Detonation and Deflagration

1 1D Combustion Wave

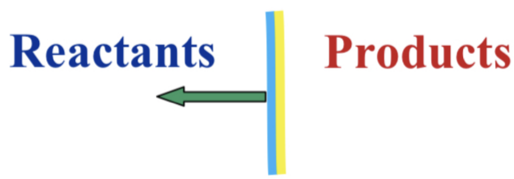

Figure 1: 1D Combustion Wave.

To simplify the problem, we usually assume the combustion wave as 1D, which means reactants on one side of "combustion/reaction zone", and products on the other. During the combustion, reaction zone moves through reactants. We define **wave propagation** as how fast does this zone travel.

2 Detonation and Deflagration

2.1 Overview

We identify 2 combustion wave regimes:

1. Deflagrations: subsonic waves (flag - slow)
2. Detonations: supersonic waves

In lab view, the combustion wave is shown below:

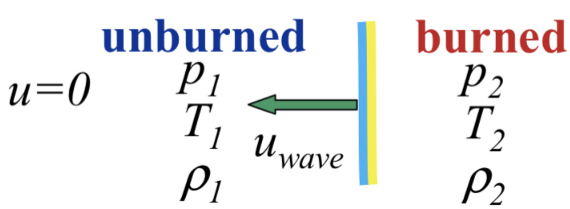

Figure 2: Lab View.

The difference between deflagrations and detonations could be shown in the table below:

	Deflagrations	**Detonations**
$M \equiv u_{wave}/a_u$	10^{-4} – 0.03	5 – 10
p_2/p_1	0.98 – 1	10 – 60
T_2/T_1	4 – 15	8 – 21
$\frac{p_2/p_1}{T_2/T_1} \approx \rho_2/\rho_1$	1/15 – 1/4	1.4 – 2.6
	expansion	**compression**

heat release

Figure 3: Difference between deflagration and detonation.

From the data, we can conclude that deflagration is a expansion wave (flag - expand), with the increase in temperature and the decrease in density and pressure. Detonation is a compression wave, with the increase in pressure, temperature and density.

2.2 Problem Setup

Now, we want to analyze this problem in a quantitative way. First we set up the problem in wave-fixed reference frame:

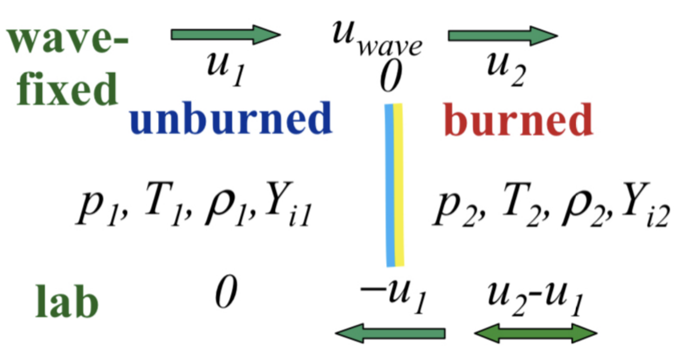

Figure 4: Wave View.

Assumptions:

1. Steady flow
2. Adiabatic
3. No work but flow work
4. Ideal gases
5. Neglect viscous effects

Now the problem is transferred to:

1. Given initial TD state $(p_1, T_1, \rho_1, Y_{i1})$
2. Find final TD state $(p_2, T_2, \rho_2, Y_{i2})$ and (u_1, u_2)

2.3 Governing Equations

Continuity:

$$\rho_1 u_1 = \rho_2 u_2 = \dot{m}'' \tag{1}$$

Where $\dot{m}''$ has the unit as $kg/(m^2 \cdot s)$
Momentum:

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

Energy: Recall the first TD law:

$$\dot{Q} = \frac{d}{dt}\int_{CV} \rho e_0 \, dV + \int_{CS} \rho h_0 (\underline{\boldsymbol{u}} \cdot \underline{\hat{\boldsymbol{n}}}) \, dA \tag{3}$$

