

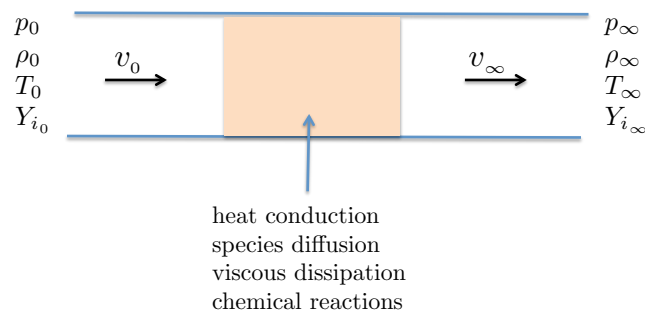
# Lecture 4

## Deflagrations and Detonations

1

### One-dimensional flow

coordinate attached to a wave propagating to the left at speed  $v_0$



plane, steady, one-dimensional flow involving exothermic chemical reactions in which the properties become uniform as  $|x| \rightarrow \infty$ .

2

steady, one dimensional  $\frac{D}{Dt} = \cancel{\frac{\partial}{\partial t}} + v \frac{\partial}{\partial x}$

$$\frac{d}{dx}(\rho v) = 0$$

$$\frac{d}{dx}(\rho v) = -\frac{dp}{dx} + \frac{4}{3}\mu \frac{d^2v}{dx^2}$$

$$\frac{d}{dx}(\rho v h) = v \frac{dp}{dx} + \frac{4}{3}\mu \left(\frac{dv}{dx}\right)^2 - \frac{dq}{dx}$$

$$\frac{d}{dx}(\rho v Y_i) + \frac{d}{dx}(\rho Y_i V_i) = \omega_i \quad i = 1, 2, \dots, N$$

$$p = \rho \mathcal{R}T/W$$

3

$$\frac{d}{dx}(\rho v) = 0$$

$$\frac{d}{dx} \left( p + \rho v^2 - \frac{4}{3}\mu \frac{dv}{dx} \right) = 0$$

$$\frac{d}{dx} \left( \rho v \left( h + \frac{1}{2}v^2 \right) - \frac{4}{3}\mu v \frac{dv}{dx} + q \right) = 0$$

$$\frac{d}{dx}(\rho v Y_i + \rho Y_i V_i) = \omega_i$$

$$\rho v = \text{const.}$$

$$p + \rho v^2 - \frac{4}{3}\mu \frac{dv}{dx} = \text{const.}$$

$$\rho v \left( h + \frac{1}{2}v^2 \right) - \frac{4}{3}\mu v \frac{dv}{dx} + q = \text{const.}$$

$$\frac{d}{dx}(\rho v Y_i + \rho Y_i V_i) = \omega_i$$

4

$$\begin{aligned}
 [\rho v]_{-\infty}^{+\infty} &= 0 \\
 \left[ p + \rho v^2 - \frac{4}{3} \mu \frac{dv}{dx} \right]_{-\infty}^{+\infty} &= 0 \\
 \left[ \rho v \left( h + \frac{1}{2} v^2 \right) - \frac{4}{3} \mu v \frac{dv}{dx} + q \right]_{-\infty}^{+\infty} &= 0 \\
 \left[ \frac{d}{dx} (\rho v Y_i + \rho Y_i V_i) \right]_{-\infty}^{+\infty} &= [\omega_i]_{-\infty}^{+\infty} \\
 q &= -\lambda \frac{dT}{dx} + \sum_{i=1}^N \rho Y_i h_i^o V_i & h &= \sum_{i=1}^N Y_i h_i^o + \int_{T_0}^T c_p dT \\
 \rho Y_i V_i &= -\rho D_i \frac{dY_i}{dx} & p &= \rho \mathcal{R} T / W
 \end{aligned}$$

