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Detonation Wave Profile

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Abstract

The Zel'dovich-von Neumann-Doering (ZND) profile of a detonation wave is derived. Two basic assumptions are required: i. An equation of state (EOS) for a partly burned explosive; $P(V, e, \lambda)$. ii. A burn rate for the reaction progress variable; $\frac{\mathsf{d}}{\mathsf{d}t}\lambda = \mathcal{R}(V, e, \lambda)$. For a steady planar detonation wave the reactive flow PDEs can be reduced to ODEs. The detonation wave profile can be determined from an ODE plus algebraic equations for points on the partly burned detonation loci with a specified wave speed. Furthermore, for the CJ detonation speed the end of the reaction zone is sonic. A solution to the reactive flow equations can be constructed with a rarefaction wave following the detonation wave profile. This corresponds to an underdriven detonation wave, and the rarefaction is know as a Taylor wave.

Explosive model

For a high explosive (HE), we assume a single-step irreversible reaction from reactants to products. The amount of reaction is characterized by a reaction progress variable, which we denote by λ. It varies from 0 to 1 as the reaction progresses. Typically, λ is taken as the mass fraction of the products.

We further assume that partially burned HE with a fixed value of λ is characterized by a thermodynamically consistent equation of state (EOS). Pressure is denoted by the function $P(V, e, \lambda)$, where V and e are the specific volume and specific energy, respectively. The reactants EOS corresponds to $P(V, e, 0)$ and the products EOS to $P(V, e, 1)$. Typically, the partly burned EOS is taken as a mixture of the reactants EOS and products EOS. Pressure-temperature equilibrium is a common mixture rule. For this mixture rule, the EOS is in general not analytic, and an iterative method is needed to evaluate the pressure.

Some pairs of EOS used for the reactants and products do not fully account for the energy of reaction and require an energy source term $Q\lambda$. The energy source term can be eliminated by shifting the energy origin of the products; *i.e.*, $\widetilde{P}_{prod}(V, e) = P_{prod}(V, e + Q)$. Here we assume that the EOS fully accounts for the chemical energy and no energy source term is needed.

Two important thermodynamic quantities are the frozen sound speed, $c(V, e, \lambda)$, and the thermicity, $\sigma(V, e, \lambda)$. They are defined by

$$(\rho c)^2 = -(\partial_V P)_{S,\lambda} = -(\partial_V P)_{e,\lambda} + P\,(\partial_e P)_{V,\lambda}\ , \tag{1a}$$

$$\sigma = (\rho c^2)^{-1}\,(\partial_\lambda P)_{V,e}\ , \tag{1b}$$

where S is the entropy. The thermicity is dimensionless and must be positive for an explosive. For the P-T equilibrium mixture rule, thermodynamic derivatives can be expressed in terms of the derivatives of the components; see [Menikoff, 2012, appendix C].

Detonation locus

The detonation locus corresponds to the possible states behind a detonation wave. It is determined by the EOS of products and the initial state of

