5 A combustion wave in a premixed gas, the Chapman-Jouguet detonation wave

Imagine a long tube closed at both ends and filled with combustible gas mixture. Now take away both ends cover rapidly and ignite the gas at one end. We will see a combustion wave propagating down the tube with constant speed of less than one meter per second. If we now repeat the experiment and only take away one cover and ignite the gas at the other end, a combustion wave starts to propagate with the same speed as in the first case but in a short while we obtain a combustion wave that propagates at a velocity several times the speed of sound of the unburned gas. If we take away the remaining cover, the wave will continue to propagate at supersonic speed. In the first case we have a deflagration wave and in the latter a detonation wave. The two combustion waves have profound differences in character which we can see in table (1) below.

	Detonation	Deflagration
u_1/a_1	5 - 10	$1 \cdot 10^{-4} - 3 \cdot 10^{-2}$
u_2/u_1	0.4 - 0.7	4 - 6
p_2/p_1	13 - 15	~0.98
T_2/T_1	8 - 21	4 - 16
ρ_2/ρ_1	1.7 - 2.6	0.06 - 0.25

Table 1: Comparison between detonation and deflagration in a coordinate system fixed to the wave.

We will start with a general description of the flow and proceed to the details later.

Consider a mixture of combustible gases in a straight pipe of constant cross section in which we have a plane combustion wave propagating along the pipe axes. The wave is described in coordinate system stationary to the wave, see figure (10).

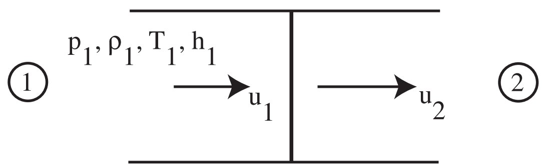

Figure 10: Notations

The governing equations preserving mass, momentum and energy are:

$$\rho_1 u_1 = \rho_2 u_2 = \dot{m_{au}} \tag{77}$$

$$p_1 + \rho_1 u_1^2 = p_2 + \rho_2 u_2^2 \tag{78}$$

$$h_1(T_1) + \frac{1}{2}u_1^2 = h_2(T_2) + \frac{1}{2}u_2^2 \tag{79}$$

where $\dot{m_{au}}$ is the mass flux per area unit. In addition, we have the ideal gas law:

$$p = \rho RT \tag{80}$$

where R is the specific gas constant (with index 1 or 2 for the inlet and outlet gases respectively). The enthalpy is as before:

$$h(T)_j = [\Sigma_i Y_i [h^\circ_{f,i}(T_{ref}) + \int_{T_{ref}}^{T} c_{p_i} dT]]_j \tag{81}$$

where j is either 1 or 2 indicating the side of the wave:

$$h^\circ_{f1}(T_{ref}) = [\Sigma Y_i h^\circ_{f,i}(T_{ref})]_1$$
$$h^\circ_{f2}(T_{ref}) = [\Sigma Y_i h^\circ_{f,i}(T_{ref})]_2$$

where $h^\circ_{f1} - h^\circ_{f2} = q$ is the **heat of combustion**, Δh_c, $(= -\Delta h_R)$, the difference between the formation of enthalpy of the inlet and outlet gases at $T = T_{ref}$. If we now look at the combustion wave problem we neither know the velocity of the inlet and outlet gas nor the combustion products. In all we have 5 unknown u_1, u_2, p_2, ρ_2 and T_2 but only 4 equations. The fifth equation relates the composition of the combustion products with the temperature T_2 and total pressure p_2 which could be determined in an equilibrium situation. However a great deal of insight into the problem is gained plotting the relation between pressure and density over the wave both as a function of the mass flux (Rayleigh line) and the heat release, q (Rankine-Hugoniot relation).

