Fundamentals of Combustion for Propulsion
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Lecture - 17
HeQu1D model- Parameter estimation

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Premixed limits and parameter estimation for calculation

That is the first part of the model which is the geometry and the thermochemistry, the second part is Parameter estimation using the premixed limits.

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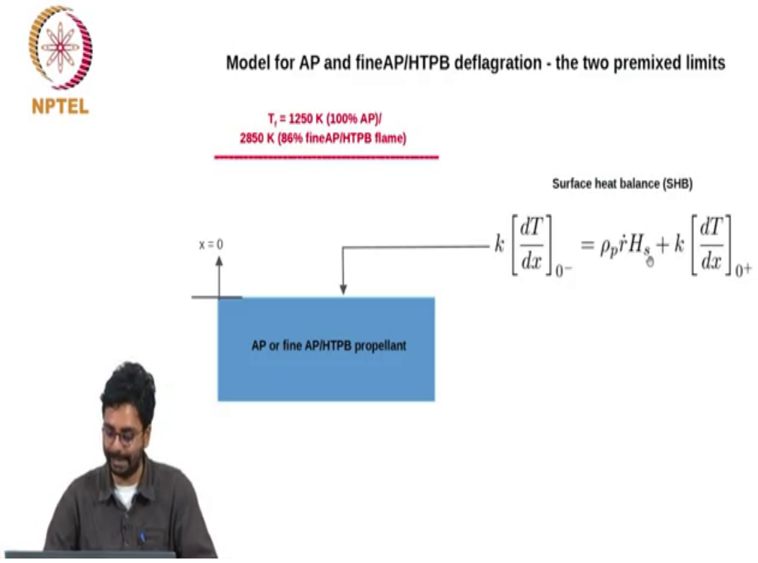

Model for AP and fineAP/HTPB deflagration - the two premixed limits

T_f = 1250 K (100% AP)/
2850 K (86% fineAP/HTPB flame)

Surface heat balance (SHB)

$$k\left[\frac{dT}{dx}\right]_{0^-} = \rho_p \dot{r} H_s + k\left[\frac{dT}{dx}\right]_{0^+}$$

I mentioned earlier that in the limits of monopropellant AP and homogenous propellant, the burning behaviour is controlled by one dimensional flame, one dimensional premixed flame and it can be represented like this; either you have a block of AP or fine AP HTPB propellant and there is a one dimensional flat flame over that surface. The flame temperature is either corresponding to the AP monopropellant temperature which is 1250 Kelvin's or corresponding to the fine AP or the homogenous propellant containing 86 percent AP which will be about 2850 Kelvin's ok.

So, the general process is that that this flame transfers heat to the surface causes decomposition and the decomposition products burn and in turn keep the flame in turn sustain the flame ok. So, the basic equation that is required to that we need to construct to get an expression for burn rate is the heat flux balance and the surface of the propellant ok, the surface of these condense faced ok.

So, the heat flux balance simply says that the heat received from the flame part of it causes decomposition at the surface and the other part goes into the condense phase. So, this is just an expression of energy conservation at a thin interface. So, this the left hand side is the flux that goes into the surface, the first term on the right hand side is the energy or the enthalpy change associated with the decomposition at the surface and k dT d x 0 plus is the heat flux that comes from the gas phase into the surface.

In some formulations you will find that this term the first term on the right hand side is actually on the left hand side, but it is only a matter of convention. Here positive values of H s are taken to be exothermic and negative values are taken to be endothermic and therefore, the term appears on the right just for consistency ok.

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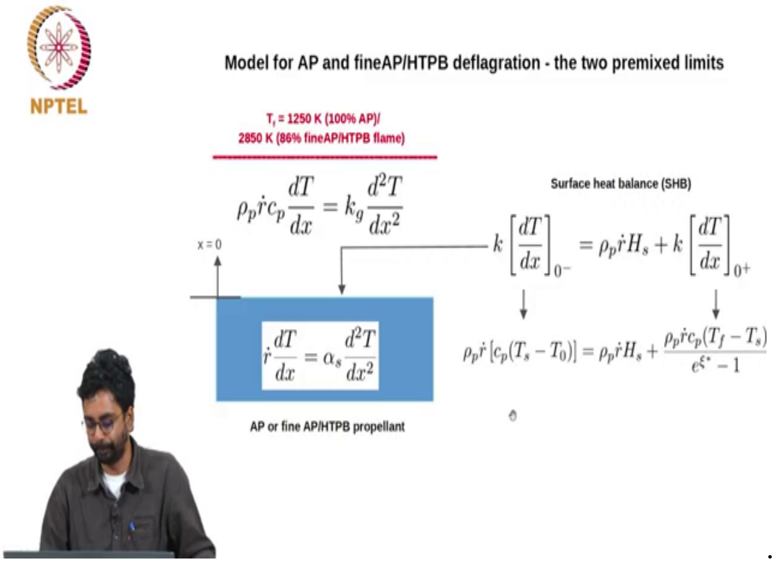

Model for AP and fineAP/HTPB deflagration - the two premixed limits

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$$\rho_p \dot{r} c_p \frac{dT}{dx} = k_g \frac{d^2T}{dx^2}$$

$$\dot{r}\frac{dT}{dx} = \alpha_s \frac{d^2T}{dx^2}$$

AP or fine AP/HTPB propellant

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$$k\left[\frac{dT}{dx}\right]_{0^-} = \rho_p \dot{r} H_s + k\left[\frac{dT}{dx}\right]_{0^+}$$

$$\rho_p \dot{r}\left[c_p(T_s - T_0)\right] = \rho_p \dot{r} H_s + \frac{\rho_p \dot{r} c_p (T_f - T_s)}{e^{\xi^*} - 1}$$

Now, we can solve for these slopes by integrating the convection diffusion, one dimensional convection diffusion in the solid phase. I am sorry one dimensional convection diffusion in the gas phase and the heat conduction equation in the solid phase and these have simple solutions.

In fact, the solutions are exponential profiles and from the profiles you can actually calculate the slopes and the slope in the condense phase is rho p r dot c p T s minus T 0. And, for this for a thin flame approximation with convection diffusion balance in the gas phase, the gradient of temperature at the surface takes this form ok.

This you we could have actually written this even without having to solve the equation. This is simply the heat that is required to raise the temperature of a burning propellant at a rate of r dot, for it to be increased for its temperature to be increased from T 0 to T s ok, this is the stem dot c p T s minus T 0 ok.

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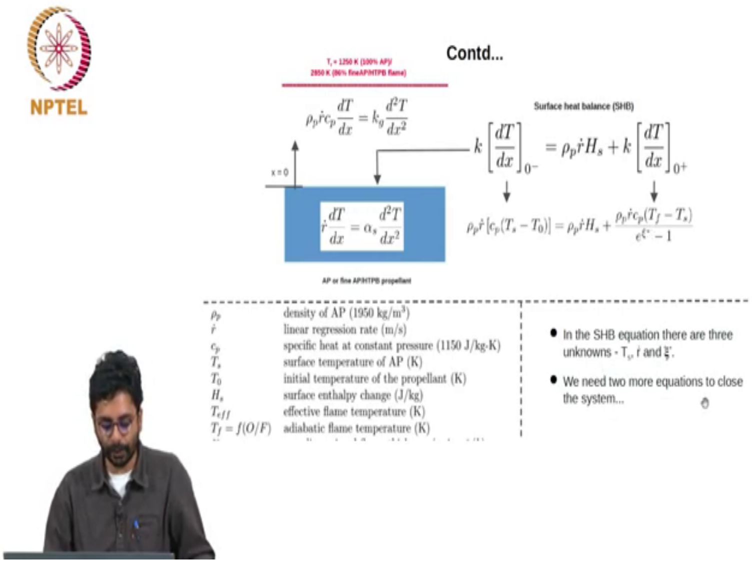

Contd...