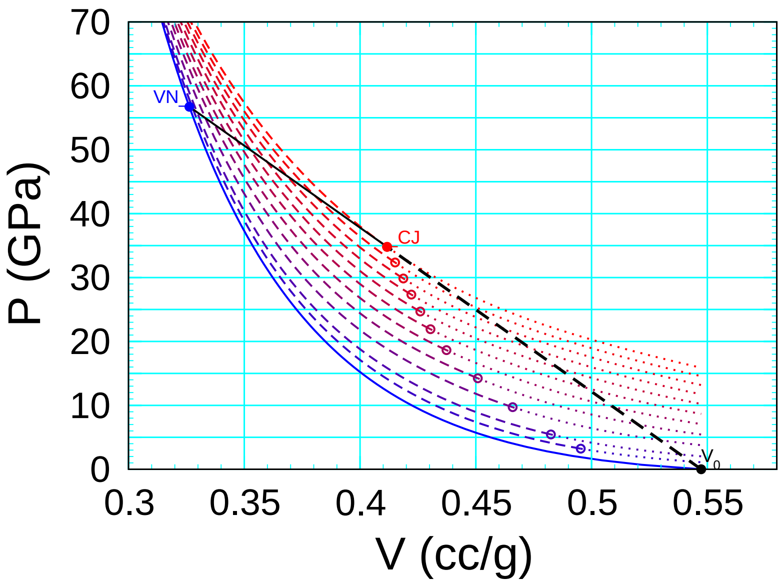

Figure 1: Partly burned detonation loci for PBX 9501. The loci are color coded for λ in steps of 0.1 from unreacted (blue, $\lambda = 0$) to fully reacted (red, $\lambda = 1$) and one additional locus with $\lambda = 0.05$. The dashed curves are the strong (subsonic) branch and the dotted curves are the weak (supersonic) branch. Open circles denote the sonic point on each locus. The black curve is the Rayleigh line through the CJ state. The CJ detonation profile corresponds to the solid portion of the Rayleigh line extending from the unreacted VN state to the fully reacted CJ state.

the reactants, denoted by the subscript '0'. More generally, partly burned detonation loci with fixed λ are defined by the Hugoniot equation

$$e = e_0 + \tfrac{1}{2}\big[P(V,e,\lambda) + P_0\big]\cdot(V_0 - V)\ . \qquad (2)$$

A family of partly burned loci, $P_h(V,\lambda)$, is illustrated in figure 1. In contrast to a shock locus ($\lambda = 0$), the initial state (V_0, P_0) does not lie on a detonation locus ($\lambda > 0$) since $\sigma > 0$ implies $P(V_0, e_0, \lambda) > P_0$. The value of $P(V_0, e_0, 1)$ corresponds to the pressure of a constant volume burn.

The following are important properties of the partly burned loci. Assuming for fixed λ that isentropes are convex and the strong EOS condition ($PV/e \geq \Gamma$) holds, see [Menikoff & Plohr, 1989], on each partially burned locus, P is monotonically increasing with decreasing V. The loci do not intersect; see proof in last section. They completely cover the region between the unreacted shock locus and the fully burned detonation locus. Each locus has a unique point which is tangent to the Rayleigh line

$$-\left(\frac{\partial P_h}{\partial V}\right)_\lambda = \frac{P_h(V,\lambda) - P_0}{V_0 - V} \ . \tag{3}$$

At a point of tangency, it can be shown that the entropy is a local extremum; see for example [Menikoff & Plohr, 1989]. Moreover, the partly burned isentrope is also tangent to the Rayleigh line; *i.e.*,

$$(\rho c)^2 = -\left(\frac{\partial P}{\partial V}\right)_{S,\lambda} = \frac{P_h(V,\lambda) - P_0}{V_0 - V} \ . \tag{4}$$

It follows from the shock jump relations that

$$u/D = 1 - V/V_0 \ , \tag{5a}$$

$$(P_h - P_0)/(V_0 - V) = (\rho_0 D)^2 \ , \tag{5b}$$

where D is the detonation speed, and u is the particle velocity. Hence, Eq. (4) is equivalent to $c^2 = (D-u)^2$, and the point of tangency is a sonic point in the frame of reference moving with the detonation front.

The sonic point splits a partly burned locus into a subsonic ($D < u + c$) high pressure strong branch and a supersonic ($D > u + c$) low pressure weak branch. For the fully burned detonation locus ($\lambda = 1$), the sonic point is referred to as the Chapman-Jouguet (CJ) state. The intersection of the Rayleigh line through the CJ state with the unreacted shock locus ($\lambda = 0$) is referred to as the von Neumann (VN) spike state. The detonation speed of the CJ state is

$$D_{\rm CJ} = V_0 \left[\frac{P_{\rm CJ} - P_0}{V_0 - V_{\rm CJ}}\right]^{1/2} \ . \tag{6}$$

It is the minimum speed of a planar detonation wave, and corresponds to a self-sustaining or underdriven detonation wave.

