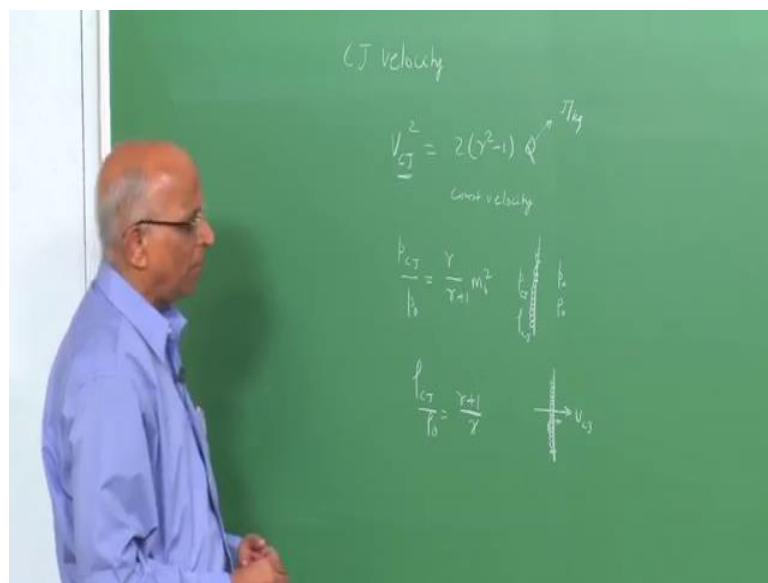


**Introduction to Explosions and Explosion Safety**  
**Prof K. Ramamurthi**  
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**Indian Institute of Technology, Madras**

**Lecture - 26**  
**Detonations: Calculation of Chapman Jouguet Velocities**  
**ZND Structure of a detonation**  
**Von Neumann Spike**

Good morning. In today's class, we continue with what we derived yesterday and you will recall we derived an expression for the Chapman Jouguet velocity of a detonation.

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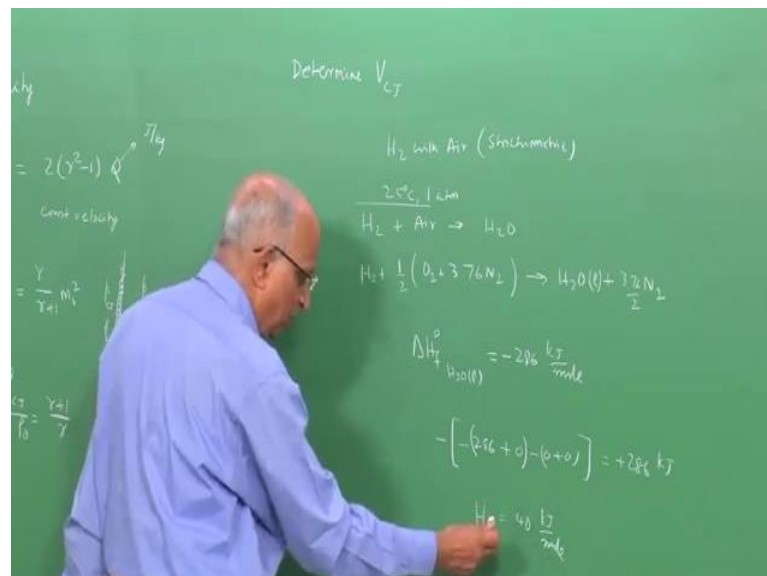
We said that the Chapman Jouguet velocity corresponds to the steady state velocity or the constant velocity with which a detonation proceeds. We found this velocity  $V_{CJ}$  square was equal to  $2(\gamma^2 - 1)Q$  where  $Q$  is the heat released by the chemical reactions which drives this shock and the unit of  $Q$  heat release was so much joules per kilogram. This gave the velocity and we said that the Chapman Jouguet velocity is a constant, since it corresponds to the tangential tangency point between the reactive Hugoniot and the Raleigh line and the velocity behind the detonation becomes equal to the sonic local sonic condition. And therefore, it is not possible for disturbances to catch up with the detonation with the result  $V_{CJ}$  velocity is a steady state or a constant velocity case.

We also derived an expression for the pressure ratio behind a detonation, we got the value of the pressure behind a Chapman Jouguet detonation and what do I call a Chapman Jouguet detonation now? You have a shock wave here chemical reactions occurring just at the shock front. Here the initial pressure  $P_0$ , here the initial density  $\rho_0$  and the condition of the condition behind the, behind the detonation which is a shock driven by chemical reactions occurring behind it.

We call it as P C J and the value of P C J by the initial value of the pressure in the un reactive medium was equal to gamma divided by gamma plus 1 into M s square. We also got, found the expression for the density behind the detonation and we got it as equal to rho C J by rho nought is equal to gamma plus 1 divided by gamma.

Therefore, let us do one problem to illustrate this, but we must not forget that when we talk of a C J detonation well we are talking of a constant velocity detonation. And in this case the shock drives the chemical reactions behind it and it is these chemical reactions which again go and reinforce the shock strain and make it go at a constant velocity which we say is V C J. Let us do one problem, let us take the problem of using the theory which was developed yesterday.

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We would like to find out let us say determine the Chapman Jouguet velocity of a detonation that is V C J for a stoichiometric mixture of hydrogen with air. Let us say the mixture is stoichiometric. We want to find out the C J velocity and also let us say the

density ratio or may be the pressure ratio or rather the pressure behind the detonation and the velocity behind the detonation such that we get a feel for what this detonation is. Let us do this problem, we must write out what is the heat liberated in a mixture which is stoichiometric hydrogen with air.

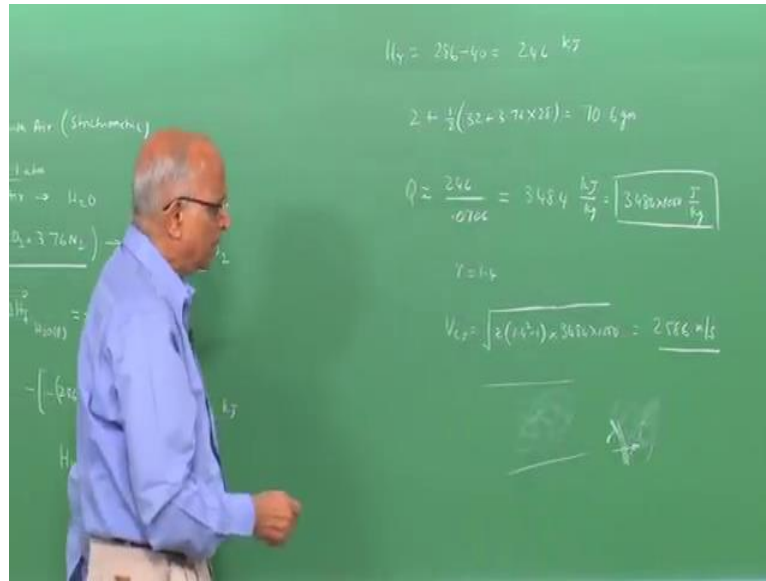
Before we say hydrogen reacting with air forms products of combustion, when we say stoichiometric mixture, we say completely burned products of combustion are formed only, either for  $H_2O$  is formed and if  $H_2O$  is formed, the amount of air which is required is  $O_2$  one mole of air is accompanied with 3.76 moles of nitrogen. And therefore, I have  $H_2$  plus  $O_2$  giving me  $H_2O$  and the balanced nitrogen is coming in the products over here  $N_2$ . Now, I have two atoms of hydrogen 2 atoms, I have 2 atoms of oxygen, here I have 1. Therefore it must be half over here and the amount of nitrogen in the product should therefore, be 3.76 divided by 2.

Well this is the reaction for the combustion or burning of hydrogen with air and I want to find out the heat released because I need to find out the heat released in order to find the C J velocity and to be able to do that we again use the heat of formation. The heat of formation of water in the liquid state we have done it earlier, the standard heat of formation. Let us presume that the hydrogen and air are at the standard condition of 25 degree centigrade. Let us also presume, it is at 1 atmosphere pressure. Therefore, this standard heat of formation of water as a liquid is equal to minus 286, we have done this before so much kilo joule per mole.

And therefore, the heat generated in this reaction is equal to minus heat of formation of the reactants which is equal to minus 1 mole of this. That is minus 286 and you have minus. Well nitrogen is a naturally occurring substance, the heat of formation is 0 at the standard condition. Hydrogen element at the standard condition is 0, oxygen again 0. Therefore, you have minus 0 minus for the products here, minus for the 0 plus 0 over here for the reactants which gives me a value of plus 286 kilo joules for the reaction.

But, in this case the water is formed as products under the, at the standard condition well it is a liquid, but you know the temperatures behind a detonation will be high and it will occur as a vapour phase. And therefore, the heat which is generated part of the heat goes into evaporating the water.

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The heat of formation, the heat of vaporisation of water is equal to 40 kilo joules per mole. This is from the standard tables for. And therefore, if I have vapour being formed, the heat of reaction is going to be 286 minus 40 which is equal to 246 kilo joules for the entire reaction. I am interested in finding out what is the energy liberated per kilogram of the mixture and I find in this particular case the mass of the reactants is equal to let us put it down  $H_2$  is 2 grams plus half  $O_2$  is 32 plus 3.76 of nitrogen is into 28 and if we now calculate 2 plus 16, 18. 18 plus 1.88 into 28, this will come out to be equal to, I wrote out this value comes out to be 70.6 grams.