5

$$\begin{aligned}
 \rho_0 v_0 &= \rho_\infty v_\infty \\
 p_0 + \rho_0 v_0^2 &= p_\infty + \rho_\infty v_\infty^2 \\
 h_0 + \frac{1}{2} v_0^2 &= \frac{1}{2} h_\infty v_\infty^2 \\
 \omega_{i_0} &= 0, \quad \omega_{i_\infty} = 0 \quad i = 1, 2, \dots, N \\
 p_0 / \rho_0 T_0 &= p_\infty / \rho_\infty T_\infty = \mathcal{R} / W
 \end{aligned}$$

assume  $c_{p_i} \equiv c_p$  and  $W_i \equiv W$  for all  $i$  (or take some average value)

$$\begin{aligned}
 h_\infty - h_0 &= \sum_{i=1}^N (Y_{i_\infty} - Y_{i_0}) h_i^o + c_p (T_\infty - T_0) \\
 &= -Q + c_p (T_\infty - T_0)
 \end{aligned}$$

$Q$  is the heat of combustion per unit mass of combustible mixture

note that  $c_p - c_v = \mathcal{R} / W$  implies  $\mathcal{R} / W = \frac{\gamma - 1}{\gamma} c_p$

6

$$\text{let } m = \rho_0 v_0 = \rho_\infty v_\infty$$

after some manipulations (and use of the equation of state to eliminate  $T$ )

$$\frac{p_\infty - p_0}{1/\rho_\infty - 1/\rho_0} = -m^2$$

Rayleigh Line

$$\frac{\gamma}{\gamma - 1} \left( \frac{p_\infty}{\rho_\infty} - \frac{p_0}{\rho_0} \right) - \frac{1}{2} \left( \frac{1}{\rho_\infty} + \frac{1}{\rho_0} \right) (p_\infty - p_0) = Q$$

Hugoniot curve

relation between thermodynamic variables only

they determine the relation between the end and initial states

7

Dimensionless variables

$$p = p_\infty/p_0, \quad \rho = \rho_\infty/\rho_0, \quad v = v_\infty/v_0 \quad (\text{also the specific volume})$$

$$\mu = m^2/p_0\rho_0, \quad q = Q/(p_0/\rho_0) = Q/(\gamma a_0^2)$$

$$\frac{p - 1}{v - 1} = -\mu$$

$$p = \frac{2q + \frac{\gamma+1}{\gamma-1} - v}{\frac{\gamma+1}{\gamma-1}v - 1}$$