With respect to the ahead flow, a detonation wave is supersonic; *i.e.*, $D_{\rm CJ} > u_0 + c_0$. Consequently, a detonation wave profile must start with a lead shock. Later we show that a steady detonation wave profile in the (V, P)-plane corresponds to the segment of the Rayleigh line starting from a point on the unreacted shock locus and ending at a point on the strong branch of the fully burned detonation locus. For now we note that the segment of the

Rayleigh line intersects every partly burned detonation locus exactly once. This structure, inert shock followed by a reaction zone, is known as a ZND wave profile; see for example [Fickett & Davis, 1979].

Finding the CJ state numerically requires a double iteration. The first to find a state on the detonation locus, Eq. (2), and the second to find the detonation state that satisfies the sonic condition, Eq. (4). It is simplest to parameterize the detonation locus by V. A bisection algorithm in V can be used to find the sonic point. A point on the detonation locus with a given V can be found with a Newton iteration for e. Linearizing Eq. (2), the iteration is $e \to e - \Delta e$, where

$$\Delta e = \frac{e - e_0 - \frac{1}{2}[P(V,e,\lambda) + P_0](V_0 - V)}{1 - \Gamma(V,e,\lambda) \cdot (V_0 - V)/(2V)} \ , \tag{7}$$

and $\Gamma = V(\partial_e P)_{V,\lambda}$ is the Grüneisen coefficient. Since Γ is slowly varying (and for products EOS, typically, a function of only V), the iteration converges in only a few steps. We note, however, that depending on the mixture rule, evaluating $P(V,e,\lambda)$ and $\Gamma(V,e,\lambda)$ may require an iterative method.

Lagrangian PDEs

The one-dimensional PDEs for reactive fluid flow in Lagrangian form are

$$\frac{\mathsf{d}}{\mathsf{d}t}V - \quad V\frac{\partial}{\partial x}u = 0 \ , \tag{8a}$$

$$\frac{\mathsf{d}}{\mathsf{d}t}u + \quad V\frac{\partial}{\partial x}P = 0 \ , \tag{8b}$$

$$\frac{\mathsf{d}}{\mathsf{d}t}e + PV\frac{\partial}{\partial x}u = 0 \ , \tag{8c}$$

$$\frac{\mathsf{d}}{\mathsf{d}t}\lambda \qquad\qquad = \mathcal{R} \ , \tag{8d}$$

where V, u, e, λ are the specific volume, particle velocity, specific energy and reaction progress variable, respectively, $P(V,e,\lambda)$ is the pressure, $\mathcal{R}(V,e,\lambda)$ is the reaction rate, and $\frac{\mathsf{d}}{\mathsf{d}t} = \partial_t + u\,\partial_x$ is the convective time derivative. The reaction and the fluid flow are coupled through the λ dependence of the pressure and the state dependence of the reaction rate.

For a steady wave, all variables are a function of the variable

$$\xi = x - D\,t \ ,$$

where D is the detonation speed. The PDEs then reduce to ODEs

$$(D-u)\frac{\mathsf{d}}{\mathsf{d}\xi}V = -V\frac{\mathsf{d}}{\mathsf{d}\xi}u \ , \tag{9a}$$

$$(D-u)\frac{\mathsf{d}}{\mathsf{d}\xi}u = V\frac{\mathsf{d}}{\mathsf{d}\xi}P \ , \tag{9b}$$

$$(D-u)\frac{\mathsf{d}}{\mathsf{d}\xi}e = PV\frac{\mathsf{d}}{\mathsf{d}\xi}u \ , \tag{9c}$$

$$(D-u)\frac{\mathsf{d}}{\mathsf{d}\xi}\lambda = -\mathcal{R} \ . \tag{9d}$$

Since a detonation wave is supersonic with respect to the flow ahead, the lead front is a shock wave. By using the variable ξ, we are in effect transforming to the frame in which the wave front is stationary. For convenience we consider a right facing wave, $D > 0$, and choose the wave front to be at $\xi = 0$. Ahead of the wave front, $\xi > 0$, the flow is in a constant state. The ahead state is denoted by the subscript '0'.

