# Fundamentals of Combustion Prof. V. Raghavan Department of Mechanical Engineering Indian Institute of Technology, Madras

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## Characteristics of combustion flame and detonation Part 4 Estimation of detonation velocity and Worked examples

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And you can see some discussions I have written here. So, since any real process going from state 1 to state 2 must satisfy the Rayleigh line equation 5 and the Rankine Hugoniot relation, both should be satisfied. So, the points between B and C on the Hugoniot curve are not realizable because no valid Rayleigh line can be drawn. So, this is the first inference.

Then, the for the upper branch of the Hugoniot there is a limiting Rayleigh line. After that the Rayleigh line cannot be drawn as a tangent basically. So, that is a tangent. So, the limiting line and this is tangent to the Hugoniot curve at the point D and this is called upper Chapman - Jouguet point or say we can also say, Chapman - Jouguet point.

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So, this point D here is called upper Chapman - Jouguet. So, CJ, I will say CJ point upper CJ point and similarly, here it is called lower CJ point; Chapman - Jouguet point. So, it can be shown. Now, I can show that Mach number will be 1 at this point D upper Chapman - Jouguet point, Mach number will be 1. Points above D are difficult to observe in the lab scale experiments.

Theoretically, it may be fine; we can solve the equation and get, but it is not practically possible to achieve this in the lab scale experiments. In some conditions, you may get it, some big engines etcetera you may get it; but not possible. Similarly, there is a limiting Rayleigh line in the lower portion which will give the tangent to the Hugoniot which is point E, we call lower CJ point or Chapman - Jouguet point.

Here, so this point E. So, this is accessible C and below E, it is not accessible. It is not practical; theoretically, you can get the value, but it is not practical; the strong deflagration and supersonic exit velocities.

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Now, let us see about the burnt gas velocity. So, for that let the wave be moving, I will come out of the wave and see the wave propagating to the mixture. So, wave propagates at  $V_w$ . So that means, you can say  $V_w = u_1$ . So, when the wave is at rest the velocity of the unburned gas approaching the wave is  $u_1$ ; so,  $V_w = u_1$ . So, that is known. Now, what is  $V_2$ , we are going to find it.

So, now  $V_1$ , this is  $V_1$ ,  $V_w$ ,  $u_1$  all the things we can write here. So, let us say. So, when I am in the laboratory frame of reference, what happens is the combustion wave is moving with the velocity of  $V_w$ . Velocity of unburned gas,  $V_1$  is see this  $u_1$  was the velocity at which the unburned gas approached wave. Now, if the wave is propagating unburned gas should be at rest.

So,  $V_1$  is the velocity of unburned gas which should be at rest, when the wave propagates over that, so that is equal to 0. Now,  $V_w = u_1$  that is known. So, either the unburned gas should approach the wave at velocity of  $V_1$ ,  $u_1$  or the wave should propagate at the same velocity towards the unburned gas. Now, the velocity  $V_2$  is  $u_1 - u_2$ . So, that is the thing here;  $u_1 - u_2$ . So, we can say  $V_2 = u_1 - u_2$  or  $-(u_2 - u_1)$ . Now, I know the expression for  $u_2 - u_1$  that is what we have derived that and kept.

$$V_2 = -(u_2 - u_1) = -(\dot{m}'')^2 \left(\frac{1}{\rho_2} - \frac{1}{\rho_1}\right)$$

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So, the  $u_2 - u_1$  which we derived here, that can be used here now  $-(\dot{m}'')^2 (1/\rho_2 - 1/\rho_1)$ . So, now, just to see the direction only we are doing this calculation. So, at point D,  $V_2 < V_1$ . Here, point D; so, this is  $V_1$ . So, this is  $V_1$  p<sub>1</sub>. Point D,  $V_2 < V_1$ . So, when  $V_2 < V_1$ , this is  $V_2$  and this is  $V_1$ ; when  $V_2 < V_1$ , this is negative. Negative of negative will be positive So,  $V_2$  is positive. So, for detonation, the burned gas follows the combustion wave; when the wave moves in the positive x direction, the burned gas also follow the wave, that we have to understand.

For deflagration at E, point E let us take. Point E, you can see that the V<sub>2</sub>; this is V<sub>2</sub> now, V<sub>1</sub> < V<sub>2</sub>. V<sub>2</sub> > V<sub>1</sub>. So, u<sub>1</sub> < u<sub>2</sub> or V<sub>2</sub> is negative. So, for deflagration, burned gas flow in the direction opposite to that of the flame. This is what we have to understand.