Therefore, we get heat which corresponds to 246 kilo joules for 70.6 grams. Therefore, the heat generated  $Q$  per kilograms is equal to 246 divided by what is generated is 0, so many kilograms you have, 246 and the value of the heat comes out to be 3484 so much kilo joules per kilogram, which is equal to 3484 into thousand joules per kilogram.

Therefore, I know the heat release in a reaction and once I know the heat release in a reaction, I want the Chapman Jouguet velocity. I know that  $V_{CJ}^2$  that velocity is equal to  $2 \gamma^2 \text{ minus } 1$  into the heat released in joules per kilogram. I need the value of gamma. Let us take a look at the mixture what is being formed, I have hydrogen gas, I have oxygen gas, I have nitrogen gas, all are diatomic.

And therefore, the gamma for this reactant is equal to gamma is equal to 1.4. And therefore, I have  $V_{CJ}$  is equal to under root of 2 into 1.4 gamma square minus 1 into the

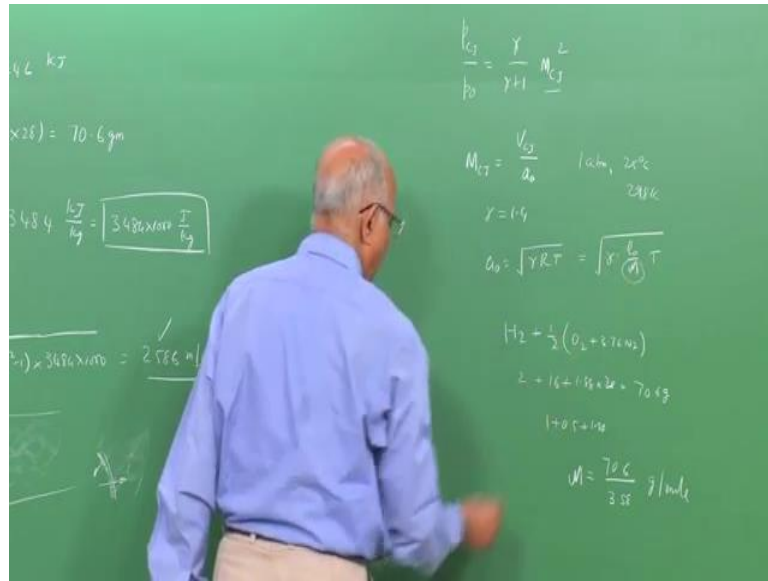
heat released that is equal to 3484 into 1000 and this gives me a value equal to 2586 metres per second. Well, this is how we calculate the Chapman Jouguet.

Therefore, if I were to have let us say a mixture of gases, stoichiometric hydrogen air mixture or a cloud of stoichiometric hydrogen air mixture is formed and suppose you had formed a shock wave. And this shockwave turns into a detonation because chemical reactions are occurring behind it. The steady velocity with which this combination of the shock and chemical reaction which we call as a detonation will move at a velocity of 2586 metres per second and this is how we calculate.

But we must remember the procedure which we adopted was somewhat quite simple and quite crude also. See we said, well chemical reactions occur completely burned products of combustion are formed from this stoichiometric mixture, but if the temperature behind a detonation, in a detonation that is behind the detonation is I then water will break like for instance let us go back into this reaction. Some of the water will break into hydrogen, may be if the temperatures are really high it will again dissociate into h atom may be into something like vibrationally excited hydrogen could also be formed.

And therefore, it could again dissociate with the result that the heat released is on the high side. And therefore, we do expect that the velocity, but we have predicted using this simplistic consideration could be on the high side. Therefore, anyway we have got the velocity of a detonation, we will debate how to improve the model a little later. Let us determine what is the value of the pressure in a, behind a detonation.

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Therefore, we say well we got the expression for pressure behind a detonation to the initial pressure is equal to gamma divided by gamma plus 1 of the marked number of the detonation. We have to find out the value of  $M_{CJ}$  and what is the value of the marked number of the detonation and  $M_{CJ}$  is equal to  $V_{CJ}$  divided by the sound speed in the mixture. I need the sound speed in the mixture, we said well the mixture is at 1 atmosphere pressure. Let us say it is at 25 degree centigrade that is 298 kelvin. I need the sound speed in the mixture at 298 kelvin. We said well, gamma is equal to 1.4.

But therefore, I need something like the molecular mass of the gases because we know sound speed is equal to  $\gamma R T$  where  $R$  is the specific gas constant we have derived this earlier and this could again be written in terms of universal gas constant as  $\gamma$  universal gas constant divided by the molecular mass into the temperature. I need to find out the mean molecular mass of the unburned gas mixture that is the stoichiometric of hydrogen and oxygen.

Well we said, well stoichiometry is  $H_2$  plus half the mixture is equal to  $O_2$  plus 3.76 of  $N_2$ . Therefore, what is the molecular mass? Well, the total mass is 2 plus 16 plus 1.88 into 28 is the, is the total molecular mass and this we got this equal to 70.6 grams earlier. And we see how many moles are associated is 1 plus half plus 1.88 that is 1 plus 0.5 plus 1.88 that is equal to 2.38, 3.38 that is equal to the mean molecular mass is equal to 70.6

divided by 3.58 so much grams per mole. Having determined the molecular mass now I can find out the value of R that is R nought by m, let us do that.

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$$R = \frac{R_u}{(70.6/3.58) \times 10^{-3}}$$

$$= \frac{8314}{20.9 \times 10^{-3}} = 398 \frac{\text{J}}{\text{kg K}}$$

$$a_0 = \sqrt{1.4 \times 398 \times 298} = 408 \text{ m/s}$$

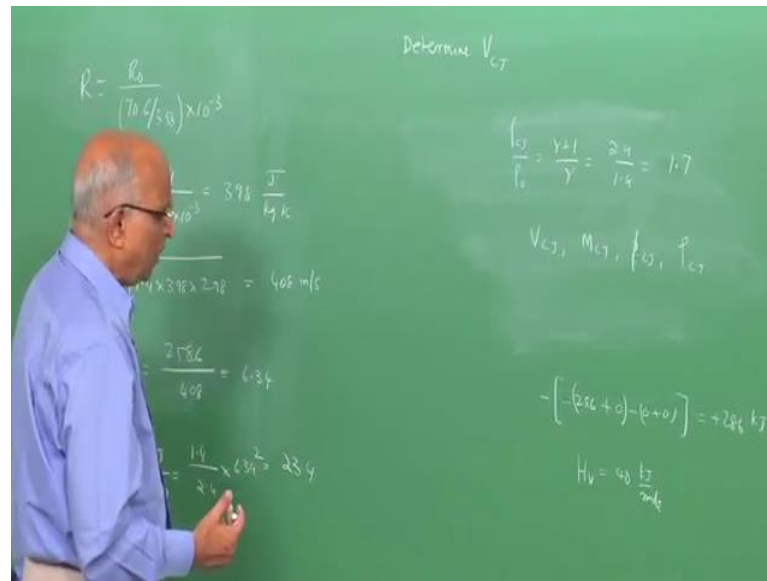
$$M_{CJ} = \frac{2586}{408} = 6.34$$

$$P_{CJ} = \frac{1.4 \times 398^2}{24} = 234$$

We have the value of R is equal to R nought universal gas constant divided by the value which we just now said is equal to 70.6 divided by 3.58 so much gram per mole. If it is kilo gram per mole it is 10 to the power minus 3 and this comes out to be R nought is equal to 8.314 joules per mole per Kelvin. And the value of the mean molecular mass is 220.9 that is 20.9 into 10 to the power minus 3 and the value of R is comes out to be 398 joule per kilogram kelvin.

This is the specific gas constant. The sound speed in the mixture is equal to under root gamma which is 1.4 into R which is 398 into the ambient temperature, this is 273 plus 25 which is 298 and this gives me the sound speed in the unburned gas mixture as equal to 408 metres per second. Therefore, the value of M C J the mark number of the detonation is the velocity of the detonation. We have calculated the velocity V C J that is the velocity of the Chapman Jouguet velocity as equal to 2586 metres per second.

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We have 2586 divided by 408. The mark number is therefore, equal to  $M_{CJ}$  is equal to 6.34. And therefore, I get now the value of  $P_{CJ}$  divided by  $P_0$  is equal to  $\gamma + 1$  divided by  $\gamma$  that is 2.4 into 6.34 square and this gives me the pressure ratio as equal to 23.4. Rather, if  $p_0$  is 1 atmosphere the Chapman Jouguet pressure behind a detonation is equal to something like 23.4 atmospheres.

Therefore, we are able to calculate the pressure behind the detonation. We are able to calculate the velocity of the detonation. Let us calculate the density behind the detonation front that means we have derived the expression as  $\rho_{CJ}$  by  $\rho_0$  is equal to  $\gamma + 1$  divided by  $\gamma$  which is equal to we have 2.4,  $\gamma$  was 1.4.