T_f = 1250 K (100% AP)/ 2850 K (86% fineAP/HTPB flame)

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AP or fine AP/HTPB propellant

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$$\rho_p \dot{r}\left[c_p(T_s - T_0)\right] = \rho_p \dot{r} H_s + \frac{\rho_p \dot{r} c_p (T_f - T_s)}{e^{\xi^*} - 1}$$

ρ_p	density of AP (1950 kg/m^3)
$\dot{r}$	linear regression rate (m/s)
c_p	specific heat at constant pressure (1150 J/kg-K)
T_s	surface temperature of AP (K)
T_0	initial temperature of the propellant (K)
H_s	surface enthalpy change (J/kg)
T_{eff}	effective flame temperature (K)
$T_f = f(O/F)$	adiabatic flame temperature (K)

- In the SHB equation there are three unknowns - T_s, $\dot{r}$ and ξ^*.
- We need two more equations to close the system...

So, now we have one equation and in the surface heat balance equation there are three unknowns, the surface temperature is unknown, the burn rate is unknown and the other thing that is not known is the flame stand of distance ok.

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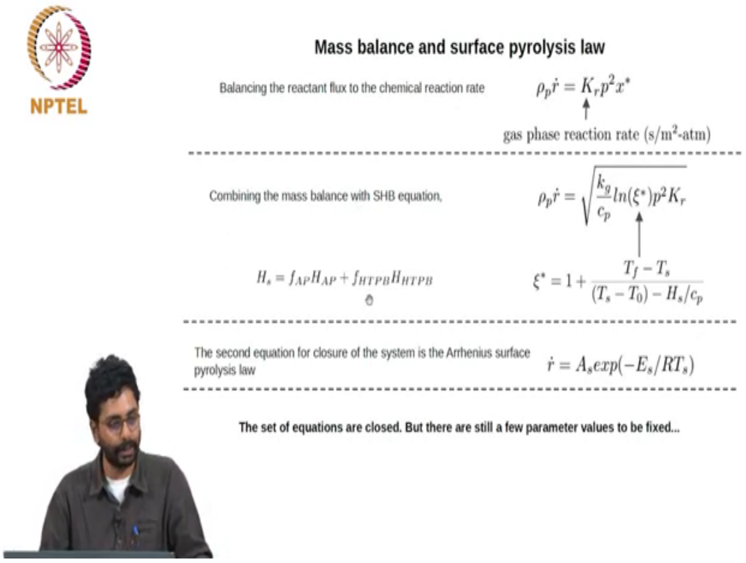

Mass balance and surface pyrolysis law

Balancing the reactant flux to the chemical reaction rate $\rho_p \dot{r} = \underset{\substack{\uparrow \\ \text{gas phase reaction rate (s/m}^2\text{-atm)}}}{K_r} p^2 x^*$

Combining the mass balance with SHB equation, $\rho_p \dot{r} = \sqrt{\frac{k_g}{c_p} ln(\xi^*) p^2 K_r}$

$H_s = f_{AP} H_{AP} + f_{HTPB} H_{HTPB}$ $\xi^* = 1 + \frac{T_f - T_s}{(T_s - T_0) - H_s / c_p}$

The second equation for closure of the system is the Arrhenius surface pyrolysis law $\dot{r} = A_s exp(-E_s/RT_s)$

The set of equations are closed. But there are still a few parameter values to be fixed...

So, we need two more equations to close the system. The two more equations come from one comes from the premixed flame theory. This we used earlier. This is exactly same as rho u s u equals omega dot delta h c I am sorry, rho u s u is equal to omega dot times delta. This we used in the premixed flame theory to get an expression for the flame speed and the flame thickness. Here it is exactly the same. The burn rate of the AP monopropellant or the homogenous propellant is balanced by the consumption rate of the reactants in the gas phase ok. Here the reaction rate is assumed to be proportional to p squared, we are assuming a bimolecular reaction let us head and stand off distance ok

So, you can combine this with the surface heat balance equation that was in the previous page and you will get an expression of this kind and the surface enthalpy is for pure AP it is the enthalpy of decomposition of AP, for a mixture of AP and HTPB it is a mass weighted average of the enthalpy of decomposition of AP and HTPB yeah. The other equation that is used to close the system of equations that we have is the pyrolysis law for the AP at the surface.

It says that the burn rate is a (Refer Time: 05:15) function of the surface temperature and we have all the equations to close the system, but we still have a few parameters. For example, we have the enthalpy of decomposition. We do not know the enthalpy of decomposition of AP at the surface or enthalpy of decomposition of HTPB in the surface.

Student: How?

Yeah

Student: How they are (Refer Time: 05:36).

We will come to that that is exactly what we are going to look at in the next line yeah.

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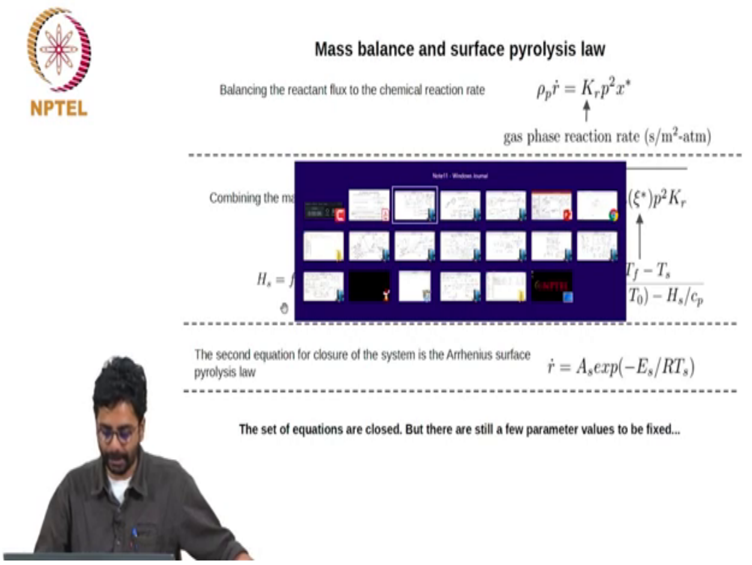

Mass balance and surface pyrolysis law

Balancing the reactant flux to the chemical reaction rate $\rho_p\dot{r} = K_r p^2 x^*$

gas phase reaction rate (s/m^2-atm)

Combining the ma

$(\xi^*)p^2K_r$

$H_s = f$

$T_f - T_s$

$T_0) - H_s/c_p$

The second equation for closure of the system is the Arrhenius surface pyrolysis law $\dot{r} = A_s exp(-E_s/RT_s)$

The set of equations are closed. But there are still a few parameter values to be fixed...

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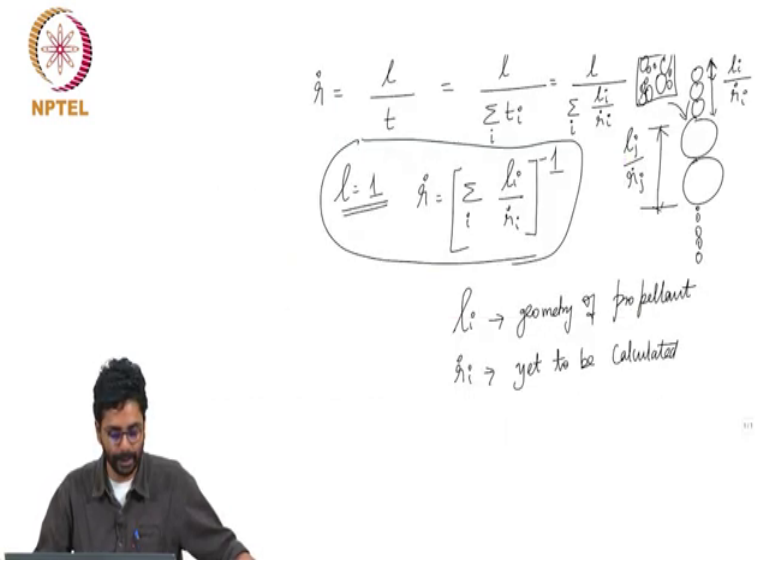

$$\dot{r} = \frac{l}{t} = \frac{l}{\sum_i t_i} = \frac{l}{\sum_i \frac{l_i}{\dot{r}_i}}$$

$$\underline{\underline{l=1}} \quad \dot{r} = \left[\sum_i \frac{l_i}{\dot{r}_i}\right]^{-1}$$

$l_i \rightarrow$ geometry of propellant

$\dot{r}_i \rightarrow$ yet to be calculated

Let me explain this in some detail.