For any quantity Q, we use the notation

$$\Delta Q = Q(\xi) - Q_0 \tag{10}$$

where $Q_0 = Q(0^+)$ denotes the value of Q in the ahead state.

Equation (9a) is equivalent to mass conservation

$$\Delta[(D-u)\rho] = 0 \ . \tag{11a}$$

Defining the mass flux $m = (D - u_0)/V_0$, then yields

$$(D-u)\rho = m \ , \tag{11b}$$

$$\Delta V = -\Delta u/m \ . \tag{11c}$$

Equations (9b) and (11b) constrain the flow to lie on the Rayleigh line in the (V, P)-plane; *i.e.*,

$$\Delta P = m\Delta u \tag{12a}$$

$$= -m^2\Delta V \ . \tag{12b}$$

Equations (9c), (9b) and (11b) imply the Bernoulli relation

$$e + PV + \tfrac{1}{2}(D-u)^2 = B_0 \ , \tag{13}$$

where $B_0 = e_0 + P_0 V_0 + \frac{1}{2}(D-u_0)^2$. With the aid of Eq. (11b) and Eq. (12b), the Bernoulli relation reduces to the Hugoniot equation (2).

Equations (11c), (12) and (13) imply that the mass, momentum and energy fluxes are constant. Hence, they are equivalent to the shock jump equations. Specifying the mass flux m is equivalent to specifying the detonation speed D. Therefore, V, e and u are the state on a partly burned detonation locus with detonation speed D, and are functions of λ; *i.e.*, $V = V_h(\lambda)$, *etc.*

A point on a partly burned detonation locus with mass flux m and given value of λ can be reduced to solving a single equation in one variable;

$$P(V, e(V), \lambda) = P_0 + m^2 (V_0 - V) \ , \tag{14}$$

where $e(V) = e_0 + \frac{1}{2}m^2(V_0 - V)^2 + P_0\,(V_0 - V)$. The equation for $e(V)$ follows from Eq. (13) and Eq. (12b). After solving for $V_h(\lambda)$, the energy is $e_h = e(V_h)$, and the particle velocity is determined by Eq. (11b); $u_h = D - m\,V_h$.

ZND wave profile

The system of ODEs (9) reduces to a single equation,

$$\frac{\mathsf{d}}{\mathsf{d}\xi}\lambda = -\frac{\mathcal{R}(V_h(\lambda), e_h(\lambda), \lambda)}{m\,V_h(\lambda)} \ . \tag{15}$$

The solution to Eq. (14) can be obtained with a Newton iteration:

$$e_h(V) = e_0 + \tfrac{1}{2}m^2(V_0 - V)^2 + P_0\,(V_0 - V) \ , \tag{16a}$$

$$P_h(V) = P(V, e_h(V), \lambda) \ , \tag{16b}$$

$$f(V) = P_h - P_0 - m^2(V_0 - V) \ , \tag{16c}$$

$$f'(V) = -(c/V)^2 + \Gamma\left[P_h - P_0 - m^2\,(V_0 - V)\right]/V + m^2 \ , \tag{16d}$$

$$V \to V - f(V)/f'(V) \ , \tag{16e}$$

where c is the frozen sound speed and Γ is the Grüneisen coefficient. Starting with the value of V from the last ODE step, only a few iterations are needed to achieve the solution $f(V_h) = 0$.

Physically, the reaction rate is finite, and the initial condition is $\lambda(0) = 0$; *i.e.*, the detonation front is an inert shock. From the analysis in the detonation locus section, a point on the partly burned detonation locus with specified detonation speed D exists for all $0 \le \lambda \le 1$ if and only if $D \ge D_{\rm CJ}$. Therefore, a detonation profile can only exist for points on the strong branch of the fully burned detonation locus.