We took it to be the same in the gas mixture and also in the products of combustion divided 1.4. This is around 0., is equal around 1.7. Therefore, we get the different values and this is how we calculate the properties of a detonation mainly the  $V_{CJ}$  mainly the mark number of the Chapman Jouguet detonation wave. The pressure behind, the pressure behind the detonation that is behind the Chapman Jouguet detonation which is the detonations travelling at constant velocity a steady state detonation and the density behind the detonation. Well, this is how we calculate the properties, but we must note a few things.

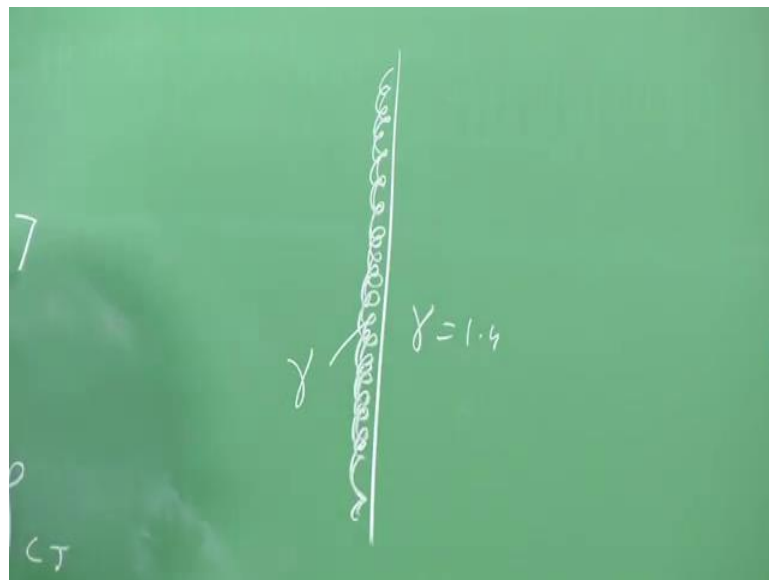


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$h_f = 28640 = 246 \text{ kJ}$   
 $2 + \frac{1}{2}(32 + 3.76 \times 28) = 70.69 \text{ mol}$   
 $\frac{246}{1.4} = 175.7$   
 $\gamma = 1.4$   
 $\frac{246}{0.0706} = 3484 \frac{\text{kJ}}{\text{kg}} = \boxed{3484 \frac{\text{kJ}}{\text{kg}}}$   
 $\gamma = 1.4$   
 $V_{C_2} = \sqrt{2(1.4-1) \times 3484 \times 1000} = 2586 \text{ m/s}$

We expect we told that we account it for a larger value of  $Q$ , we did not take into account that the dissociation taking place at high temperatures. We also did not consider a few things like in a detonation we said well I have a shock.

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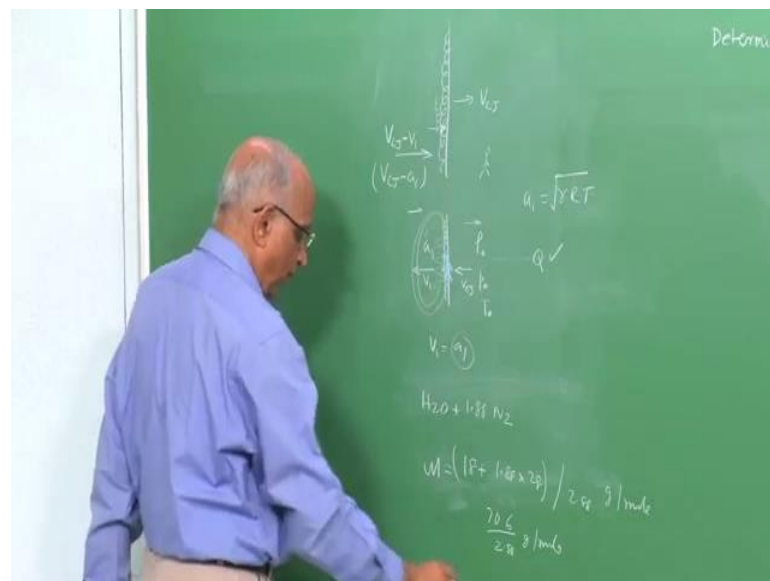


Behind the shock the chemical reaction are occurring and we took the gamma in the gas mixture ahead of a detonation and the value of gamma both as equal to 1.4. Well, when I have products of combustion which are something like water something like  $\text{H}_2\text{O}$  being formed, gamma here will be definitely different. We did not account for these

differences. And therefore, maybe our numbers may not be very accurate, but we will compare it with numbers for which this difference has been taken, but it gives us a good picture of what velocities, pressures and density to expect in a detonation.

See, one another parameter we would also like to calculate. Like for instance, we would like to calculate the velocity with which the products of combustion follow the wave.

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Like for instance, I have a detonation taking place. Let us also do this, I have a detonation that means a shock driven by chemical reaction occurring behind the shock wave, let us say this wave is travelling at the Chapman Jouguet velocity. I want to find out, when I have products of combustion over here at what velocity is it going to follow the wave. You know this is a, this is an important parameter because when I have an explosion and somebody is standing over here and he gets a detonation, it is not only the shock front which hits him afterwards the blast of wind is going to go and hit him.

And therefore, this is also equally important. To be able to determine this well what did we consider in the problem. In the problem, which we formulated we said well I have a Chapman Jouguet detonation travelling at constant velocity into a medium of  $\rho_0, P_0, T_0$ . Well, I am, I formulated the problem in the frame of reference of my detonation that means that is with respect to the wave station. That is I sit on the detonation.

Therefore, I see  $V_{CJ}$  approaching me with these properties and what leaves me is  $V_1$  with these properties and we found that for a Chapman Jouguet detonation  $V_1$  is equal to the sound speed behind the detonation  $V_1$  is equal to  $a_1$ . We got this from the point of view of the tangency condition of the Rayleigh line with respect to the reaction Hugoniot. And therefore, if we can find out the value of  $a_1$  in the product gases it is same as  $V_1$  and the velocity with which the gases follow me.

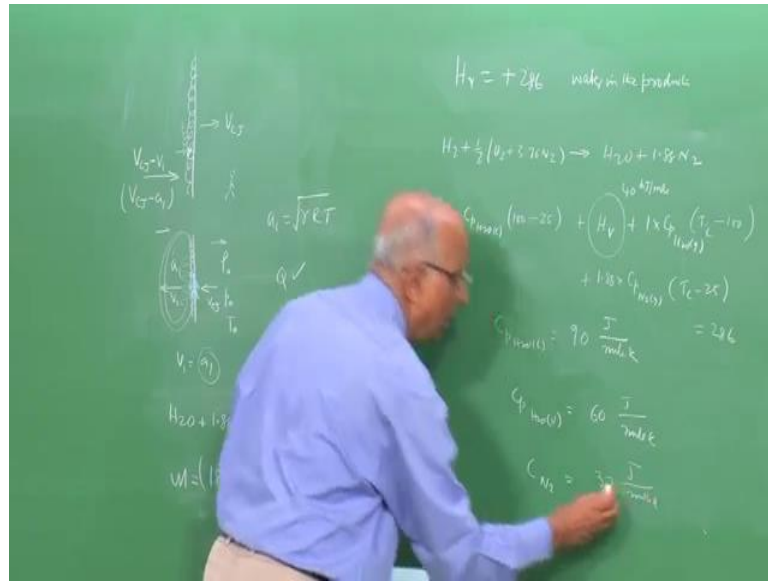
Therefore, I say well the thing now I have to again translate it in the frame of reference of a person standing outside and watching it. Therefore, I have  $V_{CJ}$  here. And therefore, the velocity with which something follows me here is equal to  $V_{CJ} - V_1$  this is equal to  $V_{CJ} - V_{sound P}$  over here. Therefore, to be able to calculate the sound speed in the products of detonation what is here I need to find out what is the composition of my products and that we have already done we said it is stoichiometric. We are assuming, it we said the products of the combustion are  $H_2O$  plus I have 1.88, 3.76 divided by to 1.88 of nitrogen. This is my products of combustion.

Now, I need to calculate the mean molecular mass of the products of combustion. Therefore, mean molecular weight of the products of combustion is equal to  $1.18 H_2O$  is 2 plus 16, 18 plus 1.88 into nitrogen is 28. This is the total molecular mass divided by the number of moles in the product of 1 plus 1.88, 2.88 so much gram per mole. Therefore, the molecular mass of the gases behind the detonation come out to be equal to let us get that done, it comes out to be equal to this is 70.6 grams divided by 2.88 so much grams per mole.

And if I want to calculate the sound speed in the product gases well the sound speed  $a_1$  is equal to  $\sqrt{\gamma R T}$  under root where  $T$  is the temperature in the products in the detonation that is after the detonation is over the products are hot, the temperature is going to be corresponding to the high temperature. I have to calculate this temperature also. How do I calculate this temperature? Well, I know the heat release, we say heat release we have calculated already using the heat release I need to calculate the temperature also.

Therefore, let us calculate this temperature such that I can calculate  $a_1$ . And therefore, find out the speed with which the products move. To be able to calculate the temperature, I again use my heat of the reaction and what is the let us write out this.