We start out with eq.(77) and (78) slightly rewritten in the following ways

$$(\rho_1 u_1)^2 = (\rho_2 u_2)^2 = (\dot{m_{au}})^2$$
$$p_2 - p_1 = \frac{\rho_1^2 u_1^2}{\rho_1} - \frac{\rho_2^2 u_2^2}{\rho_2}.$$

Eliminating the velocity we get

$$p_2 - p_1 = (\dot{m_{au}})^2 (\frac{1}{\rho_1} - \frac{1}{\rho_2}). \tag{82}$$

This is a straight line in a $(p, 1/\rho)$ diagram always with a negative slope

$$\frac{p_2 - p_1}{\frac{1}{\rho_2} - \frac{1}{\rho_1}} = -(\dot{m_{au}})^2. \tag{83}$$

Thus from the inlet conditions at 1 we have our outlet condition somewhere along the straight line also called the Rayleigh line. For later use we rewrite the equation (83) expressing the mass flux in terms of inlet and outlet Mach numbers

$$(\dot{m_{au}})^2 = (\rho_1 u_1)^2 = \rho_1^2 M_1^2 a_1^2 = M_1^2 \gamma p_1 \rho_1$$
$$(\dot{m_{au}})^2 = (\rho_2 u_2)^2 = M_2^2 \gamma p_2 \rho_2$$
$$M_1^2 = -\frac{1}{\gamma p_1 \rho_1} \frac{p_2 - p_1}{\frac{1}{\rho_2} - \frac{1}{\rho_1}} \tag{84}$$

and

$$M_2^2 = -\frac{1}{\gamma p_2 \rho_2} \frac{p_2 - p_1}{\frac{1}{\rho_2} - \frac{1}{\rho_1}} \tag{85}$$

Let us now divide the energy equation, eq.(79), with the momentum equation, eq.(78)

$$\frac{h_2 - h_1}{p_2 - p_1} = -\frac{1}{2}\frac{u_2^2 - u_1^2}{\rho_1 u_1^2 - \rho_2 u_2^2}.$$

Bring the factor $1/\rho_1$ in front of the right hand term and divide both the numerator and the denominator with u_1^2

$$\frac{h_2 - h_1}{p_2 - p_1} = -\frac{1}{2\rho_1}\frac{(\frac{u_2}{u_1})^2 - 1}{1 - \frac{\rho_2 u_2^2}{\rho_1 u_1^2}}. \tag{86}$$

To eliminate the velocities we use the continuity equation, eq.(77),

$$\frac{u_2}{u_1} = \frac{\rho_1}{\rho_2}$$

and finally obtain

$$\frac{h_2 - h_1}{p_2 - p_1} = \frac{1}{2}(\frac{1}{\rho_1} + \frac{1}{\rho_2}). \tag{87}$$

This equation is referred to as the Rankine-Huginot relation.

Let us now express the enthalpy jump, $h_2 - h_1$, with the help of eq.(81)

$$h_{f2}^{\circ}(T_{ref}) - h_{f1}^{\circ}(T_{ref}) + \int_{T_{ref}}^{T_2} c_{p2} dT - \int_{T_{ref}}^{T_1} c_{p1} dT = \frac{1}{2}(\frac{1}{\rho_1} + \frac{1}{\rho_2})(p_2 - p_1) \tag{88}$$

If we assume constant $c_{p1} = c_{p2} = c_p$, making use of the relations $q = h_{f1}^{\circ}(T_{ref}) - h_{f2}^{\circ}(T_{ref})$ and

$$c_p T = \frac{\gamma}{\gamma - 1} p/\rho$$

equation (88) becomes

$$\frac{\gamma}{\gamma - 1}(\frac{p_2}{\rho_2} - \frac{p_1}{\rho_1}) - \frac{1}{2}(\frac{1}{\rho_1} + \frac{1}{\rho_2})(p_2 - p_1) = q. \tag{89}$$

In the case of $q = 0$ this is recognized as the Hugoniot relation for a shock.

(The assumption that the specific heat capacity is constant is questionable considering both the large temperature difference between upstream and downstream condition and the high output temperature.)