The negative sign on the right hand side of Eq. (15) is because the profile for a right facing wave is in the region $\xi \le 0$. Moreover, the mass flux m is strictly positive, and the denominator is non-zero. Typically, $\mathcal{R} \propto (1-\lambda)^n$ as $\lambda \to 1$; *i.e.*, the rate vanishes as the reactants are depleted. For hot-spot reaction in a solid explosive, the factor $(1-\lambda)^n$ corresponds to the scaling of the hot-spot surface area and $n < 1$. In this case, the reaction zone width is finite.

The solution to Eqs. (15, 16) determines spatial profiles at fixed time and time histories at fixed spatial position; for example, with $\xi = x$ the pressure profile is given by $P(x) = P_h\big(\lambda(x)\big)$, and with $\xi = -D\,t$ the time history by $P(t) = P_h\big(\lambda(-D\,t)\big)$.

A physical quantity of interest is the reaction time along a particle path. From Eq. (9d) the differential of the reaction time τ is given by

$$\mathsf{d}\tau = \frac{\mathsf{d}\lambda}{\mathcal{R}} = -\frac{\mathsf{d}\xi}{D-u} \ . \tag{17}$$

It can be calculated along with the wave profile by adding an auxiliary ODE to Eq. (15)

$$\frac{\mathsf{d}}{\mathsf{d}\xi}\tau = -\frac{1}{D-u_h(\xi)} \ . \tag{18}$$

In terms of the reaction zone width, w such that $\lambda(-w) = 1$, the reaction time is bounded by

$$\frac{w}{D} < \tau < \frac{w}{D-u_h} \ , \tag{19}$$

where u_h is the particle velocity on the detonation locus; *i.e.*, the end of the reaction zone. The upper bound follows from the monotonicity of $u(\xi)$, which results from Eq. (12a) and the monotonicity of $P(\xi)$. More generally, a Lagrangian time history can be expressed parametrically; for example the pressure time history along a particle path $P(t)$ is given by $t(\xi)$ and $P_h\big((\lambda(\xi)\big)$ for ξ in the interval $-w \le \xi \le 0$.

High accuracy of the detonation wave profile is sought for verification studies. Three ordered tolerances need to be set. The highest tolerance is for the iteration to evaluate the EOS of the partially burned HE. The next is the tolerance for the iteration to determine a point on the partially burned detonation locus, Eq. (16). The lowest tolerance is for the ODE, Eq. (15).

Unsupported detonation wave

For a CJ detonation wave, the reaction zone profile can be extended with a Taylor wave. The Taylor wave is just a rarefaction wave. A rarefaction is a simple wave for which the entropy and one Reimann invariant are each constant. For a right facing wave, the hydrodynamic state is constant along the right facing characteristics, $\mathsf{d}x = (u + c)\,\mathsf{d}t$, and the left Riemann invariant is constant, $\mathsf{d}u - \mathsf{d}P/(\rho c) = 0$. The characteristic speed, $u + c$, is a function of the right Riemann invariant and decreases with pressure. Consequently, a rarefaction waves spread out in time between the characteristics corresponding to the head and tail of the wave. Since the CJ state is sonic, the head of the rarefaction wave travels at the same speed as the detonation wave; see figure 2.

The hydro state for a right facing rarefaction is determined by the ODEs

$$\frac{\mathsf{d}}{\mathsf{d}V} e = -P(V, e) \ , \tag{20a}$$

$$\frac{\mathsf{d}}{\mathsf{d}V} u = -\rho\, c(V, e) \ . \tag{20b}$$

Here, we use the EOS of the HE products, and take the initial condition of the ODEs to be the CJ state. Then Eq. (20a) defines the CJ release isentrope, $P_{\mathrm{CJ}}(V)$. We assume the release isentrope is convex. It can then be shown that the characteristic velocity $q = u + c$ is a monotonically decreasing function of P, or increasing function of V. Therefore, the rarefaction curve can be parameterized by q.