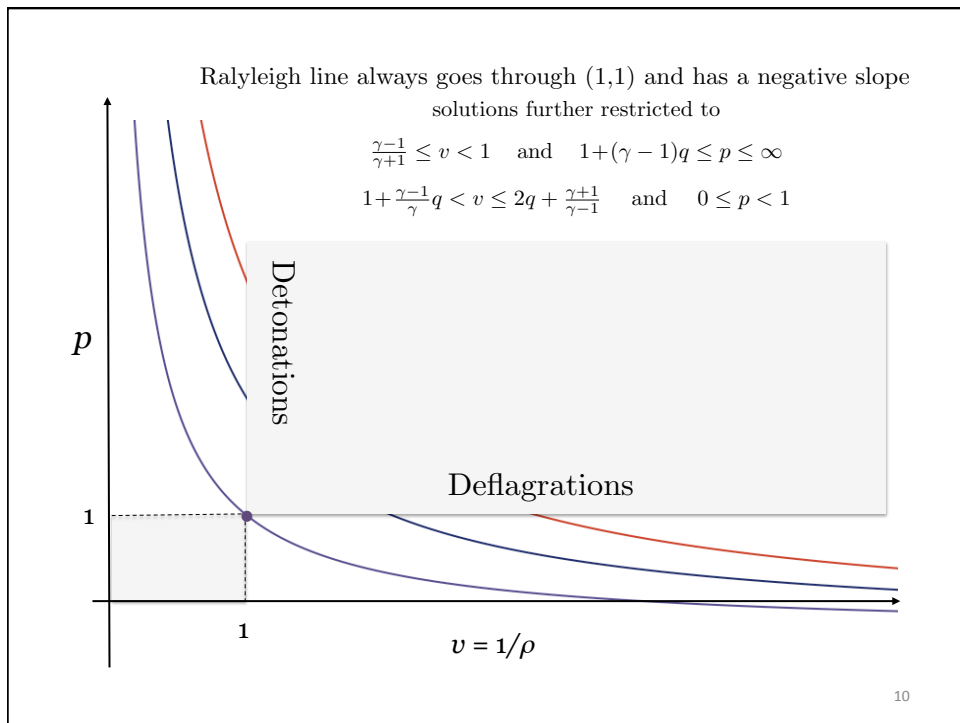
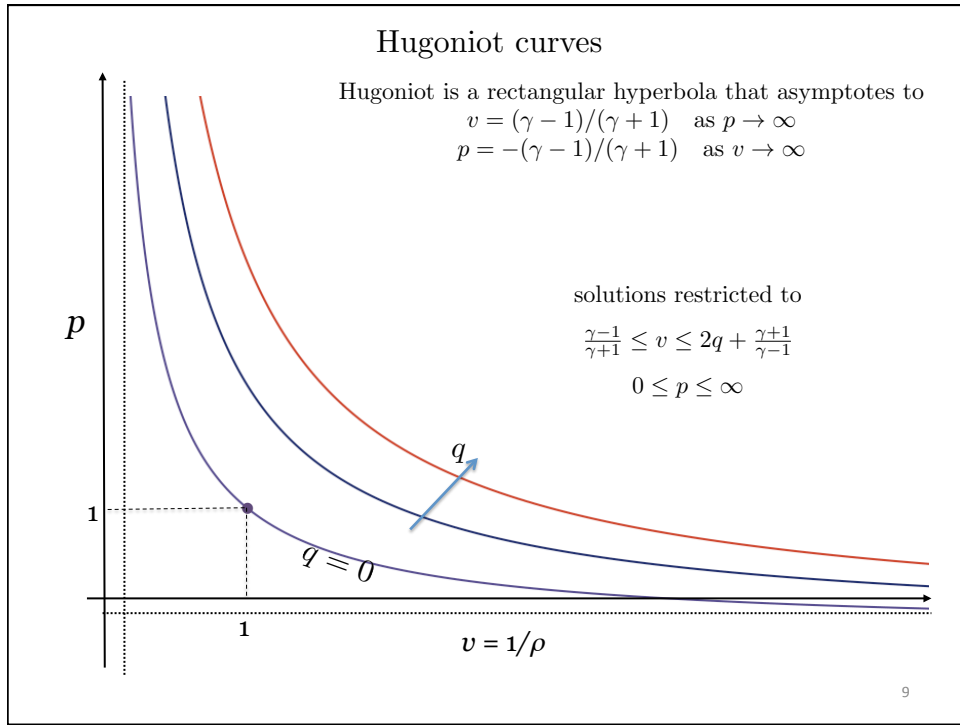
provide  $p, v$  (and consequently  $\rho, T$ ) for a given  $\mu$