5.0.1 Discussing the inlet outlet conditions

Drawing the Rankine-Hugoniot, (R-H), curve and the Rayleigh line, eq.(83), in the same diagram, gives us the visual aid to discuss where a solution to the equations is to be found. Figure (11) shows the R-H curve and Rayleigh line in a normalized $p/p_1 - \rho_1/\rho$ diagram with the inlet condition at (1, 1). The curve drawn with a full line is the R-H curve for $q > 0$, whereas the dash-dot line shows the case when $q = 0$, i.e. the shock Hugoniot curve. The full straight lines are Rayleigh lines for a few different mass fluxes. Now the solutions, the outlet conditions, are found at the intersection of the Rayleigh line and the R-H curve. But are all physically realizable?

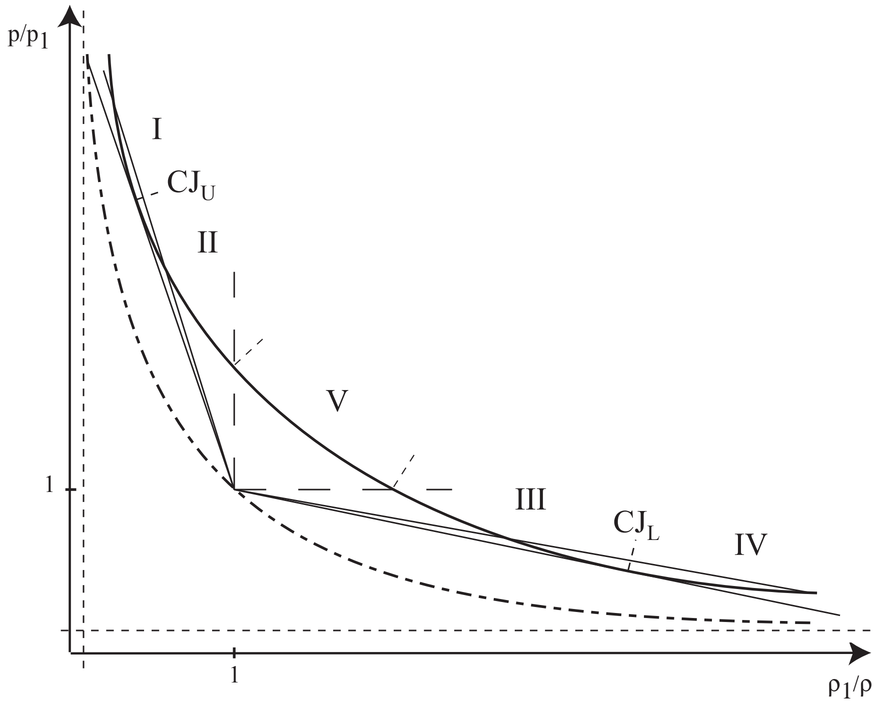

Figure 11: Rankine-Hugoniot curve and Rayleigh line. Straight lines are Rayleigh lines for different massfluxes. The dash-dot curve is the shock Hugoniot curve.

To discuss the matter we have divided the R-H curve into five segments, $I-V$. Region I is from the highest output pressure to the point on the R-H curve where the Rayleigh line touches it, the so called **upper** Chapman-Jouguet point, CJ_U. Region II extends from CJ_U to where the vertical dashed line crosses the R-H curve. Region V (it is customary to call this region V) is the next part and covers the curve down to where the horizontal dashed line intersects the R-H curve. Region III covers the part of the curve down to where the Rayleigh line is tangent to the R-H curve, the **lower** Chapman-Jouguet point, CJ_L, and IV covers the R-H curve to the right of CJ_L. The different regions, based on the pressure change over the wave, are called strong detonation (region I), weak detonation (II), weak deflagration (III) and strong deflagration (IV)

The inlet Mach number, M_1, is positive. From equation (84) we directly see that the slope of the Rayleigh line has to be negative and thus region V is not a physical solution. What about M_1 in the other regions, is it larger or smaller than 1?