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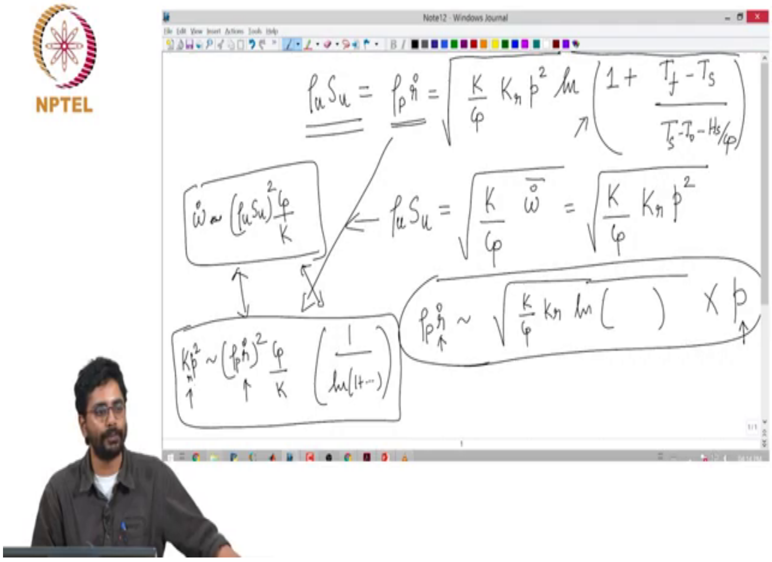

$$\rho_u S_u = \rho_p \dot{r} = \sqrt{\frac{K}{c_p} K_r p^2 \ln\left(1+\frac{T_f - T_s}{T_s - T_0 - H_s/c_p}\right)}$$

$$\boxed{\dot{\omega} \sim (\rho_u S_u)^2 \frac{c_p}{K}}$$

$$\rho_u S_u = \sqrt{\frac{K}{c_p}\bar{\dot{\omega}}} = \sqrt{\frac{K}{c_p} K_r p^2}$$

$$\boxed{K_r p^2 \sim (\rho_p \dot{r})^2 \frac{c_p}{K}\left(\frac{1}{\ln(1+\cdots)}\right)}$$

$$\rho_p \dot{r} \sim \sqrt{\frac{K}{c_p} K_r \ln(\quad)} \times p$$

So, that we have this is what we have before we go to the parameter estimation. I just want you to recognize I have gone through the slides fairly quickly, but I want you to recognize the similarity between these two equations. This is what we had yesterday, you remember and all that has happened here is that if I assume omega dot to be a constant multiplied by pressure squared which is what it will be for a bimolecular reaction, these two expressions are exactly the same ok.

The extra term which is logarithm 1 plus T f minus T s by T s minus T 0 minus H s by c p simply comes because of the presence of the condense phase into which part of the heat is going and this is also the reason. Now, you can I can also write it like this simply because the solid surface is regressing at a certain rate. It is giving off gases that is mass balance at the interface and therefore, the mass of the propellant that is getting converted from solid to gaseous phase should be equal to the mass flux in the gas phase ok, this is also the reason.

Now, you can see that rho p r dot goes as square root of k by c p K r logarithm of some factors multiplied by the pressure squared when it comes out of the square root goes as pressure ok. So, when the burning rate is controlled by a premixed flame, the r dot will be proportional to p raised on exponent that is close to 1 ok. This is exactly why the AP limit and in the AP limit and in the homogeneous propellant limit, the index is close to 1 ok. It is slightly lower than 1 because of certain parameters that change in a certain way with pressure in condensed phase that comes from this logarithm term, but otherwise the index is very close to 1 and it is 0.82 and 0.77.

And when diffusion lateral diffusion f x becomes significant this index will come down as we will see later ok. So, you can go through the derivation slowly, but I you know at your own time, but please recognize I want you to recognize these important similarities between what we did for premixed flame analysis and it is being simply extended to a case where the fuel is issued by a solid which is decomposing and giving premixed gases.

Yeah. So, now, we now that we have this expression, what is not what are all not known yes we do not know what K r is which is the reaction rate constant we do not know what H s is we know we do not know what T s is, but what we are going to do is use the known burn rates, remember that it is easier to measure flame speed than measuring reaction rates. So, you get a accurate estimate of the overall reaction rate from the flame speed that is exactly what we are going to do here to calculate the gas phase reaction rates.

We know the measured burn rates of the AP and the homogenous propellant and from the known burn rates we are going to actually calculate the reaction rates ok. So, from this equation where we have rho p r dot equals square root k by c p logarithm term p squared K r with a known value of r dot we are going to calculate K r ok.

So, we remember this from here we got omega dot is proportional to rho u S u squared C p by K for a gaseous flame and from this equation we can again show that K r will be dependent on rho p r dot squared with other factors appropriately plugged in divided by c p by k, a pressure dependence is explicitly accounted for and 1 by logarithm 1 plus something ok. I want you to notice the similarity between these two equations ok.

Reaction rate goes as rho u s u squared c p by k, here the reaction rate is K r p squared it goes as o p r dot squared c p by k is an additional logarithmic factor coming from the condense phase heat transfer considerations ok. So, this is same this is the strategy that we are going to use to calculate K r ok. From the known burn rate of AP at 20 atmospheres and the burn rate of the homogenous propellant at 20 atmospheres, we are going to calculate the value of K r and use it for calculating or predicting the burn rate of other compositions which have a variety of particle sizes.

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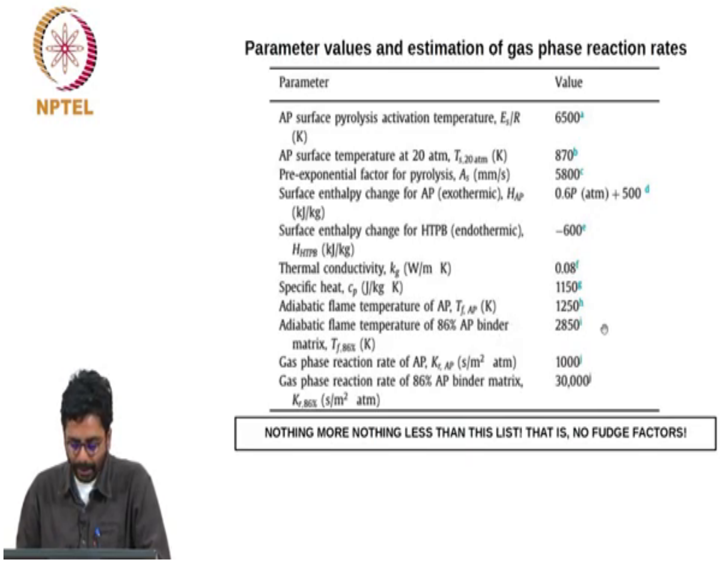

Parameter values and estimation of gas phase reaction rates

Parameter	Value
AP surface pyrolysis activation temperature, E_s/R (K)	6500[a]
AP surface temperature at 20 atm, $T_{s,20\,\mathrm{atm}}$ (K)	870[b]
Pre-exponential factor for pyrolysis, A_s (mm/s)	5800[c]
Surface enthalpy change for AP (exothermic), H_{AP} (kJ/kg)	0.6P (atm) + 500 [d]
Surface enthalpy change for HTPB (endothermic), H_{HTPB} (kJ/kg)	−600[e]
Thermal conductivity, k_g (W/m K)	0.08[f]
Specific heat, c_p (J/kg K)	1150[g]
Adiabatic flame temperature of AP, $T_{f,AP}$ (K)	1250[h]
Adiabatic flame temperature of 86% AP binder matrix, $T_{f,86\%}$ (K)	2850[i]
Gas phase reaction rate of AP, $K_{r,AP}$ (s/m^2 atm)	1000[j]
Gas phase reaction rate of 86% AP binder matrix, $K_{r,86\%}$ (s/m^2 atm)	30,000[j]

NOTHING MORE NOTHING LESS THAN THIS LIST! THAT IS, NO FUDGE FACTORS!