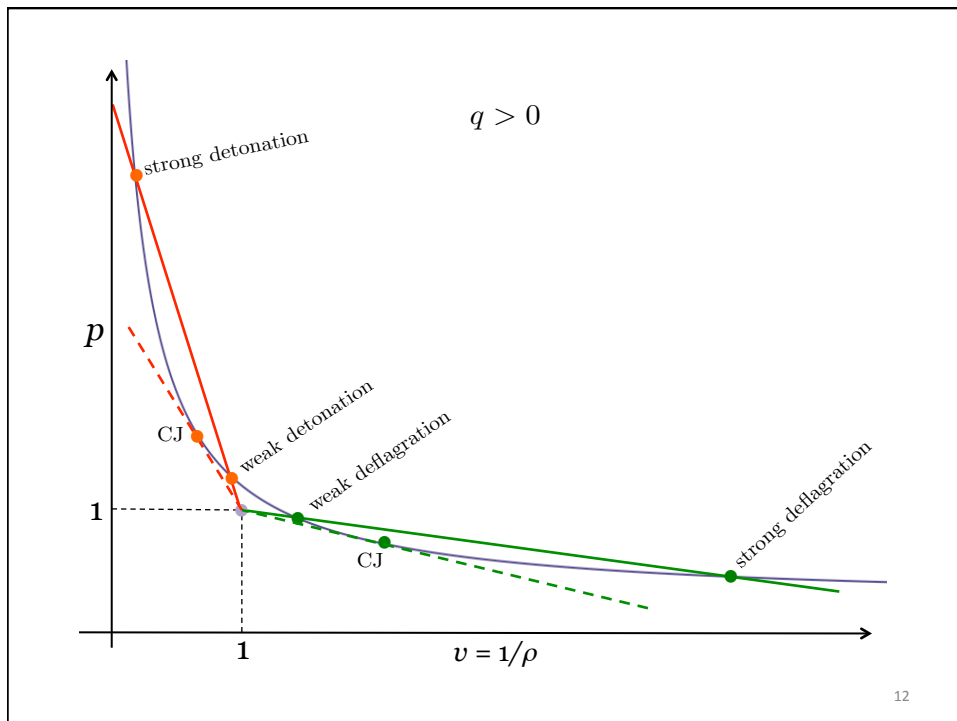
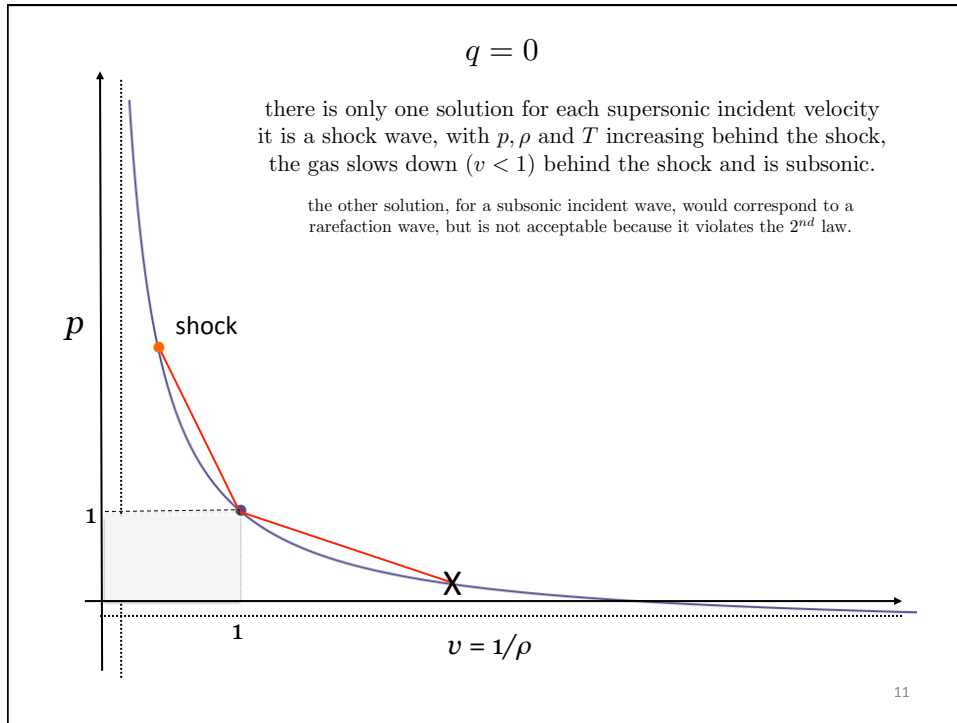
upstream state corresponds to  $p = v = 1$

possible downstream states are intersections of the Hugoniot and Rayleigh line

$$\mu = \gamma M_0^2 \quad \text{where } M_0 = v_0/a_0 \quad \text{is the upstream Mach number}$$