Plug in the continuity equation:

$$\dot{m}_2'' h_{02} - \dot{m}_1'' h_{01} = 0 \tag{4}$$

We know the mass flow rate is a constant, therefore:

$$h_1 + \frac{u_1^2}{2} = h_2 + \frac{u_2^2}{2} \tag{5}$$

We know the enthalpy has two parts:

$$h = h_{sens} + h_{chem} \tag{6}$$

Based on the definition of heat release:

$$q = h_{1,chem} - h_{2,chem} = \sum (Y_{i,1} - Y_{i,2}) \Delta h^0_{f,i,T_{ref}} \tag{7}$$

$$h_{1,sens} + \frac{u_1^2}{2} + q = h_{2,sens} + \frac{u_2^2}{2} \tag{8}$$

Ideal Gas Law:

$$p = \rho \frac{\bar{R}}{\bar{W}} T \tag{9}$$

Caloric Perfect Gas Law:

$$h_i = \int_{T_{ref}}^{T} c_{p_i}(T') \, dT' \tag{10}$$

Now we have 5 equations but 6 unknowns $(p_2, \rho_2, h_2, T_2, u_1, u_2)$, we need to find other limitations to solve the equations.

2.4 Rayleigh Line

Combine continuity and momentum equations, we have:

$$p + \rho u^2 = p + \frac{\dot{m}''^2}{\rho} = const \tag{11}$$

Since we know the mass flux is a constant, rearrange the equation we get:

$$\frac{dp}{d(1/\rho)} = -\dot{m}''^2 = const \tag{12}$$

Therefore, we can get the **Rayleigh Line**:

$$-\dot{m}''^2 = -(\rho_1 u_1)^2 = -(\rho_2 u_2)^2 = \frac{p_2 - p_1}{1/\rho_2 - 1/\rho_1} \tag{13}$$

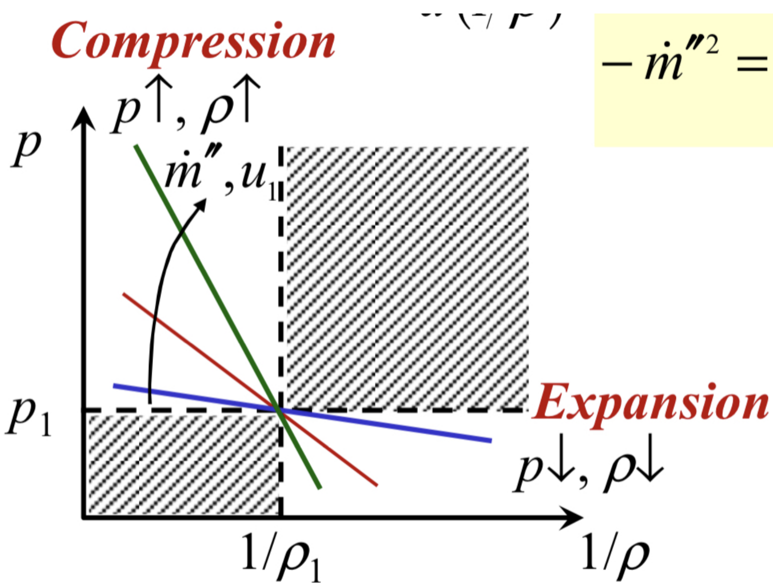

Figure 5: Rayleigh Line.

Notice that the mass flux must be positive, so p and ρ **must change in same direction**.

Using this relation, we can find the wave speed in terms of p and $1/\rho$:

$$-(u_1\rho_1)^2 = \frac{p_2 - p_1}{1/\rho_2 - 1/\rho_1} \tag{14}$$

$$u_1 = \frac{1}{\rho_1}\sqrt{\frac{p_2 - p_1}{1/\rho_1 - 1/\rho_2}} \tag{15}$$

Also the product speed:

$$u_2 = \frac{1}{\rho_2}\sqrt{\frac{p_2 - p_1}{1/\rho_1 - 1/\rho_2}} \tag{16}$$

It is also very important to compare the wave speed and the product speed. From the continuity equation, we have:

$$\frac{u_1 - u_2}{u_1} = 1 - \frac{\rho_1}{\rho_2} \tag{17}$$

Then:

1. **Compression:** $\rho_2 > \rho_1$, so $u_1 - u_2 > 0$, products move with wave
2. **Expansion:** $\rho_1 > \rho_2$ so $u_1 - u_2 < 0$, products move away from wave