And that is what is done here. Some information about how AP behaves under deflagration is already known. For example, it is known that the AP surface pyrolysis activation temperature is around 6500 Kelvin and we already know that AP starts burning only when it starts melting. And therefore, the 20 atmosphere is when it starts burning at 3.3 millimetres per second the surface temperature must be 870 Kelvin's this is something that we already know.

This information combined with the activation temperature is used to calculate a pre exponential factor from the known burn rate of AP at 20 atmospheres which is 3.3 millimetres per second. And, some information on what is the enthalpy of decomposition of AP at a surface is also known it is known that 60 to 70 percent of all AP decomposes at the surface ok. Surface enthalpy of HTPB is also known to some degree, but this does not as we will see later.

The choice of this number is not the results are not very sensitive to the choice of this number because the H S which is a surface enthalpy decomposition always appears as logarithm of 1 plus b and in that term in the denominator. So, even though H S can change by even if you change H S by a large value, the logarithm of 1 plus that term will change only be a small magnitude. So, the results are not sensitive to the choice of the endothermic decomposition enthalpy of HTPB.

Thermo physical values appropriate values have been chosen, adiabatic flame temperature of AP is known 1250 Kelvin's, adiabatic flame temperature of 86 percent AP binder can be calculated or was calculated from NASA CEA using NASA CEA and with all these numbers and from the equation that I showed in the previous slide ok. We can calculate the gas phase reaction rate for AP from the burn rate of AP and the gas phase reaction rate for the homogenous propellant from the burn rate of the homogenous propellant.

The burn rate of these compositions are equivalent to the flame speed and the important thing is these are all this is a set of parameters that we are going to use for all the calculations and there are no adjustable constance ok. Any questions at this point? We have completed the first 2 parts, the geometry part and the parameter estimation part. The parameter estimation part I I would like to reemphasize its connection to the premixed flame behaviour that we discussed yesterday, but if you have any questions now we can discuss.

Student: (Refer Time: 14:39) doing that.

Correct.

Student: (Refer Time: 14:43)

K r for the homogenous binder AP mixture.

Student: Yes.

Yeah.

Student: So, if let us say I have a composition how these how it will be (Refer Time: 14:52) in between whatever you are saying how these 2 numbers are related are they.

I will I will come to that. Actually these two reaction rates these two numbers are treated as reaction rates at 2 different temperatures and therefore, we know the reaction rate at 2 different temperatures. So, a plot of logarithm of K r versus 1 by T the slope of it will give me an activation temperature for the gas phase reaction

Student: Are you trying to say that a and e exponential by e and r T of fitting these 2 points.

Correct.

Student: Ok.

Yes yeah that is what is done exactly, yeah. The burn rate of AP is related to its surface temperature through an Arrhenius Pyrolysis law and therefore, the significance of the activation temperature is that it determines the burn rate once the surface temperature is known. That is that is just a simple statement. The is the question how it is your question how it is determined?

It is not easier it is not straight forward. Measurement of any reaction parameter is tricky ok. So, this particular temperature was temperature range was arrived at by a certain kind of calculations that were that was done by professor P R Ramakrishna during his PhD.

So, this is a number that was arrived at in through a series of calculations where every other parameter was fixed based on the range that was known for those parameters. Calculations were run for AP deflagration for various values of v s by r and it was found that that only for a range of e s by r values that is between 6000 and 7000 Kelvin's that the calculations showed that AP can undergo steady deflagration.

For every other condition the deflagration was unsteady, but the experimental observation was that AP deflagration is always steady. So, it was it is based this calculation is called or this approach is called fixing e s by r based on intrinsic stability ok, any other questions, no.

So, the first 2 parts are done. We have converted the complex geometry into a statistical representation. We have also got parameter estimates. Now if you remember the formula for the burn rate, we know l i, we have to know r dot i to calculate the burn rate of the propellant that is what we will go to.

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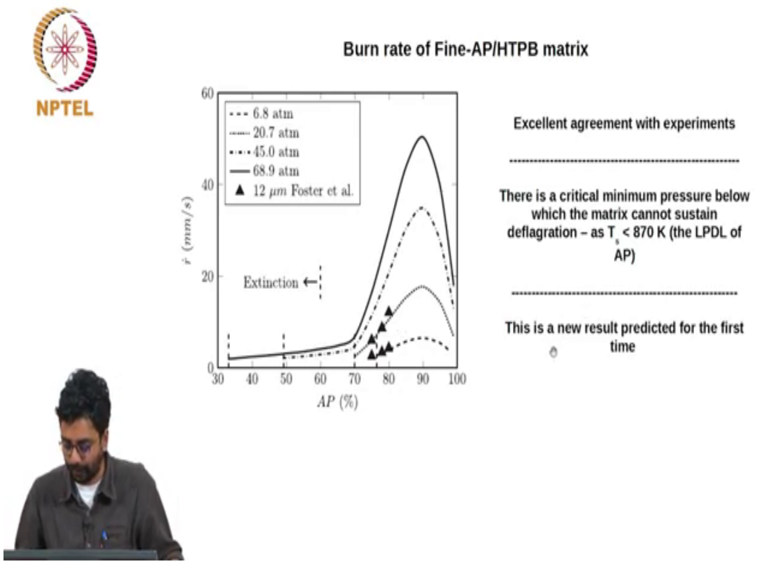

Burn rate of Fine-AP/HTPB matrix

Excellent agreement with experiments

There is a critical minimum pressure below which the matrix cannot sustain deflagration – as T_s < 870 K (the LPDL of AP)

This is a new result predicted for the first time

But before that how do we know that this parameter set is good enough? So, using this parameter set calculations were made for homogenous compositions of you know variety of compositions with AP fraction ranging from as low as 30 percent to as high as 95 98 percent. Some limited experimental data was available and the productions and the comparisons were in reasonable agreement.

More importantly, you see a vertical line that is marked here and to the left of it is marked as extinction ok. This is something that I would like to explain. If you for example, if you have a mixture a homogenous mixture of AP and HTPB, lets say with 70 percent AP ok, what the theory says is that that the surface temperature of this composition act 6.8 atmospheres would be lower than 870 Kelvin’s. This is the prediction of the theory.

It says that if I have a homogenous mixture of AP and HTPB with 70 percent AP and if I try to burn it at 6.8 atmospheres, the theory says that since the temperature of the surface is going to be lower than the melting temperature of AP, it will not burn that is the production of the theory. And another prediction that the theory makes is that the question that we can ask is: what is the pressure at which it will start burning ok?

What the theory says is that it will start burning at 20 atmospheres or 20.7 atmospheres as it is indicated here ok. How do we know that this is correct ok? Similarly extinction limits have been shown at different pressures. For example, if you go to even higher pressures 45 atmospheres, compositions containing even 50 percent AP can burn. We go to even higher pressures. So, 68.9 atmospheres, compositions containing even 30 percent AP can burn that is what the theory says.

