_i V_i \left(1 + \frac{2t_b}{d_i} \right)$; $\frac{0.13}{1950} \left(1 + \frac{2 \times 1.8}{400} \right) + \frac{0.43}{1950} \left(1 + \frac{2 \times 1.8}{20} \right)$
 $\frac{1}{L_{400} + L_{20}} = \frac{1}{0.46 + 0.54} = 0.46 (46\%)$
 $L_{20} = 54\%$



So this is AP rich, this is fuel rich, ok. Let me make quick table, AP, percentage AP. Let me call it diameter A P in micrometres, percentage AP, the corresponding adiabatic flame temperature, line average fraction and the burn rate, ok. 400 micron, 20 micron, this percentage AP is 98.7; this is 76.2, t_b the binder thickness micrometre for both this 1.8.

We are assuming that all particles are coated with the same thickness and therefore, the binder thickness is same. Recall that overall percent AP which we started with is 86; that is the average of these two numbers, mass weighted average of these two numbers. So, the flame temperature calculated from NASA CEA is 1706 Kelvin's for the 400 micron particle and 1960 Kelvin's for a the 20 micron particle.

We will next move on to the problem of calculating, the line average fraction; remember that, line average fraction is defined as V_i is 1 plus 2 t_b by d_i divided by sum V_i 1 plus 2 t_b .

Recall that line average fraction of a particle of size d_i is the fraction of the length of the line occupied by that particle size and it is proportional to the volume fraction of that particle. Therefore, l_{400} is simply I have, already calculated the volume fraction; volume fraction is actually 0.43 divided by 1950 that is the volume of 430 grams of AP, so that is 0.02567, ok.

It is V_{400} , volume of the 400 micron particle multiplied by $1 + 2 \times 1.8 \times 400$ divided by sum of both; so, $V_{400} = 1 + 2 \times 1.8 \times 400$, ok. This V_{400} may be a little misleading, this is not the binder volume; this is the volume fraction of AP particles. I will explicitly write this is 0.43 divided by 1950 0.43 divided by 1950 plus the 20 micron is also 0.43 divided by 1950 and $1 + 2 \times 1.8 \times 20$. This will be the fraction of the length of the line occupied by 400 micron particles, this number turns out to be 46 or 0.46 46 percent.

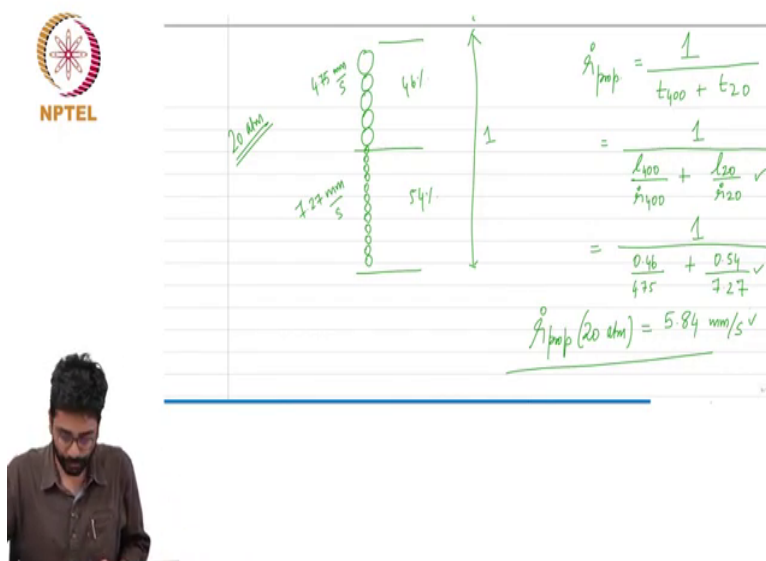
Similarly l_{20} is the rest of the line; it is 54 percent, ok. So, if you cut through this propellant, a large number of random lines and calculate for each of the lines what fraction of the line is occupied by particles of size 400 micron and 20 micron. And average it for a large number of lines; the statistical particle path will, if it has a length if it is assumed to have unit length, 46 percent of that line will be occupied by 400 micron particles and 54 percent of that unit length will be occupied by 20 micron particles 400 microns, 20 microns, ok.

So, now, we are ready to fill more entries into this table; l_i for 400 microns is 0.46 and this is 0.54. I will not go into the details of how to calculate $r \cdot d_i$; I have explained the theory behind it. The procedure is a little bit involved and that there is a reason why the equations have been coded into MATLAB and the burn rate calculation is done in MATLAB.