Sometimes, it is better to express the velocity using Mach number:

$$u = Ma = M\sqrt{\frac{\gamma p}{\rho}} \tag{18}$$

$$(u_1\rho_1)^2 = M_1^2 \gamma_1 p_1 \rho_1 \tag{19}$$

Therefore:

$$\gamma_1 M_1^2 = \frac{(u_1\rho_1)^2}{p_1\rho_1} = \frac{\frac{p_1 - p_2}{1/\rho_2 - 1/\rho_1}}{p_1\rho_1} = \frac{1 - p_2/p_1}{\rho_1/\rho_2 - 1} \tag{20}$$

Similarly:

$$(u_2\rho_2)^2 = M_2^2 \gamma_2 p_2 \rho_2 \tag{21}$$

$$\gamma_2 M_2^2 = \frac{(u_2\rho_2)^2}{p_2\rho_2} = \frac{\frac{p_1 - p_2}{1/\rho_2 - 1/\rho_1}}{p_2\rho_2} = \frac{p_1/p_2 - 1}{1 - \rho_2/\rho_1} \tag{22}$$

2.5 Rankine-Hugoniot Relation

In Rayleigh line, we only consider mass and momentum conservation. Now we add energy into the consideration, which is called Rankine-Hugoniot Relation.

Recall the energy equation:

$$h_{1,sens} + \frac{u_1^2}{2} + q = h_{2,sens} + \frac{u_2^2}{2} \tag{23}$$

or:

$$h_2 - h_1 = \frac{1}{2}(u_1^2 - u_2^2) \tag{24}$$

Recall the Rayleigh Line relation:

$$u_1^2 = \frac{1}{\rho_1^2}\frac{p_2 - p_1}{1/\rho_1 - 1/\rho_2} \tag{25}$$

$$u_2^2 = \frac{1}{\rho_2^2}\frac{p_2 - p_1}{1/\rho_1 - 1/\rho_2} \tag{26}$$

$$
\begin{aligned}
u_1^2 - u_2^2 &= (\frac{1}{\rho_1^2} - \frac{1}{\rho_2^2})\frac{p_2 - p_1}{1/\rho_1 - 1/\rho_2} \\
&= (\frac{1}{\rho_1} + \frac{1}{\rho_2})(\frac{1}{\rho_1} - \frac{1}{\rho_2})\frac{p_2 - p_1}{1/\rho_1 - 1/\rho_2} \\
&= (\frac{1}{\rho_1} + \frac{1}{\rho_2})(p_2 - p_1)
\end{aligned} \tag{27}
$$

Therefore:

$$h_2 - h_1 = \frac{1}{2}(p_2 - p_1)(\frac{1}{\rho_1} + \frac{1}{\rho_2}) \tag{28}$$

Recall the definition of sensible enthalpy:

$$h_{2,sens} - h_{1,sens} = c_p(T_2 - T_1) = c_p(\frac{p_2}{\bar{R}\rho_2} - \frac{p_1}{\bar{R}\rho_1}) \tag{29}$$

Here $\bar{R}$ is the specific universal constant.

$$\bar{R} = R/M \tag{30}$$

Where R is the universal constant and M is the molar mass. Also:

$$\frac{c_p}{\bar{R}} = \frac{c_p}{c_p - c_v} = \frac{\gamma}{\gamma - 1} \tag{31}$$

Therefore:

$$h_{2,sens} - h_{1,sens} = \frac{\gamma}{\gamma - 1}(\frac{p_2}{\rho_2} - \frac{p_1}{\rho_1}) \tag{32}$$

Assembling:

$$
\begin{aligned}
q &= (h_{2,sens} - h_{1,sens}) - (h_2 - h_1) \\
&= \frac{\gamma}{\gamma - 1}(\frac{p_2}{\rho_2} - \frac{p_1}{\rho_1}) - \frac{1}{2}(p_2 - p_1)(\frac{1}{\rho_1} + \frac{1}{\rho_2})
\end{aligned} \tag{33}
$$

From this equation, we can get a family of curves given initial conditions and heat release q. All of them are rectangular hyperbole, they are called **Rankie-Hugoniot** curves:

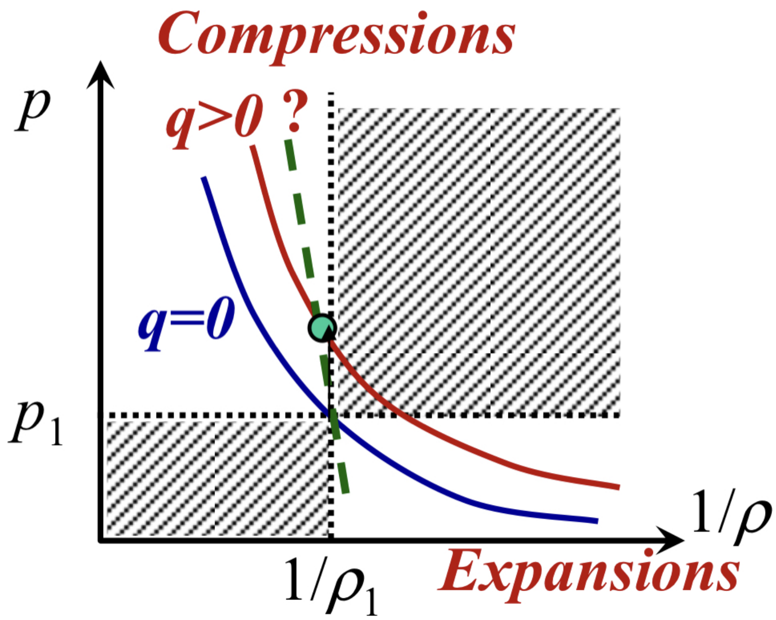

Figure 6: Hugoniot Curves.

Notice that if there is no heat release, we call this is **shock Hugoniot**. The final state will be the intersection between Rayleigh line and Hugoniot curve.

To prove $q > 0$ curve is above $q = 0$ curve, we assume $\rho_1 = \rho_2$, then:

$$q = \frac{\gamma}{\gamma - 1}(p_2 - p_1)\frac{1}{\rho} - (p_2 - p_1) = \frac{1}{\rho(\gamma - 1)}(p_2 - p_1) \tag{34}$$

To achieve $q > 0$, we need $p_2 > p_1$, so the curve is above $q = 0$ curve.

We can also prove that deflagration is subsonic and detonation is supersonic using Hugoniot curve:

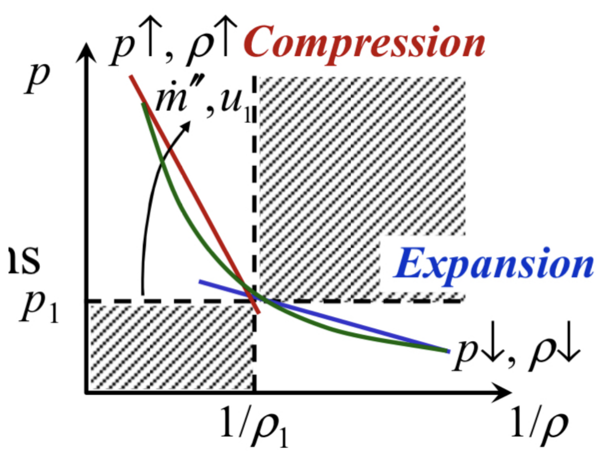

Figure 7: Subsonic, Supersonic Proof.

First, we define detonations as compressions, deflagrations as expansions.

Recall the wave speed expression:

$$\gamma_1 M_1^2 = \frac{1 - p_2/p_1}{\rho_1/\rho_2 - 1} \tag{35}$$

From the graph, in the expansion region:

$$\rho_1/\rho_2 >> 1, p_2/p_1 < 1 \rightarrow M_1 < 1 \tag{36}$$

In the compression region:

$$\rho_1/\rho_2 < 1, p_2/p_1 >> 1 \rightarrow M_1 > 1 \tag{37}$$

Therefore, deflagrations are subsonic and detonations are supersonic.

3 Allowed Solutions

3.1 Chapman-Jouget Point

We define the points where Rayleigh and Hugoniot are tangent as **Chapman-Jouget Points**. Why this point is special?

Recall the Hugoniot equation:

$$(h_2 - h_1) = \frac{1}{2}(p_2 - p_1)(\frac{1}{\rho_1} + \frac{1}{\rho_2}) \tag{38}$$

Derivative form:

$$dh_2 = \frac{1}{2}[(p_2 - p_1)d(\frac{1}{\rho_2}) + (\frac{1}{\rho_1} + \frac{1}{\rho_2})dp_2] \tag{39}$$