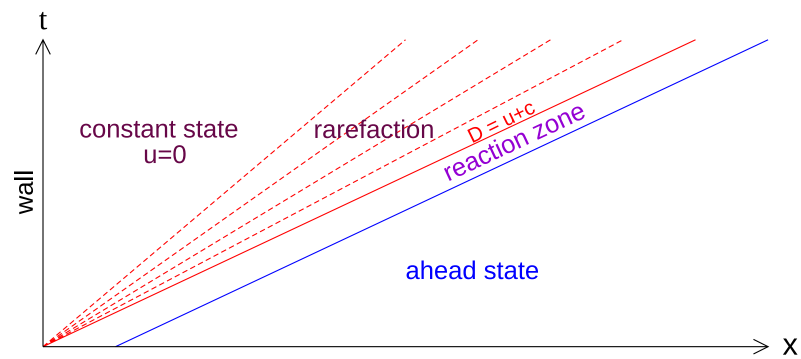

Figure 2: Underdriven detonation wave in (x,t)–plane. The ZND reaction zone is steady, while the rarefaction (Taylor wave) spreads out in time. The constant state is determined by the boundary condition behind the wave; zero particle velocity at the wall.

A solution to the reactive fluid equation for an unsupported detonation wave can be constructed as follows. Let Q represent a hydrodynamic variable; V, e, u, P or c. Let the subscript 'r' denote the rarefaction curve parameterized by the characteristic speed, and q_t and $q_h = D_{\rm CJ}$ denote the tail and head of the rarefaction, respectively. Let the subscript 'ZND' denote the CJ reaction zone profile determined in the previous section, but shifted in space such that $\xi_{\rm CJ} = 0$ and $\xi_0 > 0$ correspond to the end and start of the reaction zone, respectively. The solution for $t > 0$ can be expressed as

$$Q(x,t) = \begin{cases} Q_r(q_t) & \text{constant state for } x \le q_t\, t \\ Q_r(x/t) & \text{rarefaction wave for } q_t\, t < x \le \xi_{\rm CJ} + q_h\, t \\ Q_{\rm ZND}(x - D_{\rm CJ} t) & \text{ZND profile for } \xi_{\rm CJ} < x - D_{\rm CJ}\, t \le \xi_0 \\ Q_0 & \text{ahead state for } \xi_0 + D_{\rm CJ}\, t < x \end{cases} \tag{21}$$

For $t \to 0$ there is a discontinuity at $x = 0$. It is resolved into a centered rarefaction for $t > 0$ with only kinks (discontinuity in spatial derivative) at the head and tail of the rarefaction wave. Because of the kinks, the head and tail of a rarefaction are often referred to as weak singularities. This is in contrast to a shock front for which the hydrodynamic variables themselves are discontinuous.

For a numerical test problem, it is convenient to chose q_t to correspond to the point on the rarefaction curve with $u_r = 0$. With this choice, $q_t > 0$

and $P_r(q_t) > 0$. Then a rigid wall can be used as the left boundary condition. Taking the initial state to correspond to some $t > 0$ spreads out the rarefaction and avoids the initial discontinuity at $x = 0$. A sequence of pressure profiles in the lab frame and in the rest frame of the shock front are shown in figure 3 and figure 4, respectively. The reaction zone is fairly narrow, on the order of tenths of mm. On the scale of several mm or greater, the reaction zone stands out as a spike.

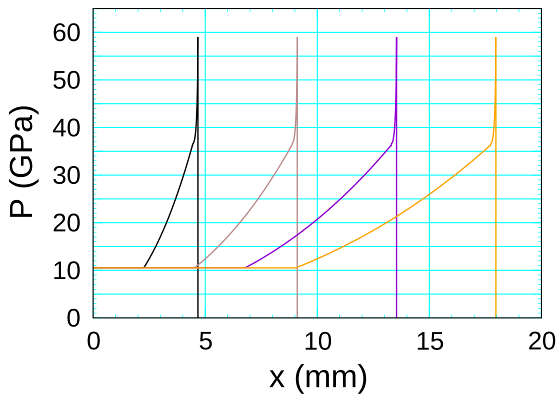

Figure 3: Pressure profile for underdriven detonation wave in the Lab frame; state ahead of the detonation at rest. Sequence of increasing times shown by color; black, brown, violet, orange.