8





## Detonations

there is a minimum value of  $\mu$  and, as a consequence, a minimum wave speed corresponding to Chapman-Jouguet (CJ) detonation

for  $\mu > \mu_{CJ}$  there are two solutions, strong and weak detonations

passing through a detonation wave

$v < 1$  the gas slows down

$\rho > 1$  the gas is compressed

$p > 1$  the pressure increases

## Deflagrations

there is a maximum value of  $\mu$  and, as a consequence, a maximum wave speed corresponding to Chapman-Jouguet (CJ) deflagration;

for  $\mu < \mu_{CJ}$  there are two solutions, weak and strong deflagrations

passing through a deflagration wave

$v > 1$  the gas speeds up

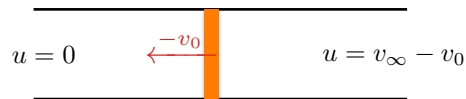
$\rho < 1$  the gas expands

$p < 1$  the pressure decreases

13

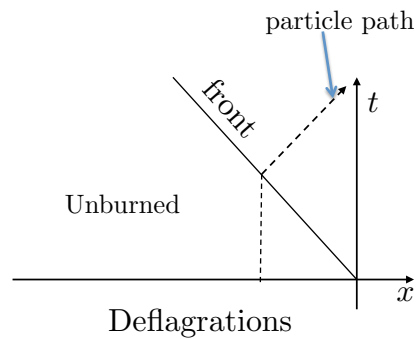
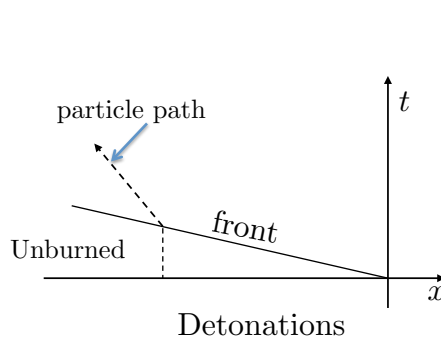


as seen by an observer moving with the wave



as seen in the laboratory frame

$u = v + V_{\text{wave}}$  is the fluid particle velocity  
 $u < 0$  for detonations and  $u > 0$  for deflagrations



14

**Deflagrations:**

- Expansion waves that propagate subsonically ( $0 < M_0 < 1$ )
- The burned gas behind the front expands and accelerates away from the front
- In a frame attached to the wave, the downstream flow beyond CJ waves is sonic ( $M_\infty = 1$ );  
 $M_\infty < 1$  for weak deflagrations,  $M_\infty > 1$  for strong deflagrations
- Strong deflagrations are not possible (there is no structure that connects the burned and unburned states)
- There is a unique solution for the (weak) deflagration, giving a definite wave speed for each gas mixture
- Weak deflagrations (flames) travel typically at 10-100cm/s and  $p_\infty/p_0 \sim 1$ ,  $T_\infty/T_0 \sim 6$ ,  $\rho_\infty/\rho_0 \sim 1/6$

15

**Detonations:**

- Compression waves that propagate supersonically ( $1 < M_0 < \infty$ )
- The wave retards the burned gas that compresses behind the front
- In a frame attached to the wave the downstream flow beyond CJ waves is sonic ( $M_\infty = 1$ ).  
 $M_\infty > 1$  for weak detonations;  $M_\infty < 1$  for strong detonations
- A strong detonation can be produced by driving a piston at an appropriate speed into the mixture
- There is only one wave speed at which a weak detonation can propagate (but weak detonations are seldom observed)
- Self-sustained detonations are CJ; in a hydrogen/air mixture  
 $v_0 \sim 2000 - 3000$  m/s and  $p_\infty/p_0 \sim 20$ ,  $T_\infty/T_0 \sim 10$ ,  $\rho_\infty/\rho_0 \sim 2$

16



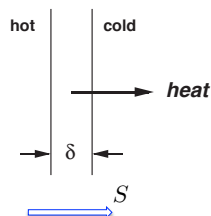
## Comment

The Rankine-Hugoniot analysis provides, for given conditions, the state of the gas downstream, but does not determine (except for the CJ waves) the wave speed  $v_0$ .