Recall the Gibb's Equation:

$$dh = Tds + \frac{1}{\rho}dp \tag{40}$$

Therefore:

$$\begin{aligned} T_2 ds_2 &= dh_2 - \frac{1}{\rho_2}dp_2 \\ &= \frac{1}{2}[(p_2 - p_1)d(\frac{1}{\rho_2}) + (\frac{1}{\rho_1} + \frac{1}{\rho_2})dp_2] - \frac{1}{\rho_2}dp_2 \\ &= \frac{1}{2}[(p_2 - p_1)d(\frac{1}{\rho_2}) - (\frac{1}{\rho_2} - \frac{1}{\rho_1})dp_2] \end{aligned} \tag{41}$$

In this problem, we assume $ds_2 = 0$, so:

$$(p_2 - p_1)d(\frac{1}{\rho_2}) = (\frac{1}{\rho_2} - \frac{1}{\rho_1})dp_2 \tag{42}$$

$$\frac{dp_2}{d(1/\rho_2)} = \frac{p_2 - p_1}{1/\rho_2 - 1/\rho_1} = -(\rho_2 u_2)^2 \tag{43}$$

Based on the definition of speed of sound:

$$a^2 = \frac{\partial p}{\partial \rho}|_s \tag{44}$$

Rearrange:

$$\frac{\partial p_2}{\partial (1/\rho_2)}|_s = -(\rho_2 a_2)^2 \tag{45}$$

Therefore, we know at C-J points, $u_2 = a_2$, $M_2 = 1$, which means the product gases move at local sonic speed in wave-fixed ref.frame.

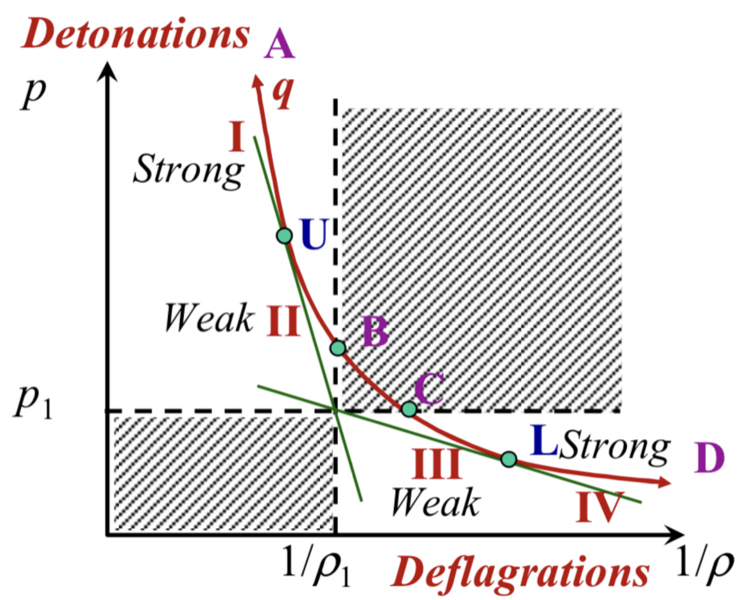

Figure 8: C-J Points.

Using C-J points, we can divide the graph into 4 different regions: strong, weak detonations and strong, weak deflagrations. Here:

1. U: upper C-J points, also the minimum detonation wave speed
2. L: lower C-J points, also the maximum deflagration wave speed

3.2 Deflagration

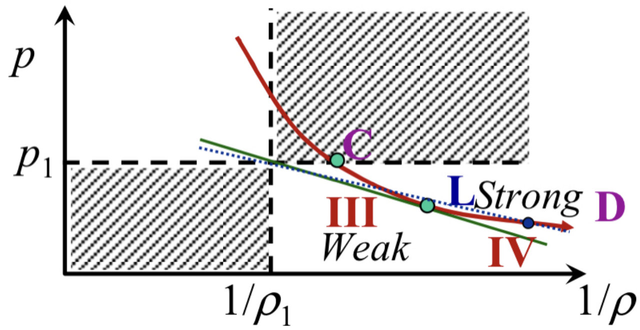

Figure 9: Deflagration.