Of course, there is no direct comparison that can be done, but there are if we look at literature carefully there are statements that are made for example, compositions that were made with 70 75 percent AP would not burn at pressures lower than 20 atmospheres and you will not I have shown data here and you will not find any data for this compositions at lower pressures or lower AP loading ok.

Therefore while this has been recognized in operational in by experimentalist when they were making propellants, it was not formally theoretically theoretically proved if I may use that word. Even now it is not proved, but there seems to be lot of evidence to indicate that that this is correct ok. I will show more evidence as we go along. This is what we call as extinction.

The basic idea is that under certain conditions when the surface temperature becomes lower than the melting temperature of AP, the propellant will not burn that is the simple idea and it manifests itself in this fashion for homogenous propellants, it manifests in a certain slightly complicated way for actual propellants. We will look at it what we will look at what it means a little later ok.

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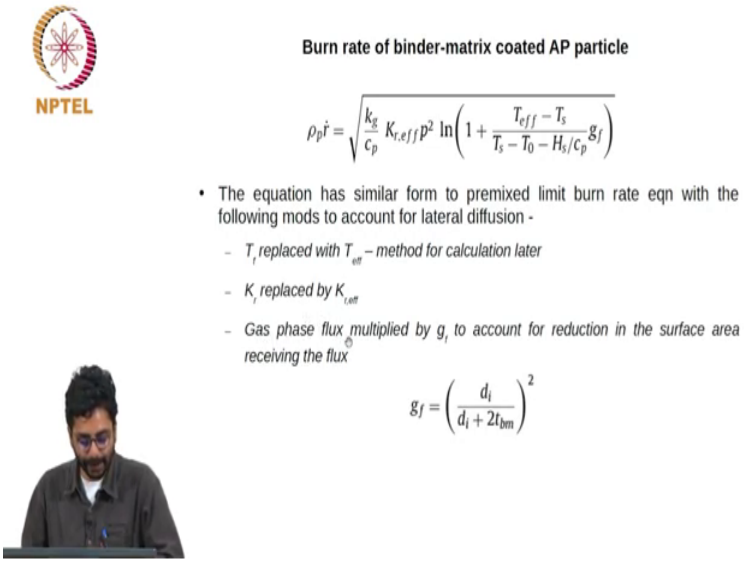

Burn rate of binder-matrix coated AP particle

$$\rho_p \dot{r} = \sqrt{\frac{k_g}{c_p} K_{r,eff} p^2 \ln\left(1+\frac{T_{eff}-T_s}{T_s-T_0-H_s/c_p} g_f\right)}$$

- The equation has similar form to premixed limit burn rate eqn with the following mods to account for lateral diffusion -
  - *T_f replaced with T_{eff} – method for calculation later*
  - *K_r replaced by $K_{r,eff}$*
  - *Gas phase flux multiplied by g_f to account for reduction in the surface area receiving the flux*

$$g_f = \left(\frac{d_i}{d_i + 2t_{bm}}\right)^2$$

Now, we move on to the third part of the theory which is a model for calculating r dot i ok, the burn rate of each individual binder matrix coated AP particles. Let me not go into the details because the ideas are essentially the same. The equation that is required for predicting r dot i has a similar form to the premixed limit burn rate equation with a few modifications to account for the effects of lateral diffusion.

T f is replaced with an effective temperature method for calculation a little late, the reaction rate is replaced with an effective reaction rate, the gas phase flux multiplied by a geometric fact that account for reduction in the surface area receiving the flux, all of this I will explain in some detail ok.

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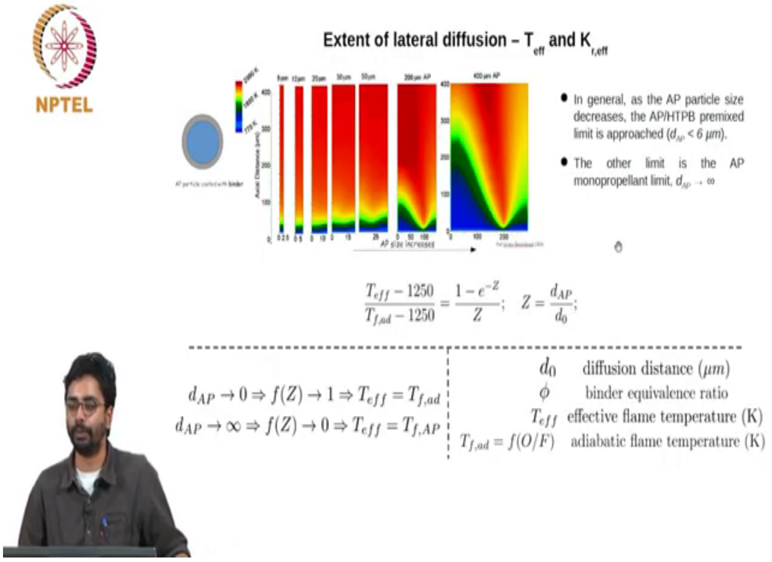

Extent of lateral diffusion – T_{eff} and $K_{r,eff}$

- In general, as the AP particle size decreases, the AP/HTPB premixed limit is approached ($d_{AP} < 6\ \mu m$).
- The other limit is the AP monopropellant limit, $d_{AP} \to \infty$

$$\frac{T_{eff} - 1250}{T_{f,ad} - 1250} = \frac{1 - e^{-Z}}{Z}; \quad Z = \frac{d_{AP}}{d_0};$$

$$d_{AP} \to 0 \Rightarrow f(Z) \to 1 \Rightarrow T_{eff} = T_{f,ad}$$

$$d_{AP} \to \infty \Rightarrow f(Z) \to 0 \Rightarrow T_{eff} = T_{f,AP}$$

d_0 diffusion distance (μm)

ϕ binder equivalence ratio

T_{eff} effective flame temperature (K)

$T_{f,ad} = f(O/F)$ adiabatic flame temperature (K)

So, far we have been looking at either pure AP or homogenous AP HTPB mixtures, but in reality we have large AP particles surrounded by binder ok. Calculations were done by Gross and Beckstead for such a configuration with AP particles of various sizes surrounded by binder matrix such that the total solid loading of AP is 86 percent. They maintain the same solid loading and that calculations for various sizes of AP particles ok.

The results are shown here. This is for a 400 micron particle 200 micron particle and all the way up to a 5 micron particle. What I would like you to observe is that the temperature distribution in the gas phase that is shown as a contour plot here becomes uniform as you go from 400 microns to 5 microns. What I mean by uniform is uniform in the horizontal direction ok.

Here if you see the 0 to 200 micron is AP, it is a 400 micron AP particle therefore, the radius is 200 micron, 0 to 200 micron is AP it has a certain temperature distribution over it. At the edge it is there is binder which is decomposing and laterally diffusing into AP creating a non-premixed flame which is at a much higher temperature than the AP monopropellant flame.

AP monopropellant flame is at 1250 degree 1250 Kelvin's, the stoichiometric binder AP flame will be at 3000 Kelvin's. Therefore, here the temperature is about 1000 200 Kelvin's here it is about 3000 Kelvin's and there is a clear 2 dimensional structure to the temperature profile. Here its monopropellant here there is another flame non-premixed flame setting and this entire assembly controls how much heat transfer goes to the surface ok.

I would like you to imagine the ethylene flame that I showed you in the morning. This is how the ethylene flame edge looks ok. Now, what is happen what they did is they did calculations by reducing the size of AP. As you keep reducing the size of AP there comes a where, the extent of lateral diffusion of a fluent deoxidiser, the distance becomes comparable to the size of AP.