To answer the question we might take help from the shock Hugoniot curve and the Rayleigh line. For an infinitely weak shock the inlet and outlet Mach numbers are 1. The Rayleigh line is tangent to the shock Hugoniot curve at the inlet point. From figure (11) we find the magnitude of the slope of the Rayleigh line is larger in region I and II but smaller in III and IV compared to the tangent. Thus equation (84) shows that the inlet Mach number is larger than 1 in I and II but less than 1 in III and IV.

Now, what about M_2, how does it vary? Let us start at the extreme outlet pressure in region I. Here eq. (89) gives us the strong shock relation

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

for an ideal gas with constant heat capacities (show that). If we use this relation in equation (85) we find that the asymptotic outlet Mach number is

$$M_2 = \sqrt{\frac{\gamma-1}{2\gamma}}.$$

Following the almost vertical R-H curve from the extreme pressure the pressure decreases drastically while the density and the magnitude of the slope only change marginally which means that M_2 increases. The outlet Mach number is monotonically increased as we move towards CJ_U.

If we now look at region II and start at a position close to region V the magnitude of the slope is infinite and likewise M_2 as pressure and density is limited. Moving towards CJ_U decreases the magnitude of the slope and increases the $p_2\rho_2$ term in the denominator in eq.(85) reducing M_2. The value of M_2 in the CJ_U point has yet to be determined.

In the subsonic inlet case, $M_1 \leq 1$, the outlet Mach number starts at $M_2 = 0$ for the horizontal Rayleigh line in region III. What is the limit value of p_2/p_1 for $\rho_2 \to 0$?

Equation (85) directly shows that in approaching the CJ_L point in region III M_2 increases whereas in region IV the Mach number decreases.

Now let us discuss if regions I, II, III, and IV are physically realizable for a flow tube with constant area. In I the inlet supersonic flow is decreased to subsonic flow through heat addition which could be done if there is also a shock. In II we have supersonic inlet condition adding heat which in turn would decrease the Mach number but could still be above one. In regions III and IV we have subsonic inlet conditions and adding heat would increase the outlet Mach number but only to one. Further increase of heat addition would cause a shock traveling upstream changing the upstream conditions, retaining sonic/subsonic outlet conditions. Thus we are limited to $M_2 \leq 1$ and exclude region IV as unphysical.

5.0.2 The Chapman-Jouguet points

The final question is the outlet Mach number at the Chapman-Jouguet points. To determine the conditions we notice that the Rayleigh line is tangent to the R-H curve at these points. Starting by taking the derivative of eq.(89) with respect to $1/\rho$

$$\frac{d}{d\ 1/\rho}\Big(\frac{\gamma}{\gamma-1}(\frac{p_2}{\rho_2} - \frac{p_1}{\rho_1}) - \frac{1}{2}(\frac{1}{\rho_1} + \frac{1}{\rho_2})(p_2 - p_1) = q\Big)$$

we get

$$\frac{dp}{d\ 1/\rho} = \frac{(p-p_1) - \frac{2\gamma}{\gamma-1}p}{\frac{1}{\rho}\frac{2\gamma}{\gamma-1} - (\frac{1}{\rho_1} + \frac{1}{\rho})}. \tag{90}$$

But the Rayleigh line from inlet (1) to outlet (2) condition, the tangent point, is just the straight line from 1 to 2

$$\frac{dp}{d\,1/\rho} = \frac{p_2 - p_1}{\frac{1}{\rho_2} - \frac{1}{\rho_1}}.$$

If we eliminate the derivative in eq.(90) we get

$$\frac{p_2 - p_1}{\frac{1}{\rho_2} - \frac{1}{\rho_1}} = \frac{(p_2 - p_1) - \frac{2\gamma}{\gamma-1} p_2}{\frac{1}{\rho_2}\frac{2\gamma}{\gamma-1} - (\frac{1}{\rho_1} + \frac{1}{\rho_2})}.$$