We already know maximum mass flux at L point, therefore:

$$\dot{m}'' = \rho_2 u_2 \leq (\rho_2 u_2)_L \tag{46}$$

3.2.1 Strong Deflagration

$$\begin{aligned}
\frac{M_{2,IV}}{M_{2,L}} &= \frac{u_{2,IV}/a_{2,IV}}{u_{2,L}/a_{2,L}} \\
&\propto \frac{\dot{m_{2,IV}}''/\rho_{2,IV}}{\dot{m_{2,L}}''/\rho_{2,L}} \sqrt{\frac{p_{2,L}/\rho_{2,L}}{p_{2,IV}/\rho_{2,IV}}} \\
&= \underbrace{\frac{\dot{m_{2,IV}}''}{\dot{m_{2,L}}''}}_{<1} \underbrace{\sqrt{\frac{p_{2,L}}{p_{2,IV}}}}_{>1} \underbrace{\sqrt{\frac{\rho_{2,L}}{\rho_{2,IV}}}}_{>>1}
\end{aligned} \tag{47}$$

Therefore, $M_{2,IV} > 1$ (**strong: subsonic to supersonic**). This requires acceleration of subsonic to supersonic flow in constant area via **heat addition**, which violates 2nd TD law. Therefore, **strong deflagration is not allowed**.

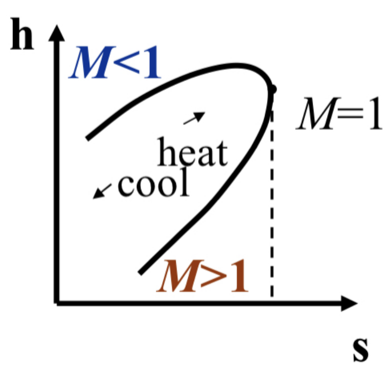

Figure 10: RayleighFlow.

3.2.2 Weak Deflagration

$$\frac{M_{2,III}}{M_{2,L}} \propto \underbrace{\frac{\dot{m_{2,III}}''}{\dot{m_{2,L}}''}}_{<1} \underbrace{\sqrt{\frac{p_{2,L}}{p_{2,III}}}}_{<1} \underbrace{\sqrt{\frac{\rho_{2,L}}{\rho_{2,III}}}}_{<<1} \tag{48}$$

Therefore $M_{2,III} < 1$. In weak deflagration, the flow is accelerated from subsonic to subsonic, and the heat release increase u_2, M_2 from u_1, M_1. This does not violate 2nd TD law, so the **whole range of weak deflagration is allowed**.

3.3 Detonation

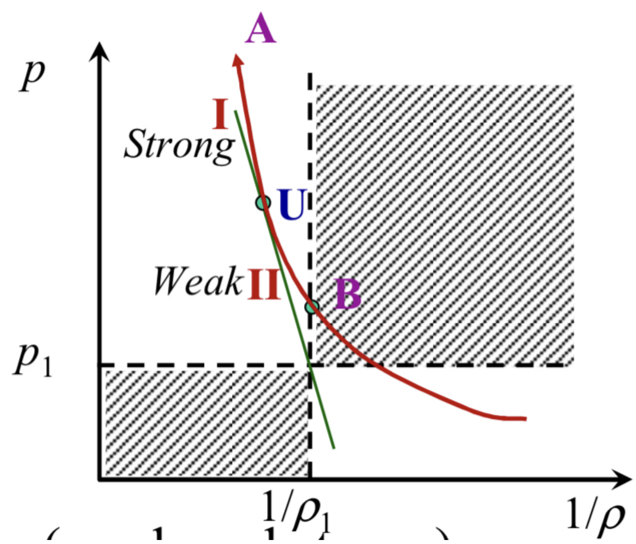

Figure 11: Detonation.

We already know U is the minimum detonation speed (M_1), we can prove that detonation is supersonic wave using another method. Based on continuity:

$$\rho_1 u_1 = \rho_2 u_2 \tag{49}$$

So:

$$M_1 = \frac{u_1}{a_1} = \frac{\rho_2}{\rho_1}\frac{u_2}{a_1} \tag{50}$$

At upper C-J point:

$$M_{1U} = \frac{\rho_2}{\rho_1}\frac{a_2}{a_1} = \frac{\rho_2}{\rho_1}\sqrt{\frac{T_2}{T_1}} \tag{51}$$

We know detonation is compression wave, so $\rho_2 > \rho_1$ and $T_2 > T_1$, so $M_1 > 1$ for all detonations.