When this happens there is a there is premixing of fuel and oxidiser before the reaction begins, this is the idea that we discussed in the morning. When you keep reducing the diameter of the fuel issuing jet when you come to a where the diameter is comparable to the lateral diffusion distance the flame will become premixed.

So, that is exactly what is happening here. Here you have a 80 monopropellant flame surrounded by a diffusion flame or a non-premixed flame. So, keep reducing the size of the AP particle. There is complete mixing of AP d composition products and fuel before the flame gets established. So, what you get is a flat premixed flame ok

So, that in this case this calculation is done at 20 atmospheres this happens at about 20 micron ok. Till about 30 micron there is some variation in the horizontal temperature profile, but at 20 microns clearly the profile has become more or less homogenous ok. This is the crux of the argument based on lateral diffusion and this is what is used to calculate the effective temperature ok.

So, for the same solid loading and at the same pressure the heat flux that is coming to the surface for a 400 micron particle is mostly controlled by the AP monopropellant flame because there is only a small zone that is influenced by the non-premixed flame. On the other hand, if you go to 20 micron particle the heat flux that is coming to the surface is completely controlled by a homogenous premixed flame at 3000 Kelvin's.

Here the heat transfer is controlled by a flame sending heat to the surface at 1250 Kelvin's, here the same solid loading same pressure, the only difference is that the diameter of the particle is smaller and this is controlled by a flame that is at 3000 Kelvin's ok. And, this is the basis for the general rule of thumb that is used that reducing the particle size increases the burn rate of the propellant simply because when you reduce the particle size, the flame the effective temperature at which heat flux is transferred to the surface is much higher and therefore, the burn rates are higher ok.

And this effect that larger particles are controlled by monopropellant flame and smaller particles are controlled by a premixed flame is captured using a simple idea based on effective temperature and this functional form. And, let us not worry about the details the functional form is dependent on should is dependent on the relative magnitude of the size of the AP particle in relation to the diffusion distance.

So, the Z is defined as a size of AP divided by the diffusion distance ok. If the diffusion distance is larger than the size of AP, you have premixed flame you have diffusion distance much smaller than the size of AP; you have AP monopropellant flame ok. So, in the limit as Z goes to 0 you should have premixed flame and in the limit as Z goes to infinite you should have monopropellant flame and as it is shown here these limits are correctly captured by this functional form.

As I will we will see later that it also captures the intermediate points correctly and now the next question is how to calculate the diffusion distance. We already know how to do it.

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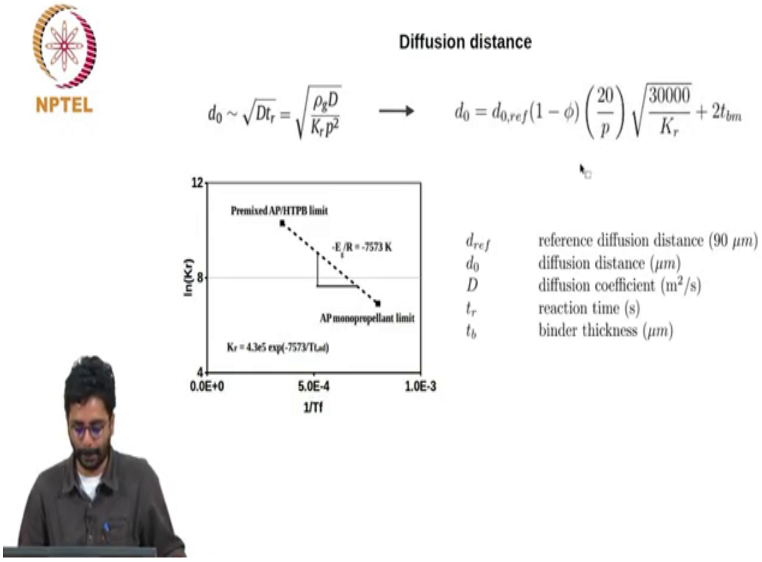

Diffusion distance

$$d_0 \sim \sqrt{Dt_r} = \sqrt{\frac{\rho_g D}{K_r p^2}} \longrightarrow d_0 = d_{0,ref}(1-\phi)\left(\frac{20}{p}\right)\sqrt{\frac{30000}{K_r}} + 2t_{bm}$$

d_{ref}	reference diffusion distance (90 μm)
d_0	diffusion distance (μm)
D	diffusion coefficient (m^2/s)
t_r	reaction time (s)
t_b	binder thickness (μm)

We already discussed this in some detail. The extent of lateral diffusion is proportional to square root Dt r this we have already discussed; t r is the reaction time which is density divided by the reaction rate that is exactly what is done here. Density is rho g divided by reaction rate which is K r p squared diffusion constant ok. This idea you can express in a slightly simpler form as shown here.

What I want you to recognize is that the diffusion distance should decrease with increase in pressure and at a given pressure it should decrease with increase in reaction rate and that is exactly what you see here; d 0 is inversely proportional to pressure and it is also inversely proportional to square root of the reaction rate ok

This is this idea clear? This is probably the most important thing that is quite here. It follows the same logic that I showed in the morning when we were discussing the ethylene flame ok; d 0 goes as square root Dt r and d 0 this gives us the relation in which d 0 is inversely proportional to pressure inversely proportional to square root of the reaction rate ok. Only that we do not know any absolute values, we have chosen some relative magnitudes to fix the constants in this expression, that is it.

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Predictions of the theory

We have all the elements required to make predictions now.

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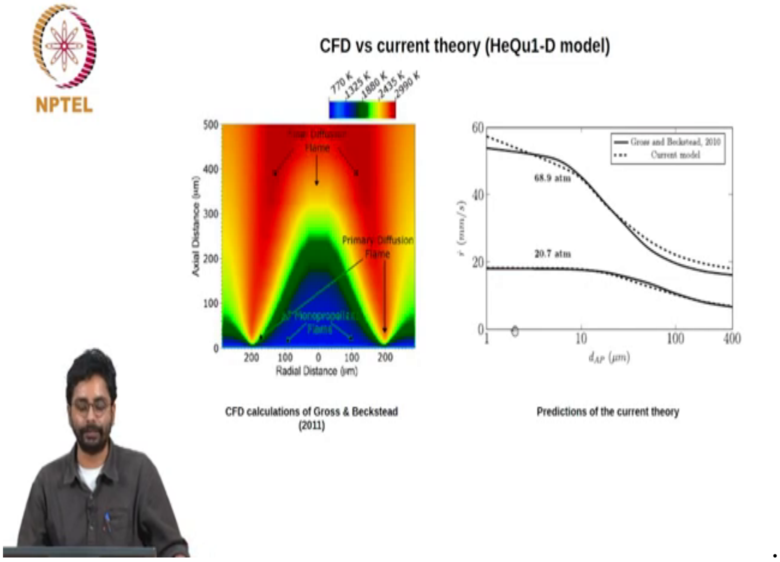

CFD vs current theory (HeQu1-D model)

CFD calculations of Gross & Beckstead (2011)

Predictions of the current theory

So, let us look at the predictions in the theory. So, as I said that at the limits we definitely know that the relationship works, but this is to show that at intermediate sizes also we get the correct results. The thick lines the continuous lines are the predictions from CFD by Gross and Beckstead, the dotted lines are the predictions of the current model they are in they are in very good match ok. In fact, this is what was used to validate the lateral diffusion model.