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Heat of the reaction is equal to minus of minus 286 that is 286, if I form water in the products of combustion and the what does this heat do? This heat increases, let us, let us again write the reaction  $H_2 + \frac{1}{2} O_2 + 3.76$  of nitrogen gives me the products namely the  $H_2O + 1.88$  of nitrogen.

And therefore, what is going to happen? The energy of the reaction goes to increase the temperature of this and what happens therefore, I have 1 mole of water into the specific heat of water and what does water do? The specific heat of water that is  $H_2O$  liquid increases from 25 degrees at standard condition to a temperature of 100 at which it begins to boil.

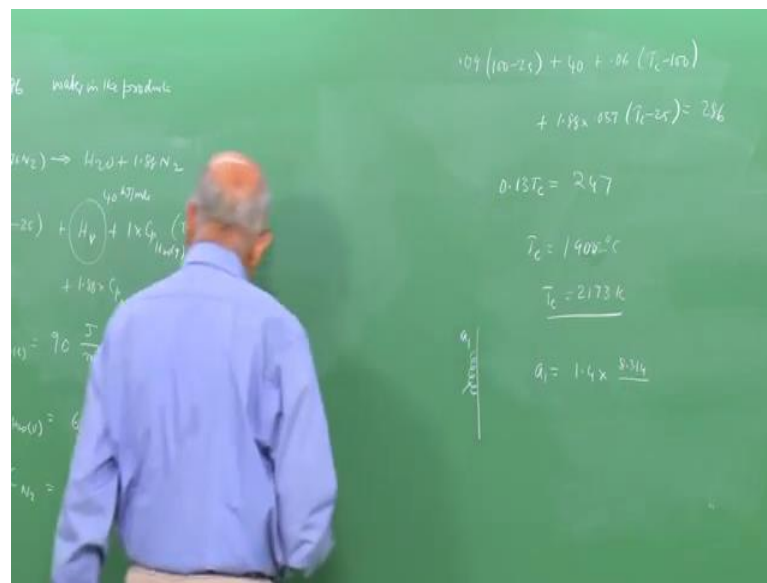
And then, I have the latent heat of vaporization of water, I call it as  $H_V$  plus the same 1 mole of water into specific heat of the water vapour  $H_2O$  as a gas increases in temperature from 100 degree centigrade to the temperature of combustion, I call it as  $T_c$  over here minus 100 plus I have 1.88 moles of nitrogen into the specific heat of nitrogen which is equal to nitrogen gas. And mean value I will take into the temperature of combustion minus 25 degrees it is a gas all along.

And this should be equal to the value of 286. We said the latent heat of vaporisation is 40 kilo joule per mole and if the value, if I can use the mean values of the specific heat of water, the specific heat of steam or water vapour and the specific of heat of nitrogen these are available to me. The specific heat of water as a liquid is equal to 90 joules per

mole kelvin. The specific heat of water vapour H<sub>2</sub>O as vapour is equal to 60 joules per mole kelvin and the specific heat of nitrogen gas is equal to 37 joules per mole kelvin.

And therefore, I plug in these values and what is it I get? I am able to now calculate the value of T<sub>c</sub>, let us quickly do this. I get since these are in joules whereas this is in kilojoules for the reaction 286 kilojoules. Therefore, I convert this to kilojoules and therefore, I write it as 0.9, 100 minus 25 plus I have 40 kilo joules latent vaporization plus 0.06 into T<sub>c</sub> minus 100 plus 1.88 into 0.037 into T<sub>c</sub> minus 25 is equal to 286.

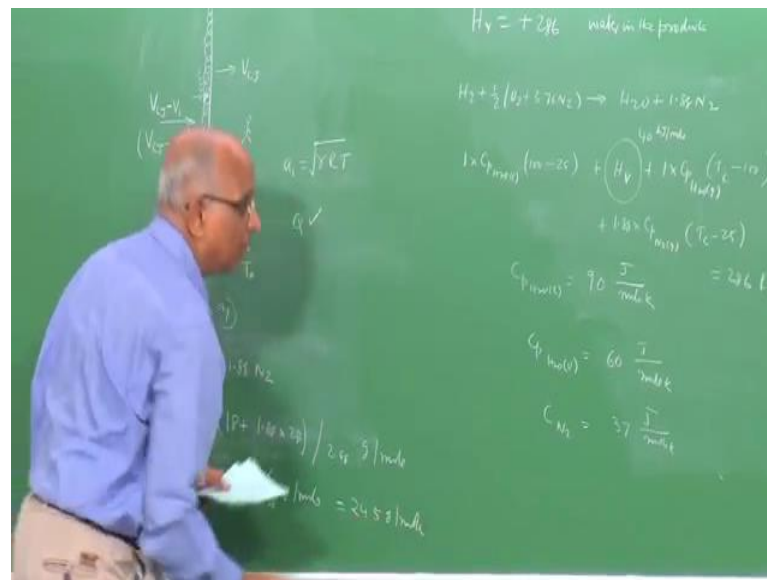
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And therefore, if I simplify this and do not go through all the steps, I find what I get is 0.13 T<sub>c</sub> is equal to 247 or rather the temperature of the combustion products in a detonation is equal to I get for this particular, this is equal to something like 1900 degree centigrade which is equal to in kelvin add 273 which is equal to 2173 kelvin.

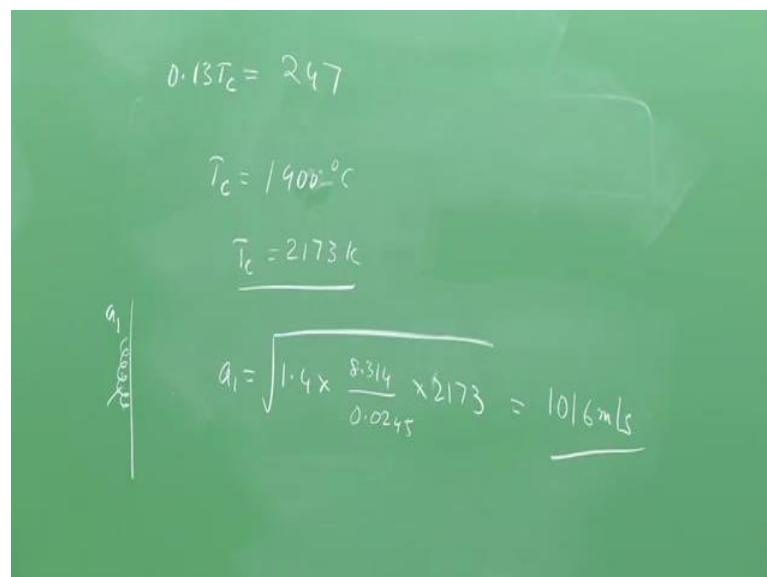
This is my temperature of the gasses in a detonation in the, in the products that means I have the shock, I have products, the temperature here is 2173. The sound speed is therefore, equal to I presume that the gamma is still the same I take the value as 1.4, I get a 1 that is the sound speed in the process gasses. That is gasses processed by a detonation is equal to 1.4 into the value of R naught is equal to 8.314. The molecular mass of the gases we have calculated here is equal to 70.6 divided by 2.88 which is equal to the it comes out to be 24.5 gram per mole.

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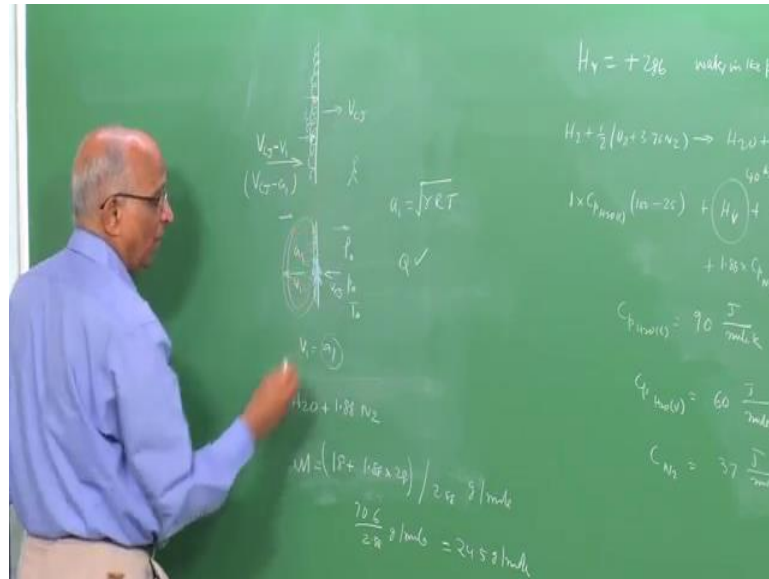
Therefore, into 8.314 divided by 0.0245 so much kilogram per mole into the value of 2173 under root which is equal to a value of 1016 meters per second.