3.3.1 Strong Detonation

We know the U point has the minimum mass flux, so:

$$\dot{m}'' = \rho_2 u_2 > (\rho_2 u_2)_U \tag{52}$$

Therefore in strong detonation region:

$$\frac{M_{2,I}}{M_{2,U}} \propto \underbrace{\frac{\dot{m_{2,I}}''}{\dot{m_{2,U}}''}}_{>1} \underbrace{\sqrt{\frac{p_{2,U}}{p_{2,I}}}}_{<<1} \underbrace{\sqrt{\frac{\rho_{2,U}}{\rho_{2,I}}}}_{>1} \tag{53}$$

Therefore, $M_{2,I} < 1$, the products are subsonic (**strong: supersonic to subsonic**). This does not violate the TD laws, **but not observed as steady, self-sustained process**.

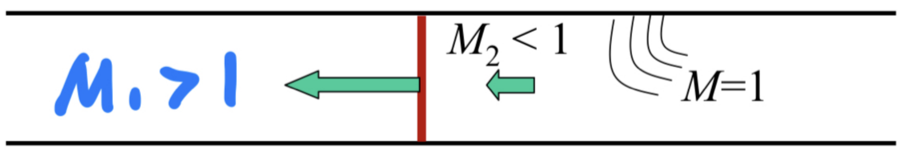

Figure 12: Strong Detonation.

From the graph, we can observe that there is an expansion wave behind the detonation wave, with increasing temperature and reducing pressure (detonation back pressure), so it will slow M_1 until $M_1 = 1$, also speed up M_2 until $M_2 = 1$. Therefore, the solution will **eventually relax to C-J point detonation.**

3.3.2 Weak Detonation

$$\frac{M_{2,II}}{M_{2,U}} \propto \underbrace{\frac{\dot{m_{2,II}}''}{\dot{m_{2,U}}''}}_{>1} \underbrace{\sqrt{\frac{p_{2,U}}{p_{2,II}}}}_{>1} \underbrace{\sqrt{\frac{\rho_{2,U}}{\rho_{2,II}}}}_{>1} \tag{54}$$

Therefore $M_{2,II} > 1$, products stay supersonic. To examine whether this solution, we need to introduce **Zeldovich, von Neumann, Doring (ZND) Model**.

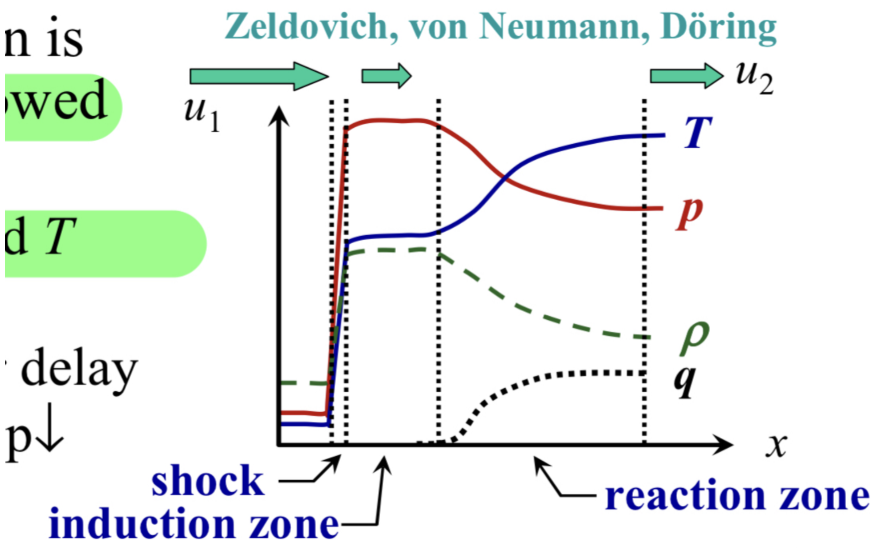

Figure 13: ZND Model

Here is the detonation structure:

1. Detonation is leading shock followed by reaction zone
2. Shock raises p and T
3. M goes subsonic
4. Autoignition after delay
5. Heat release, temperature increases, pressure decreases like deflagration

After leading shock wave, flow is reduced to subsonic. To achieve weak detonation, flow must reaccelerate to supersonic. If induction/reaction zones only have heat release, this will violate 2nd TD law.

3.3.3 Summary

No weak (unallowed), strong (unstable) detonation, only leaves C-J solution, which is a planar detonation solution. A planar detonation is a type of explosion where the detonation wave (the shock wave causing the actual explosion) propagates in a planar (flat, two-dimensional) manner. This is in contrast to spherical or cylindrical detonations where the detonation wave propagates outward in a spherical or cylindrical fashion.