I already ran this code and got the burn rates for these particles, this is 4.5, I am sorry 4.75 millimetres per second and this is 7.27 millimetres per second. A good reference to remember yes this is at 20 atmosphere; a good reference to remember is that the AP burns at 3.3 millimetres per second at 20 atmosphere, adding a little bit of fuel increases the burn rate. Of course this is the proportion of AP and fuel for the 20 micron particle is lot more favourable; because the flame temperature itself is much higher than the 400 micron AP particle and proportionally the burn rate is also higher.

So, now we have everything that is required to calculate the burn rate of the propellant. Remember that, this is a statistical particle path; the burn rate of the propellant is the length of this line divided by time it takes for the 400 micron particle to burn plus the time it takes for the 20 micron particle to burn, I will continue this in the next page.

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So, we have this 400 micron particle occupying 45 plus 46 percent of the line and 20 micron particle occupying 54 percent; this is 54 percent, this is 46 percent, this burns at 4.75 mm per second sorry 7.5 mm per second. And, this burns at 7.27 mm per second, this is at 20 atmospheres; so pressure changes these numbers will also change.

The burn rate of the propellant is simply; the burn rate of the propellant is simply the length of this line which is taken to be 1 divided by time for the 400 micron to burn plus time for 20 micron to burn which is equal to 1 by. The time for 400 micron to burn is the length of 400

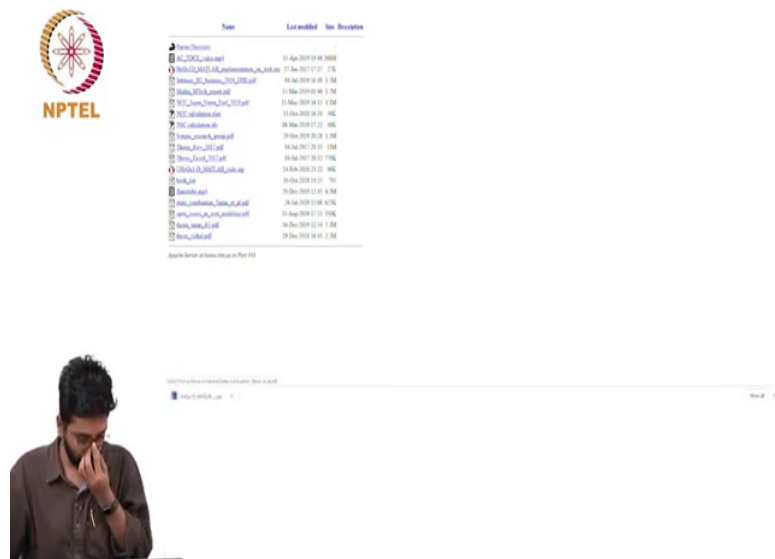
divided by $r \cdot 400$, lengths my velocity is time, length of 20 by $r \cdot 20$. All the numbers we have already calculated, l is 0.46; $l \cdot 400$ is 0.46 and it burns at 4.75.

And $l \cdot 20$ is 0.54 and it burns at 7.27; 7.27 not 25. And therefore, $r \cdot \text{prop}$ at 20 atmospheres is 5.84 mm. I will just go over this quickly one more time, we start with calculation of binder thickness by equating the volume coated with the actual volume of the binder and we found it to be 1.8, around 1.8 microns. From that we calculate from the; first we calculate binder thickness, then we calculate the percentage AP from the size of the AP and the binder thickness, and then look up from the table tabulated temperature flame temperature values, we look up the flame temperature values.

And from using the heterogeneous quasi 1 D theory or the quasi 1 D model, we can calculate these burn rates which I have not explained in this video; but there is a MATLAB code that is available, I will show it to you at the end of the. I will show you where you can get a copy of that code at the end of this lecture. And, one other information it is required for calculating the burn rate is; how much of the statistical particle path or what fraction of the statistical particle path is occupied by particles of different sizes.

And, the simplified in the simple example that we have considered; we found that, the 400 micron particle occupy is 46 percent of the line and 20 micron occupies 54 percent of the line. At all this information, we could calculate the burn rate of the propellant to be simply length divided by time, and length divided by the time is length of individual particles divided by the burn rate of the propellants. That is this when we plug in the numbers; we get burn rates of the propellant ok. So, that brings us to the end of this video; before I close, I just want to show you where you can get a copy of this code.

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You can get a copy of this code from my home page, which is `home dot i i t m dot a c dot in slash varun s`. Here you will see this particular file called `da he H e Q u 1 D`, we call it He Quad MATLAB implementation on web.

[illegible]

It will ask for whether you want to run the cases for propellants from Miller 19182 or Friedrich 1988 or some of the recent publications. You can run the code and check for yourselves how it works; feel free to look at the source code. And you will understand, you can better understand the procedure for calculating the binder thickness, oxidized into fuel ratio and more importantly the burn rate of individual particles. Of course, you will need

MATLAB to run this, ok. So, well with this I would like to conclude this problem solving session.

Thank you.