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Now, estimation of detonation velocity. So, at the upper Chapman - Jouguet point, CJ point velocity is sonic. Above D, the velocity is subsonic and between B and D, the velocity is supersonic. When I say velocity it is the approaching velocity, please understand this is the approaching velocity; not the burnt gas velocity. Burnt gas velocity is different, we have already seen that. This is approaching velocity

So, when we want to do this, the approaching velocity should be in between the B and D and is supersonic. So, the continuity equation, I can write as  $\rho_1 u_1$ , the approaching velocity is  $u_1$  equal to  $\rho_2 c_2$ ; so, now,  $u_1 = (\rho_2/\rho_1)c_2$ . What is  $c_2$ ?  $c_2$  is the speed of sound which is nothing but  $\sqrt{\gamma RT}$ ;  $c = \sqrt{\gamma RT}$ . So,  $c_2 = \sqrt{\gamma R_2 T_2}$ . So, this is the expression I get.

$$u_1 = \frac{\rho_2}{\rho_1} c_2 = \frac{\rho_2}{\rho_1} (\gamma R_2 T_2)^{1/2}$$

Now, I can relate this  $\rho_2/\rho_1$  and T<sub>2</sub> to state 1 quantities or other quantities. Now, further I make important assumption that  $p_2 >> p_1$ . So, when I say the momentum equation  $p_1 + 1/2 \rho_1 u_1^2 = p_2 + 1/2 \rho_2 u_2^2$  for example. So, now,  $p_1 = 0$  because I can neglect  $p_1$  and consider the value of  $p_2$ .

So,  $p_1$  is very low. So, I write this equation. Please understand that, I write this when I use this momentum equation, I can write  $\rho_1 u_1^2 / \rho_2 u_2^2 - p_2 / \rho_2 u_2^2$ . Just divide throughout by  $\rho_2 u_2^2$ . So, I have to put 1 here; 1 and 2 here.

So, momentum equation.  $p_1 + 1/2 \rho_1 u_1^2 = p_2 + 1/2 \rho_2 u_2^2$ , by this assumption I say  $p_1 = 0$ . So, I can write this. From that, I can get the value of  $\rho_2/\rho_1$  as this Now,  $u_2 = c_2$ ; so, using that I can write  $\rho_2/\rho_1$ . Then, using the definition of the  $c_p$  etcetera plus the equation of state  $p = \rho RT$ , I can get a simple formula for  $\rho_2/\rho_1$  as  $(\gamma+1)/\gamma$ .

$$\frac{\rho_2}{\rho_1} = \frac{\gamma + 1}{\gamma}$$

So, you can just use it very simple derivation here. (Refer Slide Time: 08:55)



So, now similarly T<sub>2</sub>, I want a relationship for  $\rho_2/\rho_1$  which I have got now; similarly, I want a relationship for T<sub>2</sub>. So, for that what I do? Solving the energy conservation equation for T<sub>2</sub>, eliminating u<sub>1</sub> using the continuity equation substituting c<sub>2</sub> = u<sub>2</sub>, I can get this and also, using the density ratio. So, much thing I do here. I am not deriving it. So, that is what the summary is.

So, what I do here is I know that  $c_pT_2 + 1/2u_2^2 = c_pT_1 + 1/2u_1^2$ . So, that I try to now take value of T<sub>2</sub>. So, T<sub>2</sub> = T<sub>1</sub> divide throughout by  $c_p$ ,  $u_1^2 + q$  is there,  $(u_1^2 - u_2^2)/2c_p + q/c_p$ . It is only energy equation, simple.

Now, this you retain, we will try to write this  $\gamma RT$ . So,  $u_2 = c_2 = \sqrt{\gamma R_2 T_2}$  that you substitute you get this equation. Now, you know that  $\gamma R_2/(\gamma - 1) = c_p$ ; similarly,  $p = \rho RT$ . So, use this equation; finally, this equation you get.

$$T_{2} = T_{1} + \frac{u_{1}^{2} - u_{2}^{2}}{2c_{p}} + \frac{q}{c_{p}}$$
$$= T_{1} + \frac{q}{c_{p}} + \frac{\gamma R_{2} T_{2}}{2c_{p}} \left[ \left( \frac{\gamma + 1}{\gamma} \right)^{2} - 1 \right]$$