Collecting the factor $(p_2 - p_1)$ we obtain after some algebraic manipulations

$$\gamma p_2 \rho_2 = -\frac{p_2 - p_1}{\frac{1}{\rho_2} - \frac{1}{\rho_1}}.$$

Comparing the equation with the Rayleigh line, eq.(85)

$$M_{2_{CJ}}^2 = -\frac{1}{\gamma p_2 \rho_2} \frac{p_2 - p_1}{\frac{1}{\rho_2} - \frac{1}{\rho_1}}$$

directly gives that the outlet Mach number at both Chapman-Jouget points is equal to one

$$M_{2_{CJ}} = 1. \tag{91}$$

5.0.3 Internal structure of a plane detonation wave. The ZND-theory (Zeldovich, Neumann, Döring)

The detonation wave although it may appear plane, it is not. Experiments show that wave front consists of both waves moving in the main propagation direction and in spanwise direction and that the front has triple points (three shocks meeting in a point) moving in spanwise direction. However the assumption that the detonation wave essentially consists of a shock wave followed by a deflagration zone, the so called ZND detonation wave, gives a good description and quantitatively correct results for the Chapman-Jouguet detonation (CJ_u-point). The internal structure is made up of a shock, a few mean free paths thick, where the pressure rises drastically, usually more than 20 times, and temperature and density to more moderate levels i.e. 4-6 times. The shock is followed by a much thicker induction zone where the state variables are almost constant, the chemical reaction starts but does not come to full rate and finally a reaction zone where density and pressure decrease by a factor of about two, while the temperature rises by a similar factor. A schematic of the internal structure is depicted in fig.(12)

5.0.4 Approximate determination of the Chapman-Jouget detonation velocity

The C-J detonation is very special as the outlet gas velocity is sonic and downstream expansion waves will not catch up with the wave and weaken its strength. Experimentally it is found that free running detonations are often C-J detonations and it is therefore of interest to calculate its characteristics as the detonation velocity and the change in pressure, temperature and density over the

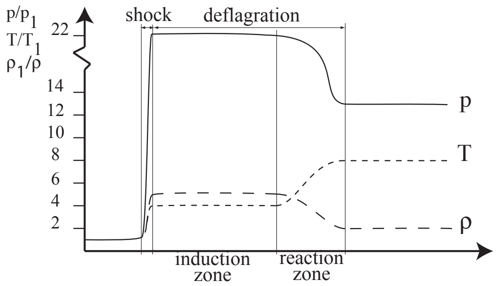

Figure 12: ZND wave

wave. An analytical solution is not possible, but with some approximations we get an estimate of the outlet condition.

Let us assume constant heat capacities of the reactants and products. The conservation equations eq.(77), eq.(78) and eq.(79) with $u_2^2 = a_2^2 = \gamma_2 R_2 T_2 = \gamma_2 p_2/\rho_2$ reads

$$\rho_1 u_1 = \rho_2 u_2 = \rho_2 \sqrt{\gamma_2 R_2 T_2} \tag{92}$$

$$p_1 + \rho_1 u_1^2 = p_2 + \gamma_2 p_2 \tag{93}$$

and

$$\frac{1}{2}u_1^2 + h_{f1}^\circ(T_{ref}) + (T_1 - T_{ref})c_{p_1} = \frac{1}{2}u_2^2 + h_{f2}^\circ(T_{ref}) + (T_2 - T_{ref})c_{p_2}.$$

Assuming $c_{p_1}T_{ref} = c_{p_2}T_{ref}$ and using $q = h_{f1}^\circ(T_{ref}) - h_{f2}^\circ(T_{ref})$ we get the energy equation in the following form

$$\frac{1}{2}u_1^2 + q + c_{p_1}T_1 = \frac{1}{2}u_2^2 + c_{p_2}T_2. \tag{94}$$

To determine u_1 we rewrite equation (92)

$$u_1 = \rho_2/\rho_1 \sqrt{\gamma_2 R_2 T_2}. \tag{95}$$

Now we have to determine ρ_2/ρ_1 and T_2. Assume $p_2 >> p_1$ in eq.(93) the momentum equation becomes