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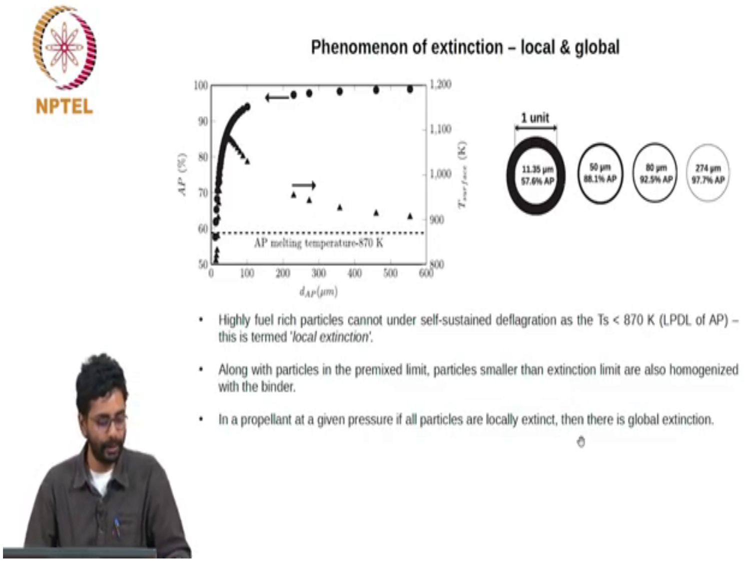

Phenomenon of extinction – local & global

- Highly fuel rich particles cannot under self-sustained deflagration as the Ts < 870 K (LPDL of AP) – this is termed '*local extinction*'.
- Along with particles in the premixed limit, particles smaller than extinction limit are also homogenized with the binder.
- In a propellant at a given pressure if all particles are locally extinct, then there is global extinction.

Let us go to the phenomenon of extinction. Even in we saw this earlier for the for a typical composite solid propellant smaller particles are fuel rich and larger particles are oxidiser rich ok. And therefore, if you look at the surface temperature, the surface temperature will be closer to the AP monopropellant temperature at large particle sizes and at small particle sizes it can become lower than the AP melting temperature. This is in fact, what the calculation shows and this is because here I have shown 4 particles of different sizes starting from 274 microns to as small as 12 microns ok.

All the diameters have been scaled by the diameters of the particles. So, they are are all of unit size. So, remember that all particles are coated with fuel of the same thickness. So, the thickness of the fuel is fixed. Therefore, the amount of binder, the amount of fuel available for the large particle is much smaller compared to a particle of smaller size. In fact, for the same binder thickness a 274 micron particle is almost pure AP it is 97.7 percent AP, but on the other hand 11.35 micron particle more than half of it or about half of it is binder 50 percent is binder.

So, therefore, the surface temperature of the smaller particle can actually become smaller than 870 Kelvin's which is the melting temperature of AP and therefore, can stop burning ok. So, highly fuel rich particles cannot undergo self sustained deflagration as the surface temperature can become less than 870 Kelvin's. This is termed as local extinction as supposed to what we discussed earlier for homogenous compositions. Along with particles in the premixed limit, particles smaller than extinction limit are also homogenized with the binder.

One thing I forgot to mention, I will go back and mention after I finish this slide. So, in a propellant at a given pressure if all particles are locally extinct then there is global extinction ok. What I missed was that I have been referring to the limit of fine AP that is nothing but once you reach 20 microns, the gas phase does not recognize that the AP is of a certain size, it does not actually matter whether it has 20 microns or 10 microns or 5 microns, all these cases will have the same burn rate because all the 3 cases are controlled by a single premixed flame ok.

In fact, you can clearly see that here. You look at the predictions as a function of particle size at 20.7 atmospheres. Once you reach a point where the size is about 20 microns, irrespective of what the size is how small you go the burn rate remains the same because they are all controlled by the same premixed flame. And, all these particles are called the fine AP particles and they are homogenized with the binder in addition to the particles that are extinct.

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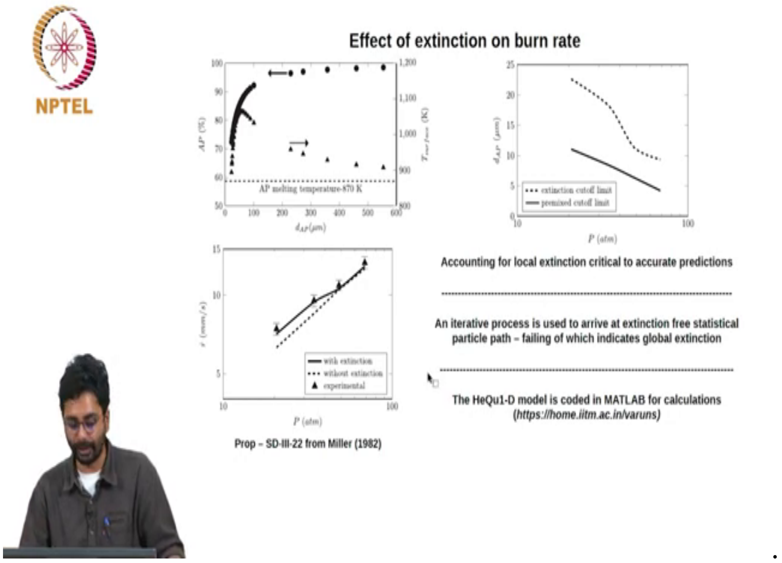

Effect of extinction on burn rate

Prop – SD-III-22 from Miller (1982)

Accounting for local extinction critical to accurate predictions

An iterative process is used to arrive at extinction free statistical particle path – failing of which indicates global extinction

The HeQu1-D model is coded in MATLAB for calculations
(https://home.iitm.ac.in/varuns)

So, I said that there is no hard data available for validating the extinction limits for homogeneous compositions, but what we found evidence in by other means this is prediction for a particular composition taken from Miller 1982. When we do not account for extinction the predictions is shown by this dotted line and the data are the triangles which are actually the error bars are about 10 percent. So, the deviation and burn rate is quite significant it is about 20 percent.

But when we account for extinction the predictions are very good and not just that it even predicts the change in the slope with pressure ok. The general impression is that you write AP raised to n and we assign a lot of significance to the n and we demand that n should not change with pressure that is not true that need not be true ok; n is constant or n can be approximated to be a constant only in certain pressure ranges ok.

So, a set of small particles or fuel rich fine particles which are not burning at low pressures can start burning at high pressures changing the index of the propellant. So, the index can itself be a function of pressure ok. This is not something that is recognized in practice it is demanded that the end should remain constant, but only over a certain pressure range it remains constant and it is a function of decomposition and other variables ok.

So, accounting for local extinction, critical to accurate predictions, an iterative process is used to arrive at extinction free statistical particle path failing of which indicates global extinction. And, this whole theory that I just described to you is available in the form of a MATLAB code that anybody can use to make predictions for a variety of composite solid propellants.

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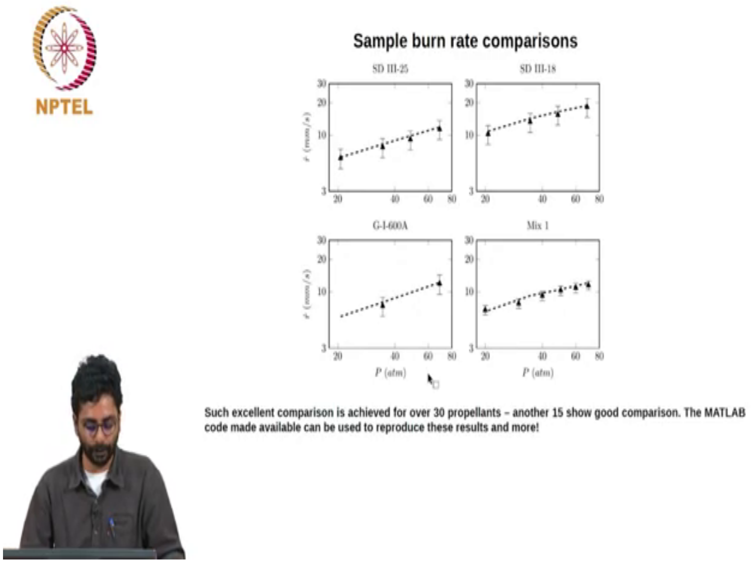

Sample burn rate comparisons

Such excellent comparison is achieved for over 30 propellants – another 15 show good comparison. The MATLAB code made available can be used to reproduce these results and more!