So, now this we have taken to this side and do some algebra, you get a simple equation for  $T_2$  as  $2\gamma^2/(\gamma-1)(T_1 + q/c_p)$ . Plus understand that this is the simple equation because we have assumed  $c_p$  to be constant.

$$T_2 = \frac{2\gamma^2}{\gamma+1} \left( T_1 + \frac{q}{c_p} \right)$$

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So, now you use this density ratio  $\rho_2/\rho_1$  and  $T_2$  and get the velocity for detonation, that is all. So, detonation velocity is nothing but the approaching velocity  $u_1 = [2(\gamma+1)\gamma R_2 (T_1 + q/c_p)^{1/2}]^{1/2}$ .

$$u_D = u_1 = \left[2(\gamma + 1)\gamma R_2 \left(T_1 + \frac{q}{c_p}\right)\right]^{1/2}$$

Now, the above expression for detonation velocity is very approximate. First of all, main assumption is  $p_2$  is much more greater than  $p_1$  and also, we have the constant physical properties.

Now, slightly we can relax it. So, what we will do? First assumption say, constant and equal specific heats say  $c_{p,1} = c_{p,2}$ , let us avoid this. When I do that, you get the expression for state 2 temperature and detonation velocity slightly better; but still it is approximate. I can get slightly better values, but it is still approximate. This is the thing. (Refer Slide Time: 11:56)



So, now I try to put instead of considering  $c_{p,1} = c_{p,2}$ , now I will consider it is not. So, I will put the ratio of  $c_{p,1}/c_{p,2}$  here. So, T<sub>2</sub> is slightly better, see if you see this, you can get  $\gamma$ . There is no  $\gamma_1$  or  $\gamma_2$ ; now, I can specify its  $\gamma_1$  or  $\gamma_2$ . So, please understand  $\gamma_1 = c_{p1}/c_{v1}$ ;  $\gamma_2 = c_{p2}/c_{v2}$ .

$$T_2 = \frac{2\gamma_2^2}{\gamma_2 + 1} \left( \frac{c_{p1}}{c_{p2}} T_1 + \frac{q}{c_{p2}} \right)$$

Now, if I assume that  $c_{p1} = c_{p2}$  and  $c_{v1} = c_{v2}$ , then  $\gamma_1 = \gamma_2$ . These are all assumptions made here to get this. But when I relax that at least this the concept of equal specific heat etcetera for the products and this if we relax, I will say I will take  $\gamma_1 = c_{p1}/c_{v1}$  and  $\gamma_2 = c_{p2}/c_{v2}$ .

Now, you can see that I will retain  $\gamma_2$  here and the ratio of  $c_{p1}/c_{p2}$  etcetera here and get this. But still it is approximate, but slightly better than the previous equation because I am now relaxing the constant property assumption here. So, I get an improved equation for this u<sub>D</sub>. So, this you can use. But please understand that more exact mathematical description of a one-dimension detonation wave.

$$u_D = u_1 = \left[2(\gamma_2 + 1)\gamma_2 R_2 \left(\frac{c_{p1}}{c_{p2}}T_1 + \frac{q}{c_{p2}}\right)\right]^{1/2}$$

Please understand one more thing, detonation is not one-dimensional phenomenon, it is 3D phenomenon. However, some assumptions can be made and one-dimensional detonation wave propagation can be adjudged. For that, know you need a numerical solution and NASA Chemical Equilibrium Code, CEC has a module to do this. (Refer Slide Time: 13:59)



Now, at last we will see a worked example. A combustion wave propagates with the mass flux of  $3500 \text{ kg/m}^2$ -s and the initial mixture has a temperature of 298 K and 1 atmospheric pressure.

The molecular weight and the specific heat ratio of the mixture burned and now, both are same. Molecular weight is 29 kg/kmol and specific heat ratio  $\gamma$ =1.3. So, that is what is given in this.

So, the heat release rate q is given as  $3.4 \times 10^6$  J/kg. So, now, determine the state of the burned gas and determine in which region, this state lies in the Rankine Hugoniot curve; then, Mach number of the burned gases. So, this is the problem. Now, let us use the equation of Rayleigh line (equation 5) Rayleigh line. So,  $p_2 = p_1 + (m'')^2 (v_1 - v_2)$ .