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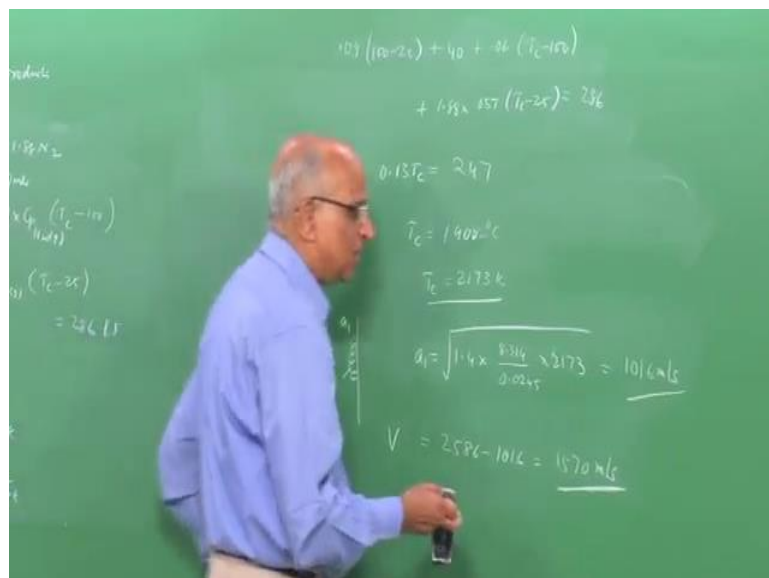
Therefore, we find that the sound speed in the medium processed by the detonation is 1016 meters per second and if it is 1016 meters per second.

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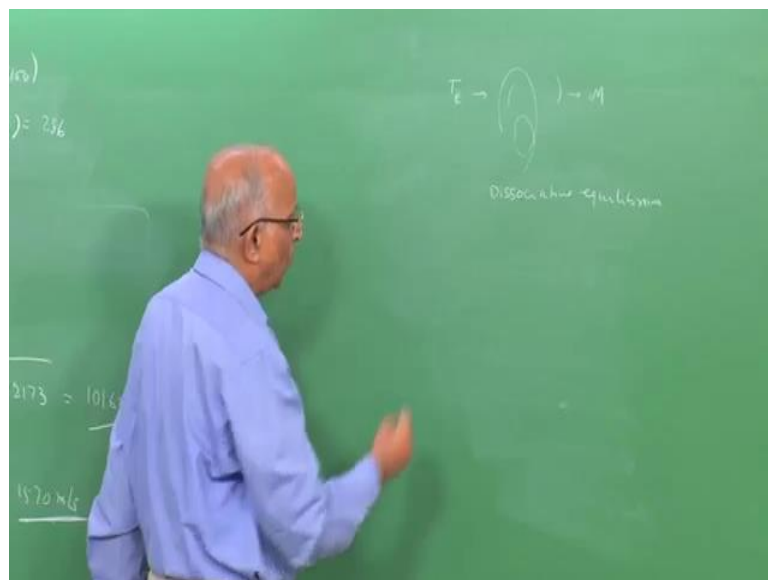
Well, we want the velocity behind in the frame of reference of this that is  $V_1$  is equal to the same as the sound speed, it is equal to 1016. And therefore, the velocity with which the products of detonation follow the shock wave is going to be the velocity of a detonation we have calculated earlier and that was equal to 2586 meters per second minus 1016 meters per second is the velocity with respect to the frame of reference that is the velocity over here.

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And this is equal to the velocity with which the products follow the detonation and it comes out to be 1570 meters per second. Therefore, we are able to get the velocity with which the products follow that detonation we know the velocity of detonation  $C_J$  velocity. We also know how to calculate the pressure and the density changes taking place in a detonation. This is how we do a problem on detonations and having done this now we have understood how to do this, but we also said these are little approximate because we did not really take care of dissociation and in practice we have to, we have to do the problem iteratively and standard codes are available in literature like cosmic and other codes which calculate the detonation velocity using the dissociation.

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And what we do is, it must be done in something like you assume a flame temperature, or assume a combustion temperature, calculate at this temperature, what is the equilibrium composition of products taking place in a detonation.

Then, you calculate the molecular mass, then you calculate what is the sound speed taking place. May be you keep on iteratively such that all these things are matching and you do it in an iterative scale and mind you this iterative scale gives values which are better than what we have calculated. But what we have calculated is representative and we can do these calculations namely these iterative calculations using the dissociative equilibrium.



We have not discussed dissociative equilibrium and if time permits towards the end of the class as I said earlier we will also take a look, we have to look at the minimization of Gibbs free energy to achieve equilibrium of the products of a detonation. Let us now quickly compare what are the results, how do these values compare with for the other gases.

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$$V_{CJ}^2 = 2(\gamma^2 - 1)Q$$

|   | Gaseous Fuel                            | (km/s) | (atm.) |
|---|---|--------|--------|
| 1 | Methane CH <sub>4</sub>                 | 1.8    | 16.05  |
| 2 | Ethane C <sub>2</sub> H <sub>6</sub>    | 1.8    | 17.0   |
| 3 | Propane C <sub>3</sub> H <sub>8</sub>   | 1.8    | 17.27  |
| 4 | Butane C <sub>4</sub> H <sub>10</sub>   | 1.8    | 17.44  |
| 5 | Acetylene C <sub>2</sub> H <sub>2</sub> | 1.87   | 18.0   |
| 6 | Hydrogen H <sub>2</sub>                 | 1.96   | 14.6   |
|   | TNT                                     | 6.94   | 1900   |

I show in this particular slide we use this expression  $V_{CJ}^2$  is equal to  $2(\gamma^2 - 1)Q$  and whether we use it or do iteratively, we do iteratively we get for different gaseous mixtures stoichiometric mixtures for which the initial condition is 1 atmosphere and initial temperature is 298 kelvin.

The detonation velocity is something like 1.8 kilometres per second for Methane air mixture stoichiometric. For Ethane air it is again 1.8, for Propane air again 1.8, Butane air again 1.8. We find for all these aliphatic hydrocarbons the detonation or C J velocity is around 1.8 kilometres per second. While for Acetylene, it is higher at 1.87, for Hydrogen it is around 2 kilometres per second.

Mind you, for the stoichiometric these are all for the stoichiometric mixtures with air and we had calculated instead of 2 kilometres per second, we had calculated a velocity of around 2586 metres because of the assumption of complete combustion. We had overestimated the heat release. When we look at the pressure behind the detonation we find that for the Methane stoichiometric Methane air mixture, the pressure when the

initial pressure is equal to 1 atmosphere is 16 times is 16 atmospheres, for Ethane it is 17, 17.2, 17.5 around 18 for Acetylene and around 15 for Hydrogen.

Therefore, this is how these are the values and what is it we immediately note. We immediately note that these velocities are typically kilometres per second. When we talk in terms of flame velocities in Methane, Ethane, Propane, we found it is around 0.5 metres per second. Here it is 1800 that means it is something like 4000 times higher that means the velocities of these detonation are high. We also find that the pressures are very high in the case of a flame we said the pressure slightly drops. In this case, we find that the pressure increases almost between 15 to 18 times or something like 15 to 20 times.

And therefore, these pressures are high. Therefore, a detonation is capable of doing much more harm and we also find that the velocities of the product gases which move behind the shock wave are also of high velocity which we just did on the board. And therefore, a detonation does much higher damage than what a burning or a flame can do. Now, we can do a similar problem see we have been illustrating for gases since we use the perfect gas equation we were able to get an expression for the reactive Hugoniot and then we calculated the upper point at which the Raleigh line is tangent to the reaction Hugoniot which we found is the gives me the Chapman Jouguet velocity.

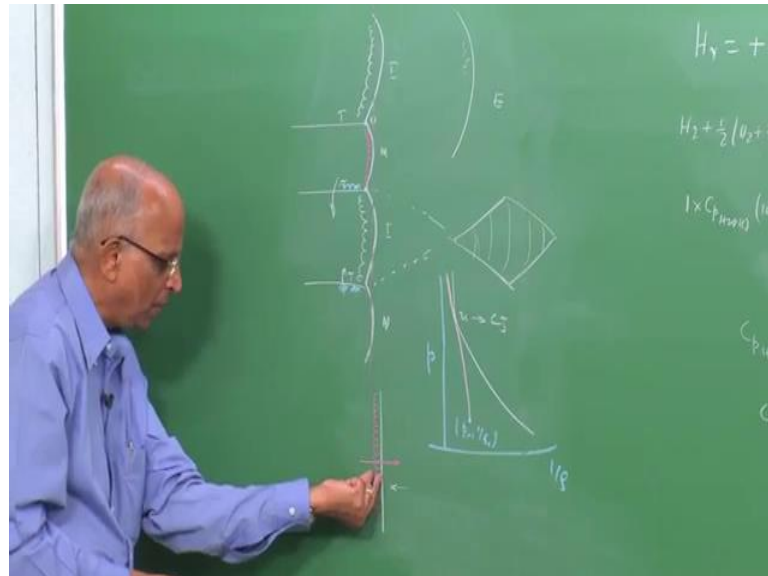
You know when we consider solids, let us say T N T which is a solid explosive, high density condensed phase. You know the equation of state for gases cannot be used. We have to estimate the reaction Hugoniot and then if you use the reaction Hugoniot and find the tangency condition, you will find that the speed of a detonation in a solid like T N T that is tri nitro toluene is equal to something like almost like 3 times the value 6.94 kilometres per second. And the pressure behind the detonation is extremely large something like 1900 atmospheres.

Therefore, we find here the detonation velocities are large, if the initial density is large well the velocity also increases and the pressure behind the detonation is also quite a large number. Therefore, these are the cases. By now, we should know we should have a feel of what a detonation is? What this Chapman Jouguet detonation is?