The possible existence of a final state based on this analysis does not guarantee the existence of the solution. One needs to ensure that the initial and final states are connected smoothly by a solution of the differential equations and that this solution is stable.

17

## Deflagrations



Thermal diffusivity  $\mathcal{D}_{th} \sim 10^{-5} \text{ m}^2/\text{s}$

Chemical time  $t_c \sim 10^{-5} \text{ s}$

Speed  $S \sim \sqrt{\mathcal{D}_{th}/t_c}$

Wave thickness  $\delta \sim \sqrt{\mathcal{D}_{th} t_c}$

$S \sim 10 - 100 \text{ cm/s}$

$p_\infty/p_0 \sim 1, \quad T_\infty/T_0 \sim 6$

18

Deflagrations (weak) are subsonic waves, so that disturbances behind the wave can propagate ahead and affect the state of the unburned gas before arrival of the wave (this depends, of course, on the rear end boundary conditions, if open or close, etc. . .).

The expansion of the products can therefore cause a displacement of the reactants so that the wave moves faster than the flame speed (burning velocity relative to quiescent mixture).

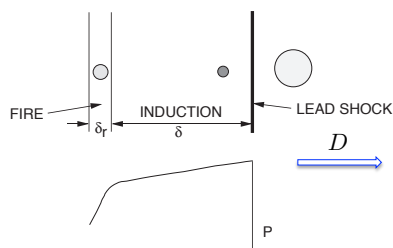
Because of intrinsic instabilities, turbulence, obstacles, etc. . . the deflagration wave may accelerate and turn into a detonation, known as Deflagration to Detonation Transition (DDT).

19

## Detonations

### The ZND structure

Zel'dovich, von Neuman, Döring



shock followed by a fast flame

Ahead of the wave - gas is quiescent, insignificant reaction

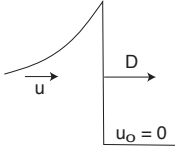
Passage through the lead shock the gas is compressed and its temperature rises thousands of degrees

The ensuing chemical reaction goes to completion very rapidly in a thin reaction zone (or fire) behind the shock

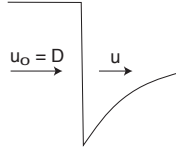
The ZND solution is an exact solution of the reactive Euler equations

20

### Steady Propagating Waves



Laboratory Frame



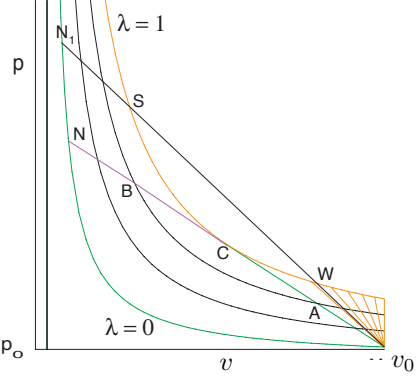
Wave-fixed Frame

State ahead  
 $p_0, v_0 (= \rho_0^{-1}), u_0, \lambda_0 (= 0)$

State within  
 $p, v (= \rho^{-1}), u, \lambda$

Here  $\lambda$  is a progress variable, that varies from  $\lambda = 0$  in the fresh unreacted gas to  $\lambda = 1$  when reaction is complete, and  $u$  is the particle velocity.