Predictions have been made for this is slightly old slide, it says over 30 propellants, but I think if I remember right now we have made predictions for over 100 propellants of variety of kinds including aluminized ones with nitramines and variety of catalyst and inhabitors the predictions are reasonably good.

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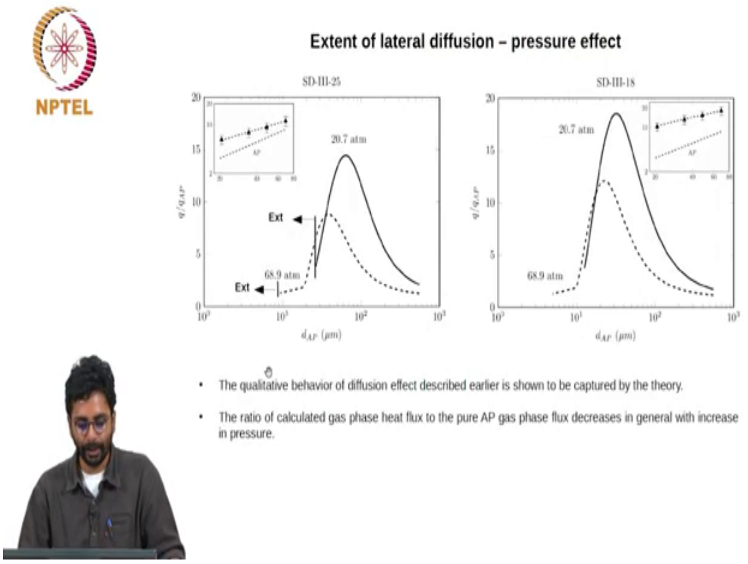

Extent of lateral diffusion – pressure effect

- The qualitative behavior of diffusion effect described earlier is shown to be captured by the theory.
- The ratio of calculated gas phase heat flux to the pure AP gas phase flux decreases in general with increase in pressure.

I think I will close with this particular slide because this is an idea that we have discussed in some detail today. I made several statements about the extent of lateral diffusion, this slides sort of summarizes or shows a good case for all those claims. The first claim is that the extent of lateral diffusion decreases with increase in pressure ok.

So, what is shown here is the heat flux that comes to a comes to the surface of AP particles constituting a propellant and the AP size varies from as small as 10 microns to about 300 400 microns ok. In you can see clearly that at 20.7 atmospheres, the contribution of heat flux to the surface because of lateral diffusion because this is normalized by the heat flux that that particle would get if it was only AP ok.

So, the contribution from lateral diffusion is much much higher than what that particle would get just from AP. It is in fact, a factor of 12 for this particular size because it is close to stoichiometry the flux is very large. For the same particle when you go to 68.9 atmospheres the contribution to the heat flux because of premixing caused by lateral diffusion is significantly lower, its a factor of 3 lower.

And therefore, this propellant will in relation to AP, this propellant will have a burn rate of this magnitude at 20 atmospheres, but as the pressure increases it will get closer and closer to AP and that is the reason why the slope for these cases decreases as you have particles of different sizes ok. Another example is shown here, a different composition SD III 18. Here again the extent of lateral diffusion significantly decreases with increase in pressure.

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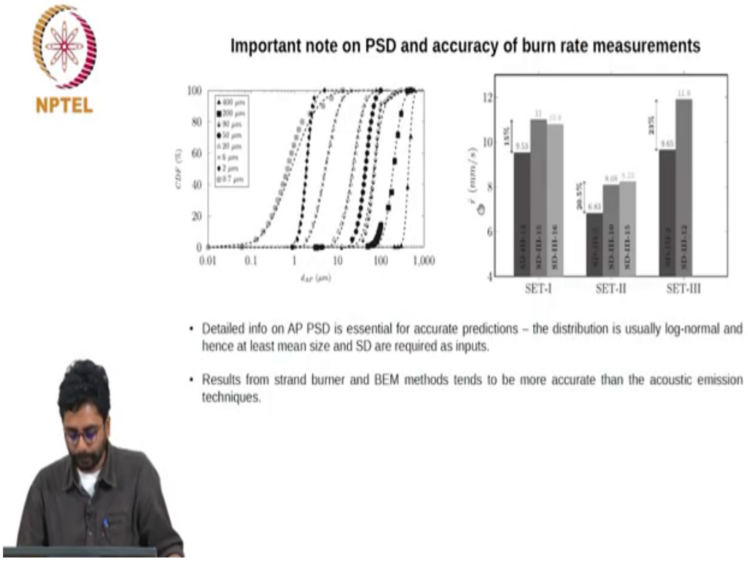

Important note on PSD and accuracy of burn rate measurements

- Detailed info on AP PSD is essential for accurate predictions – the distribution is usually log-normal and hence at least mean size and SD are required as inputs.
- Results from strand burner and BEM methods tends to be more accurate than the acoustic emission techniques.

I will skip this part ok.

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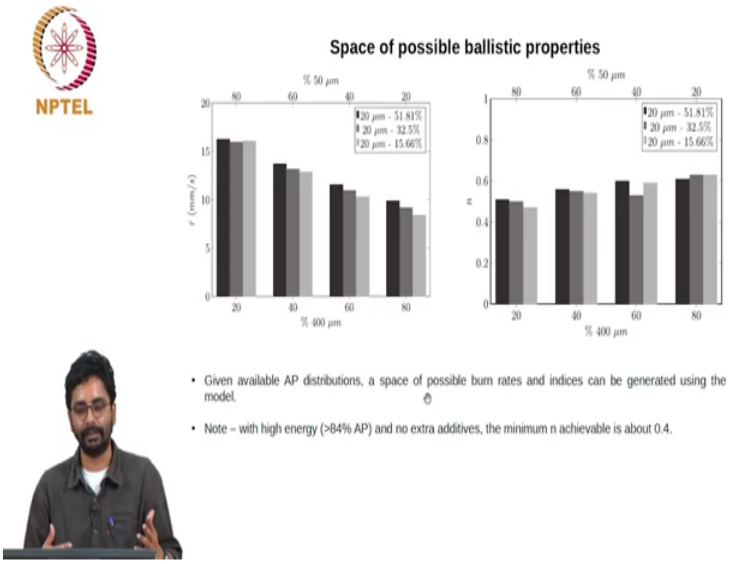

Space of possible ballistic properties

- Given available AP distributions, a space of possible burn rates and indices can be generated using the model.
- Note – with high energy (>84% AP) and no extra additives, the minimum n achievable is about 0.4.

One thing that we can do with this code is that which is value to practitioners is if you are looking for a particular composition that will satisfies that will satisfy the demands of certain mission and you know what AP particle sizes you have, you can use the code to get space of all possible combinations of index burn rate and temperature sensitivity and from there you can pick a few for experimental validation.

This will significantly bring down the number of trials that you need to do to choose or design a propellant for a particular application ok. We will just close with by saying that I still have not answered the question of the connection between low index and instability and at this point I want to emphasize that with all the effects that I have described AP monopropellant flame, the lateral diffusion because of the fuel and the oxidiser, particle size effects, extinction all taken into account.

High energy compositions will have a the lowest possible index seems to be about 0.4. There is no provision or there is no mechanism by which a high energy AP HTPB composition can have an index it is lower than 0.4. So, the index can come below 0.4 only with some additives which could be a combination of aluminium brings down the index a little bit down from 0.4 which we will see tomorrow, but some special additives are required to bring it below 0.3 as to what the mechanisms that are at play will discuss in subsequent lectures ok.