And now let us proceed further, let us see the structure of a detonation because the structure of a detonation also has some information. Before getting into the structure, I want to spend a couple of minutes to sum up what we have done so far in detonation so

that we know what are the assumptions made? How we are looking at the problem? We found that well a detonation front consists of a series of shock waves.

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It is not a single shock wave we have something like an incident shock, we have a mark shock, we have an incident shock, we have a mark shock and we also have transverse waves which move behind it. We have these transverse waves moving here and these things the triple point where in you have the transverse waves and the shocks combining these are known as the triple point.

These triple point generate something like a cell, a cell of a detonation and within a cell of a detonation these shocks completely are in a shape of continuous decay, but however you know you have these cells of detonation within which the lead shock travels and it is in a state of decay it gets energised when the two transverse waves meet here and then it progresses. But then for a small cell size that is when the cell size is small and also to have a feel for what a detonation is, we said it could be approximated as a planar case and instead of saying well behind the incident shock, incident shock is weaker it takes a longer time for the reaction to occur if behind a marked shock well the marked shock is stronger.

Therefore, reaction occurs faster behind this well it takes longer, we are talking of incident shock. I also have chemical reactions occurring behind the transverse wave, some chemical reactions occurring here, the chemical reactions occurring over here.

Therefore, this is the type of chemical reaction zone in an actual detonation. I have simplified the whole picture into something like a planar shock and we found we said well the chemical reactions are occurring behind the detonation over here. And we found well this combination of a shock driven by chemical reactions is what constitutes the detonation in practice.

We have the chemical reaction zone spread out here and here, but I just take a mean value and this is what I found. And for this well, this corresponded to the case when the velocity was such that we had something for a one dimensional case, I had pressure into  $1/\rho$ . I had this is my initial point 1 by 1 or let us say  $P_0$  into  $1/\rho_0$  was my initial condition. I had my reaction Hugoniot over here when the Raleigh line from the initial point to this was tangent to this, mind you the reaction Hugoniot was over here.

Well, this corresponds to the upper tangency condition and this gave me the condition for a C J in which case, the velocity behind it in the frame of reference of the shock wave that means the gases are moving towards it. I have the velocity here this was equal to the sound speed behind and this is the constant velocity picture of a detonation and in practice we do observe that the V C J what we calculate and what is measured is very near saying that even though the structure is 3 dimensional the Chapman Jouguet velocity gives a fairly reasonable estimate of the velocity of a detonation.

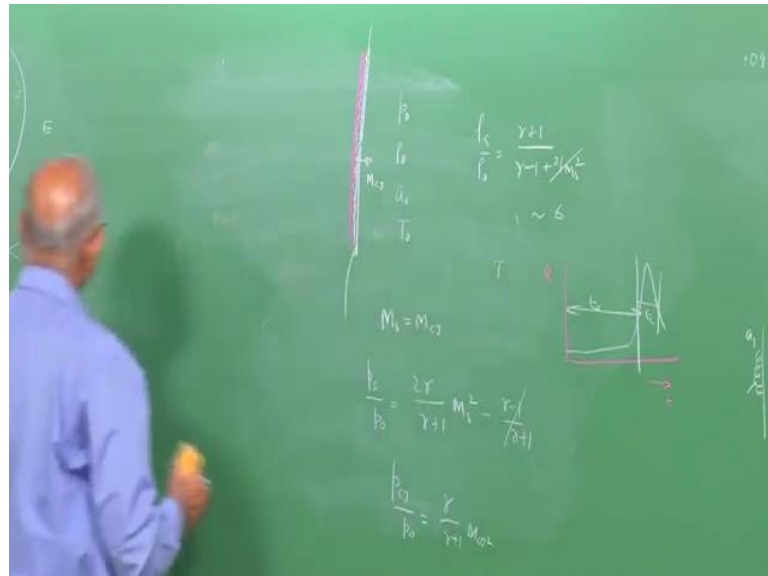
The pressure behind a detonation could be measured using the one dimensional model. The density could be measured, the mean velocity at which the particles follow could be measured. We did a problem for calculating this, but now we ask one last question you know what is the use of all this. You know, we use the three dimensional structure to be able to calculate what this mean cell size is, we found out this as a characteristics of detonation.

We also calculated using a shock wave followed by chemical reactions. We were able to calculate the energy required to start a detonation, we found that this energy is several kilo joules. We related it to a blast initiation, we also said well if in practice I cannot have such high energy released.

And therefore, a flame if formed by a ignition source it can always transit to a detonation if shocks are generated and this is all what we have learned for detonation. Now, if I look at this picture a little more closely what is it I observe? I observe the following. Well, I

have something like a shock and still in my 1 dimensional representation, I have a shock, I have the initial pressure let us say  $P_0$ , I have the density  $\rho_0$ .

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Let us say the sound velocity in the, in the un burn gas mixture or the mixture in which the shock has not travelled and cost chemical reactions let it be a 0 metres per second. Temperature could be initial temperature  $T_0$  and what happens?

When I say detonation is nothing but a shock followed by chemical reactions, what is happening this frontal shock also travels at the same velocity as the Chapman Jouguet detonation. That is the strength of the shock wave is same as the C J value of the detonation and behind the C J detonation well I have the chemical reactions which are occurring.

Now, what is it I perceive? I find that well there is shock behind the shock the pressure and temperature will go up and how do I get it? Well, we have done these things earlier. We said that the shock pressure divided by initial pressure is equal to  $\frac{2\gamma}{\gamma+1} M_0^2 - \frac{\gamma-1}{\gamma+1}$  into the shock mark number square minus gamma minus 1 divided by gamma plus 1.

Well, this is a small number  $M_0$  is large for detonation that is a Chapman Jouguet mark number is quite high. And therefore, it is  $\frac{2\gamma}{\gamma+1} M_0^2$ . Whereas, when we derived the expression for the C J detonation for  $P_0$ , we had it equal

to gamma divided by gamma plus 1 into  $M C J$  square. In other words, what is it we are talking of? Behind this shock, a zone of high pressure is created not only is it a zone of high pressure the density is also high  $\rho_s$  by  $\rho_0$  is equal to gamma plus 1 divided by gamma minus 1 plus 2 over the mark number of the shock square. Well, this is the small term gamma plus 1 divided by gamma minus 1 is our around 6 over here.

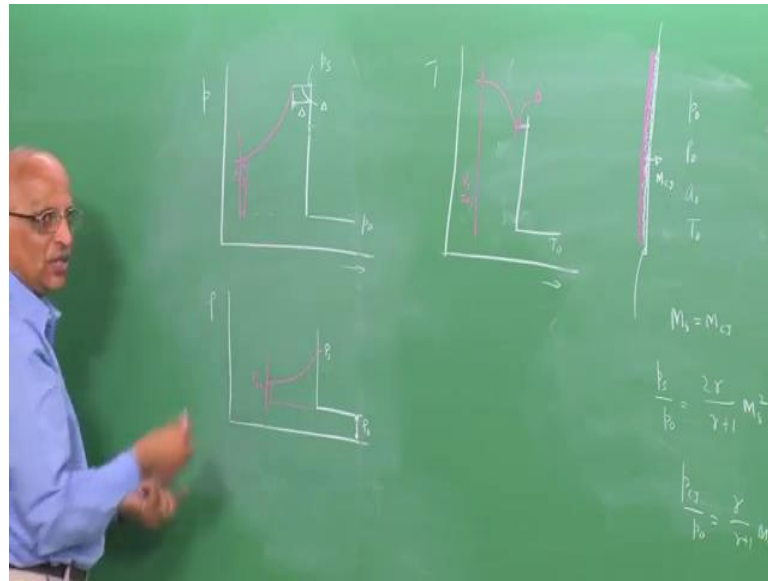
And therefore, we find yes high pressure high density gases are generated. Therefore, temperature is also quite high over here. And therefore, chemical reactions begin to get started behind the shock wave, behind the shock wave chemical reactions get started. But you remember when we talked of explosive gas mixtures we found normally the activation energies are large and whenever the activation energies are large what did we plot?

We found that the time taken versus the heat released  $Q$  and what did we find during the initial time? Well, there is not much heat being released. There is an induction time during which chains are being formed and when large number of chains are formed we have a sudden increase in chemical reaction, this is your induction time  $T_d$ . This was your chemical reaction time  $T_c$  over here.

And therefore, what is happening due to the high temperature and pressure you have some induction time taken for the chemical reaction to occur and after the chemical reactions are occurring you have the zone at which heat is getting liberated. And when heat is getting liberated, I find that at this particular condition when heat liberation is getting stopped here for a  $C J$  detonation the velocity of the particles here in the frame of reference of the front is equal to the sound velocity in the medium and the density here is much smaller than this is the value of 1.7.

The pressure was around half that in across a shockwave. And therefore, what is the picture I get? The picture I get is I have something like a shock front. If now I were to plot the value of pressure and density in a detonation, what is it I get?