21

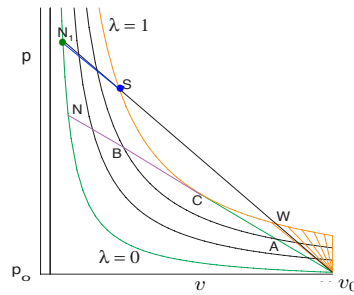


The two extreme Hugoniot curves correspond to  $\lambda = 0$  and  $\lambda = 1$ .  
 For a given  $D$ , all states within the reaction zone must lie on the corresponding Rayleigh line.

$$p = p_0 = -\rho_0^2 D^2 (v - v_0)$$

Since the Hugoniot reaction must be satisfied, the portion of the Rayleigh line relevant is bounded by the extreme Hugoniot corresponding to  $\lambda = 0, 1$ .

22

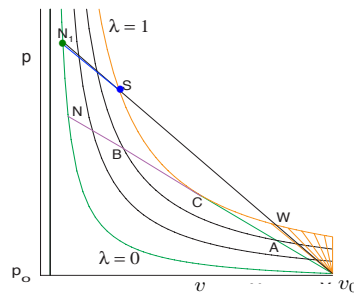


Starting with an initial state, the state of the gas will jump to the point  $N_1$  along the shock-Hugoniot (corresponding to  $\lambda=0$ ) as it traverse the led shock.

As the particle reacts,  $\lambda$  increases and the state of the particles slides down to  $S$  along the Rayleigh line crossing Hugoniot curves with varying  $\lambda$ .

At the end of the reaction zone,  $\lambda=1$ , and the particle reaches the state  $S$ .

23



The lowest possible Rayleigh line is the one tangent to the Hugoniot, corresponding to  $\lambda=1$ . The final state in this case will be  $C$ , the CJ state and the propagation speed in this case is  $D_{CJ}$ .

ZND structure is not possible for weak detonations.

ZND structure does not restrict the propagation speed  $D$  for strong detonations. Therefore, wave speeds depend on the experimental configuration, or on the rear BCs.

24

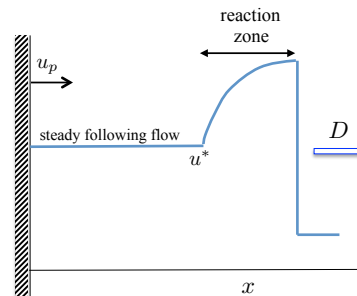
The rear BC can be thought to be a hypothetical piston following the wave. The question is to determine  $D$  for a given piston velocity  $u_p$ .

We denote by  $u^*$  the particle speed at the end of the reaction zone and  $u_{CJ}^*$  the corresponding value for the CJ detonation.

$$\underline{u_p > u_{CJ}^*}$$

The detonation speed  $D$  is chosen such that  $u_p = u^*(D)$

The same qualitative picture remains as  $u_p$  is reduced towards  $u_{CJ}^*$

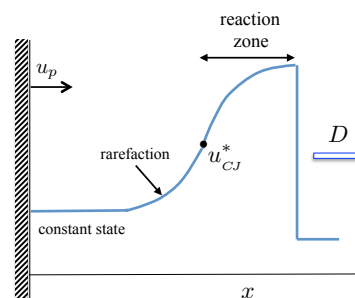


25

As before,  $u^*$  is the particle speed at the end of the reaction zone and  $u_{CJ}^*$  the corresponding value for the CJ detonation.

$$\underline{u_p < u_{CJ}^*}$$

The detonation wave (including the reaction zone) propagates at  $D_{CJ}$ .



The following flow must be reduced to match the BC. this corresponds to a time-dependent rarefaction wave, which is then followed by a constant state (as necessary).

26

The conditions across the shock follow from the RH relations. The spatial distribution behind the shock is determined from

$$\frac{D\lambda}{Dt} = r \quad r = k(1-\lambda)^n e^{-R/\mathcal{R}T}$$

which in a frame attached to the shock is given by

$$(u + D) \frac{d\lambda}{dx} = k(1-\lambda)^n e^{-R/\mathcal{R}T}$$

and can be integrated to give

$$x = \int_0^\lambda \frac{[u(\lambda) + D]}{k(1-\lambda)^n} e^{R/\mathcal{R}T} d\lambda$$

and when  $\lambda = 1$  we find the end state.