$$\rho_1 u_1^2 = p_2 + \gamma_2 p_2. \tag{96}$$

Elliminating $\rho_1 u_1$ using eq.(92) we get

$$\rho_2/\rho_1 \gamma_2 p_2 = p_2(\gamma_2 + 1)$$

and accordingly the density ratio is

$$\rho_2/\rho_1 = \frac{\gamma_2 + 1}{\gamma_2} \tag{97}$$

(less than for a strong shock where $\rho_2/\rho_1 = \frac{\gamma+1}{\gamma-1}$). To determine T_2 we use the energy equation, eq.(94) rewritten

$$q + c_{p_1}T_1 = c_{p_2}T_2 + \frac{1}{2}u_2^2\Big(1 - (\frac{u_1^2}{u_2^2})^2\Big). \tag{98}$$

With the following relations:

$$\frac{u_1}{u_2} = \frac{\rho_2}{\rho_1} = \frac{\gamma_2 + 1}{\gamma_2},\ u_2^2 = \gamma_2 R_2 T_2 \text{ and } R_2 = \frac{\gamma_2 - 1}{\gamma_2} c_{p_2}$$

eq.(98) becomes

$$T_2 = \frac{2\gamma_2^2}{\gamma_2 + 1}\Big(\frac{q}{c_{p_2}} + \frac{c_{p_1}}{c_{p_2}} T_1\Big). \tag{99}$$

The detonation velocity u_{CJ} is obtained substituting T_2 (eq.(99)) and density ratio (eq.(97)) in eq.(95)

$$u_{CJ} = \frac{\gamma_2 + 1}{\gamma_2}\sqrt{\gamma_2 \frac{\gamma_2 - 1}{\gamma_2} c_{p_2} \frac{2\gamma_2^2}{\gamma_2 + 1}\Big(\frac{q}{c_{p_2}} + \frac{c_{p_1}}{c_{p_2}} T_1\Big)}$$

and finally

$$u_{CJ} = \sqrt{2(\gamma_2^2 - 1)(q + c_{p_1} T_1)} \tag{100}$$

5.0.5 Gas motion in a coordinate system fixed to the unburned gas

In most cases we look at the gas motion with the coordinate system fixed to the wave as in fig.(10) but from time to time it is of interest to have the gas velocities related to an other coordinate system. In figure (13) we have the wave and gas velocities related to a new coordinate system $\acute{x}$ which moves with velocity $u_{\acute{x}}$ to the right relative system x.

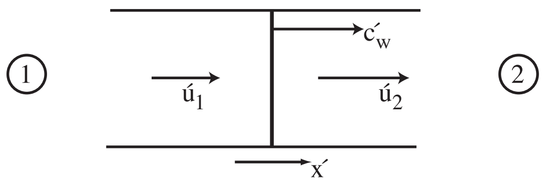

Figure 13: The wave in a coordinate system moving with speed $u_{\acute{x}}$

If the coordinate system $\acute{x}$ is moving with speed u_1 the inlet gas is standing still $\acute{u_1} = 0$, and the measured velocities will be:

$$\acute{u_2} = u_2 - u_1 \tag{101}$$
$$\acute{c_w} = 0 - u_1$$

Let us now determine the outlet and wave velocies, ($\acute{u}_2$, $\acute{c_w}$) in the case of detonation and deflagration. Use the continuity equation

$$u_1 = \rho_2/\rho_1 u_2$$

in eq.(101) and we obtain:

$$\acute{u}_2 = u_2(1 - \frac{\rho_2}{\rho_1}). \tag{102}$$
$$\acute{c_w} = -u_2 \frac{\rho_2}{\rho_1}$$

Since u_2 is always positive and the factor ρ_2/ρ_1 is greater than one for a detonation the outlet gas moves in the negative direction (but away from the wave, the difference is u_2). In a deflagration the factor ρ_2/ρ_1 is less than one and consequently the gas moves in the positive direction.