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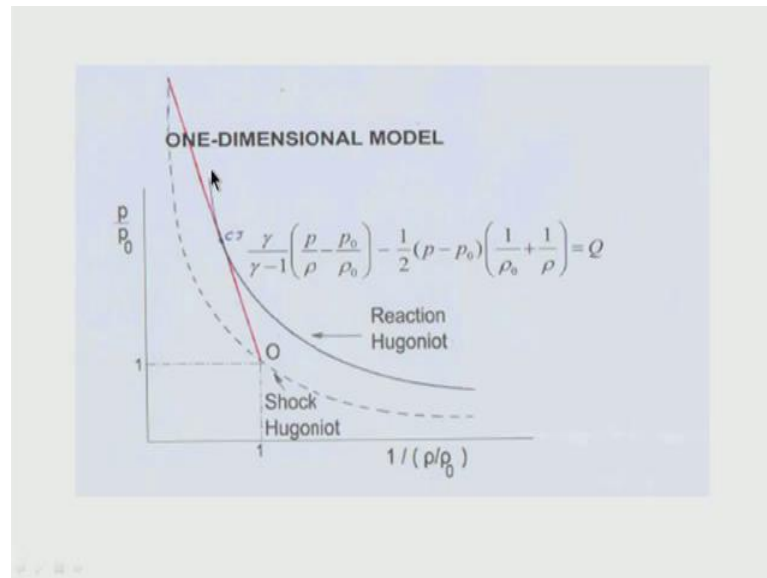
Well, I say well I am plotting the value of pressure as a function of the frontal shock over here. The pressure initially is  $P_0$  behind a shock the value is  $P_s$  and so also if I were to plot the value of density and the value of density as a function of the distance well I have the shock over here. This is the value of the initial density  $\rho_0$ , well I get the shock value as  $\rho_s$  over here. This is the value of  $P_0$  over here and so also if I were to plot the temperature I get temperature as a function of the distance, I have a shock here and the ambient temperature is  $T_0$ , let us say 300.

Here the temperature is quite high over here and then behind this what is going to happen? There is going to be an induction time, a time taken for chemical reaction to occur equivalently a small distance  $\delta$  which is the distance for the induction time to be over. I call it as the time for the chain reactions to be over or the distance for the induction time or the induction distance and once the induction distance is over what is going to happen?

The temperature will further increased to the value corresponding to the temperature of the chemical reactions. And what is going to happen here? Well, I have the induction distance over here  $\delta$ , this is equal to  $\delta$  and what is going to happen behind it? Well, the pressure is going to fall to the value of  $P_{CJ}$  and what is going to happen to that density? Here, the density ratio is around 6.

Well, the density falls to a value around 1.7 that is  $\rho_{CJ}$  such that this is smaller now, this is smaller now. And at this particular condition wherein all the chemical reactions are over I have the value of  $V_1$  is equal to a 1. Well, this becomes the actual picture in the case of a 1 dimensional detonation. And therefore, let us take a look at it through these slides over here. Now, for what is it we are talking of?

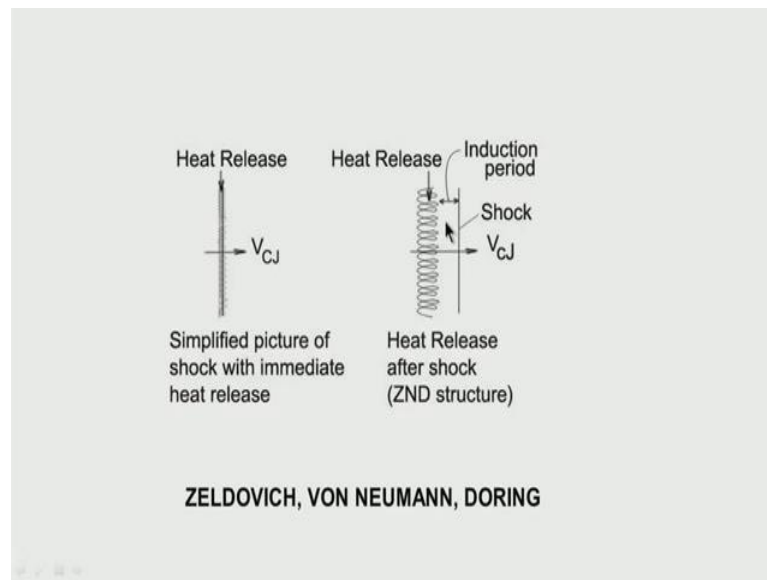
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We are saying in the 1 dimensional model, we had the reaction Hugoniot over here. We had the initial point over here. We drew the Rayleigh line, this is the upper point at which it was tangential, we called it as  $CJ$  point, over here we said well this is the steady state velocity of a detonation.



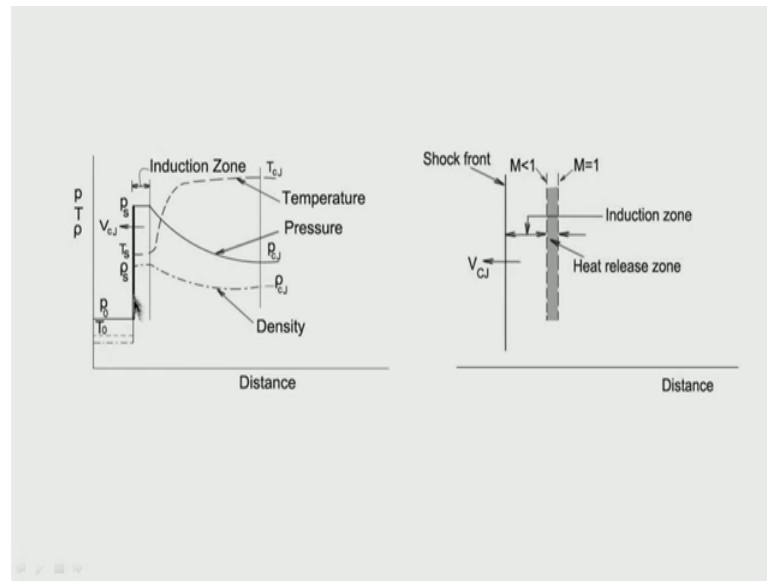
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And once we are able to translate it into the structure of a detonation, we find well I have a shock here, I have a induction period over here in which may be there is not much heat released at all. But it is at a high temperature and followed by a zone of reactions in the, in the picture what I had when I talk in terms of a Chapman Jouguet detonation, I just presumed that the heat is getting released. I never looked at this mechanism of an induction tank heat being released a little later.

And therefore, now we are talking of a detonation as comprising of a shock followed by some distance after which the heat is getting released and such type of a structure of a detonation was postulated independently by Zeldovich. These are all our pioneers Zeldovich, Von Neumann and Doring and it is known as Zeldovich Von Neumann Doring structure or an z n d structure of a detonation. Therefore, the 1 dimensional structure of a detonation consists of a shock front followed by an induction distance followed by the heat released.

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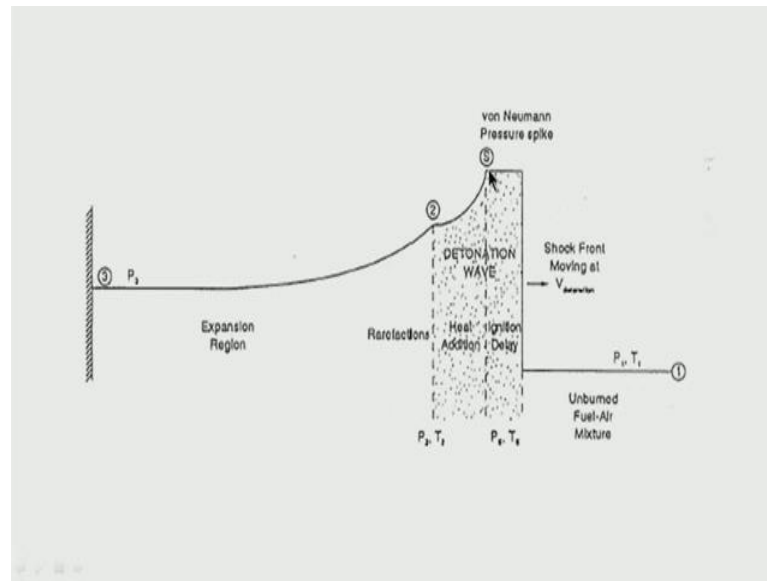


If we were to quantify it further, I show you this in this particular figure, I have a frontal shock moving at C J velocity. At the front, the pressure increases from  $P_0$  to  $P_s$ . During the induction time or induction zone thickness well, the pressure is remaining constant that means no chemical reactions are occurring and then when heat release gets started well the pressure falls from the high value of  $P_s$  which is equal to  $2\gamma$  by  $\gamma + 1$  into  $M_s$  square, the expression was here  $2\gamma$  by  $\gamma + 1$  into  $M_s$  square. And therefore, the pressure reaches the high value and then gradually falls to the C J value which is equal to  $\gamma$  by  $\gamma + 1$  into  $M_{CJ}$  square and this is what happens in the chemical reaction zone.

Similarly, the density increases to a value around  $6\gamma$  plus 1 by  $\gamma$  minus 1 and then the density drops to a smaller value of  $\gamma$  plus 1 divided by  $\gamma$ . And the temperature increases behind the shock to high values and then further increases due to chemical reaction to the Chapman Jouguet value. Therefore, this becomes Z N D structure or the two dimensional structure of a detonation and what is it we have? We have the shock front behind the shock.