Similarly, equation 8 is written like this; equation 8, that is the Rankine Hugoniot curve equation. Now, I want to fix the state. So, what is  $v_1$ ?  $p = \rho RT$ ; so,  $v_1 = RT_1/p_1$ . So, I get 0.843 m<sup>3</sup>/kg, that is the volume 1; pressure is 1 atmosphere, initial pressure is 1 atmosphere. So, initial state is fixed as 1 atmosphere and specific volume as 0.843 m<sup>3</sup>/kg.

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Now, p<sub>2</sub>; p<sub>2</sub> this equation, Rayleigh line equal to p<sub>1</sub>. Here all the values. So, you can see  $p_1 + (m'')^2$ ,  $m'' = 3500 \text{ kg/m}^2$ -s, then  $v_1$  and  $v_2$ . So,  $v_1$ , but I do not know  $v_2$ . So, I form a equation for p<sub>2</sub> in terms of  $v_2$  here like this; form an equation for p<sub>2</sub> in terms of  $v_2$ 

Similarly, heat addition, this equation 8 that is the Rankine Hugoniot equation, I can substitute the values here; but please understand I do not know both  $p_2$  and  $v_2$ , but I know now from this equation, Rayleigh line equation, I know  $p_2$  in terms of  $v_2$ .

So, now substituting for  $p_2$  from the Rayleigh line equation, you get a quadratic equation in  $v_2$  and this is a quadratic equation, when I solve I get 2 volumes  $v_2$ 's that is 0.723 m<sup>3</sup>/kg and 0.239 m<sup>3</sup>/kg.

You can readily see that  $v_1$  was 0.843 m<sup>3</sup>/kg and we got two  $v_2$ 's from the quadratic equation, both are less than that. That means, we are on the detonation curve. So, if you see here this is the initial point, but both  $v_2$ 's are less than this now.

So, either I will be here or here somewhere, I am going to be there in this regimes. So, both  $v_2$ 's are less than the  $v_1$ , initial  $v_1$  what I got. So, now that is the 2 values I get. Now, for both we will try to fix the state

So, corresponding to the  $v_2$  of 0.723,  $p_2$  value is got as this is the same 1.57 MPa Similarly, for  $v_2$  of 0.239, I get 7.5 MPa. So obviously, you can see the higher, we are travelling in that curve to a higher value of pressure.

Now, the velocities are calculated now I know the pressure, let us say state 2 is fixed now. Pressure for corresponding each state is fixed. Now, how will we calculate velocities? I know the mass flux; mass flux, mass flow rate is what? Mass flow rate is  $\rho$ AV, mass flux is  $\rho$ V. So, divided by A; so,  $\rho$ V. So, this is  $\rho$ V. But  $\rho = 1/v$ .

So, capital V is a velocity; so, velocity by specific volume. So, velocity will be equal to mass flux into specific volume. So, for specific volume of point 2 0.723, velocity will be 2530 m/s, state 2 velocity. For this  $v_2$  equal to 0.239, it will be 836.5 m/s. So, I am getting 2 velocities ok; 2530 for the specific volume of 0.723 which is slightly less than less than the initial 0.843.

If it is much less than the initial this  $v_2$  equal 0.239, pressure is very high. For that, I am getting a lower velocity of 836.5 correct.

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Now, I calculate the speed of sound  $(\gamma RT)^{1/2}$ . For that, I need temperatures. So, for each volume, again I calculate temperature as for 0.723, I get the temperature as 3963 K and for 0.239, I get temperatures of 6253 K.

So, now, 6000 etcetera, I cannot realize in the lab scale, that is what we are trying to make a point here. It is not realizable in the lab scale. So, now from this, I can calculate the value of the speed of sound  $a_2$  for 0.723 m<sup>3</sup>/kg, it is 1215 m/s and for 0.239, it is 1526 m/s. So, Mach numbers will be for the specific volume 0.723, it is 2.08. That means supersonic. So, that will be in between the B and D value correct; B and D that portion and this is subsonic; that will be above D. For 0.239, it is above D. So, both specific volumes are less than state 1. So, this state corresponds to subsonic velocity lies in the upper CJ point; above the point D, 7.5 MPa, 0.239.

Subsonic velocity 0.55 that is above that above D and this 1.57 MPa, 0.723 m<sup>3</sup>/kg that lies in the region between the point B and D because it has a supersonic velocity. So, you can see that the very high mass flux causes detonation. If you reduce the mass flux etcetera, then you go to the deflagration part. So, I will stop here.