Well, the flow is sub sonic in the sub sonic you have the induction time and after when once the chemical reactions are occurring well the flow gets accelerated and it reaches a value  $m$  is equal to 1 and this is where the chemical reaction stop and this is the heat released zone and this is the induction zone.

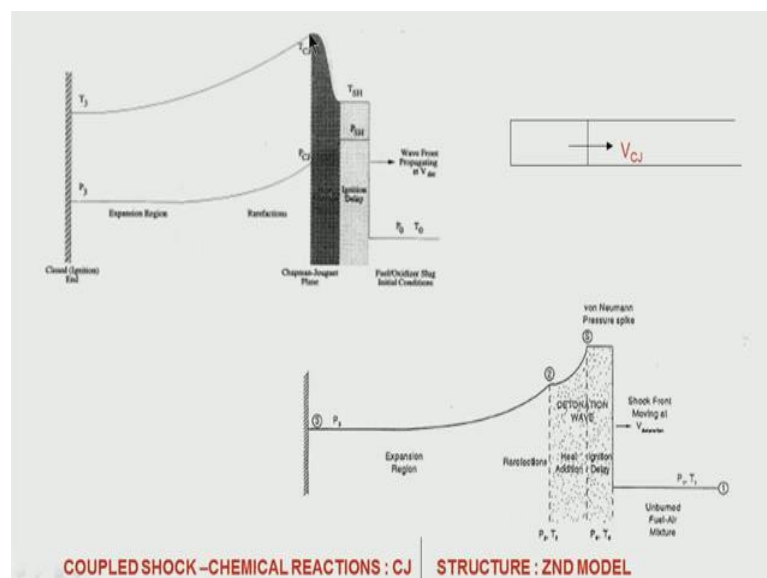
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If I try to look it in a slightly different format well I have the initial temperature here, a shock moves. I have a pressure which is formed here I have the pressure behind the shock we said is higher than the detonation pressure which is coming over here. And the gases further expand over here.

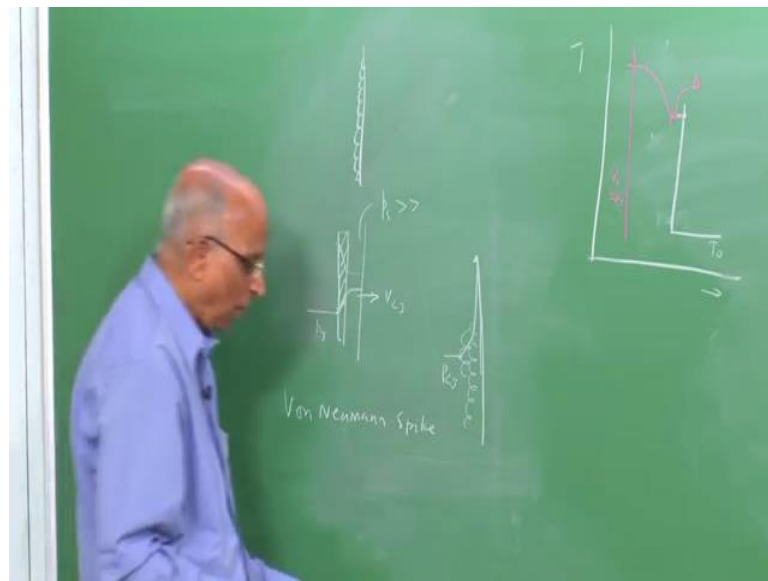
And therefore, at this point the sound speed in the medium is same as the velocity. Therefore, none of this expansion disturbances can catch with this. This travel with a constant speed and we have a pressure spike in a shock followed by a lower pressure.

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And the same thing is again represented here in terms of temperatures have the shock temperature increasing behind this to a higher value corresponding to chemical reactions. You have the temperature corresponding to the Chapman Jouguet value with chemical reactions. The pressure increasing and falling to the Chapman Jouguet value and similarly, the density will also fall and this is the Z N D or we call it as the Zeldovich Von Neumann Doring structure of a detonation. Therefore, let us quickly sum up what little we have learnt about detonation.

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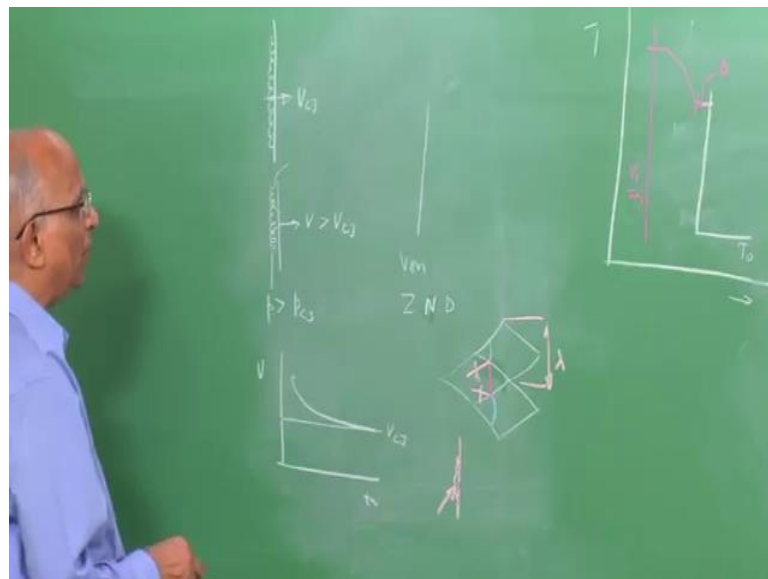
We sell ourselves in the 1 dimensional model we had a shock front followed by chemical reactions which we call as the Chapman Jouguet detonation corresponding to the point u and we also said well if I were to consider the induction time, I have a zone of chemical reaction. This is the shock front moving at a value V C J. This is the zone of chemical reaction in this case may be the temperature increases to high value the pressure falls to the C J value.

Then we know we have also found that pressure behind the shock that is P s is very much higher than the mean value of pressure or the value of pressure behind the detonation. In other words, whenever I talk in terms of a detonation, what is going to happen? I have a shock followed by chemical reactions in the zone following the shock, I have a spurt in the value of pressure which is higher than the value behind the detonation

that is the C J value. And this spike in the pressure is known as Von Neumann pressure spike.

That means the pressure behind the shock wave is what is referred to as Von Neumann spike and it falls down in the zone of chemical reactions to the C J value which is around half the Von Neumann value. If I want to estimate the value of the Von Neumann spike in a particular mixture well all what I do is, I use the shock wave relations  $P_{\text{shock}} / P_0$  divided by initial pressure is equal to  $M^2$  this corresponds to the C J value and for the C J value using this equation I estimate the pressure. Well, this is all about detonations and I think it is time to sum up what we have learnt about detonations.

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We find that well a detonation is a shock which is followed by chemical reaction which are induced by the shock, but these chemical reactions drive the shock at a constant velocity which is the Chapman Jouguet velocity, point one.

We also find that if I supply much more initiation energy, I create a shock velocity that is shock velocity which is greater than the Chapman Jouguet velocity and in this case what is going to happen? The pressure behind the detonation is going to be let us say pressure behind is going to be greater than the C J pressure with the result these the velocity over here is less than the acoustic or the sound velocity in the medium.

Therefore, disturbances keep catching and if I have if I start a detonation with a high value of velocity and with respect to time I look at it the velocity will decay till it reaches a constant  $c_j$  value, this comes from the 1 dimensional model. We also talked in terms of induction time, we talked in terms of structure of a detonation. Therefore, if I talk in terms of a structure of a detonation, I have something like a Von Neumann pressure spike followed by the pressure falling to the  $C_J$  value.

And therefore, we talk in terms of Von Neumann spike and also the Zeldovich Doring and Von Neumann model or let us say Von Neumann and Doring model Z N D model of a detonation. But, we also recognise that even though the 1 dimensional model gives excellent predictions for the Chapman Jouguet velocity constant velocity of a detonation, the pressure and density behind a detonation.

The actual structure of a detonation follows that means we have multiple shocks interacting and when these multiple shocks interact the triple point that is at the interaction of the three shocks incident mark and the transverse shock traces something like cells of detonation. And this is the structure by which a detonation proceeds. We have something like a mark same shock and you have an incident shock over here. We have a mark shock over here and behind it you have the transverse waves. That means waves which are travelling normal to it and this is the 3 dimensional structure in which case i have a multiples shocks at the front.

I have these transverse waves behind it chemical reaction that distributed all along, but even in this the measured velocities match well with the 1 dimensional model what we have. Here, we were able to get the energy required for starting a detonation. We also found out that the energy required is proportional to the cell size of a detonation and in general we find well the pressures are very high. In a detonation that is the Chapman Jouguet pressures or the pressure behind a detonation wave are something 22 for a solid is extremely high and for solids.

Well, the method used is the same, but you have to use the equation of state for a solid is different from a perfect gas equation which we used. And we have to use the reaction Hugoniot for a solid along with the Raleigh line for a solid to be able to find out it is detonation velocity. Now, that we have learnt about all these features of detonation, we find it much more catastrophic than what a flame is. You have high pressure, high

velocity and in the next class what we do is, we will examine some case studies of some explosions. Let us say some three or four case studies of explosion in which detonation have occurred and assess the damage.

Well, thank you.