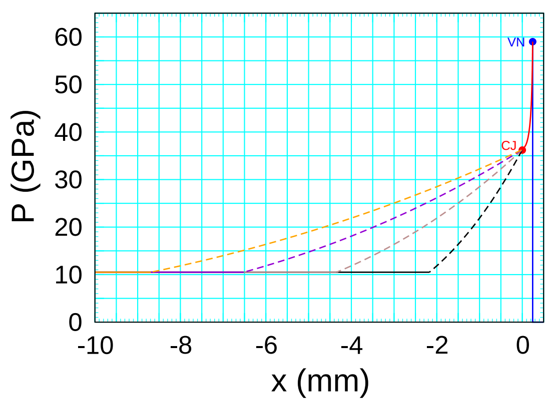

Figure 4: Pressure profile for underdriven detonation wave in the frame in which the detonation front is at rest. Sequence of increasing times; black, brown, violet, orange.

A solution with a non-centered rarefaction can also be constructed by specifying the boundary condition at $x = 0$ to have a time dependent Riemann invariant. This is equivalent to a time dependent inflow boundary in which the inflow state is on the rarefaction curve and the pressure decreases with time.

ZND profile in neighborhood of CJ state

The unsupported detonation wave solution in the preceding section assumes that the reaction zone length is finite. Near $\lambda = 1$ this requires that the rate is proportional to a depletion factor $(1-\lambda)^n$ with $0 < n < 1$. The depletion factor dominates the behavior of the profile in the neighborhood of the CJ state. It has to vanish suitably slowly as $\lambda \to 1$ in order for the reaction zone to be finite; namely $n < 1$. Moreover, we will show that $n = \frac{1}{2}$ has the special property that the pressure derivative is finite and non-zero at the CJ state.

To leading order in $1-\lambda$, near the CJ state Eq. (15) reduces to

$$\frac{\mathsf{d}}{\mathsf{d}\xi}\lambda = -(1-\lambda)^n \frac{\mathcal{R}_{\rm CJ}}{m\, V_{\rm CJ}} \ . \tag{22}$$

In the neighborhood of the CJ state, $\xi - \xi_{\rm CJ} \ll 1$, the solution is

$$\lambda(\xi) = 1 - \left[(1-n) \frac{\mathcal{R}_{\rm CJ}}{m\, V_{\rm CJ}} \cdot (\xi - \xi_{\rm CJ}) \right]^{\frac{1}{1-n}} \ , \tag{23}$$

where $\xi_{\rm CJ}$ is the coordinate at the CJ state. Below we will show as a result of the tangency condition of the detonation locus, Eq. (3), at the CJ state

$$\frac{V_{\rm CJ} - V_h(\lambda)}{V_{\rm CJ}} \to \left[\frac{\sigma}{\mathcal{G}} (1-\lambda) \right]^{1/2} \qquad \text{as } \lambda \to 1, \tag{24}$$

where $\mathcal{G} = \frac{V^2}{2\rho\, c^2} \left(\frac{\partial^2 P}{\partial V^2} \right)_S$ is the fundamental derivative, and σ is the thermicity, Eq. (1b), both evaluated at the at the CJ state. The fundamental derivative is a dimensionless measure of the convexity of an isentrope.

Combining Eq. (23) and Eq. (24), at the end of the ZND profile yields

$$\frac{\mathsf{d}}{\mathsf{d}\xi} V_h\big(\lambda(\xi)\big) = \frac{\mathsf{d}}{\mathsf{d}\lambda} V_h(\lambda) \cdot \frac{\mathsf{d}}{\mathsf{d}\xi}\lambda \tag{25a}$$

$$\propto -(1-\lambda)^{n-1/2} \tag{25b}$$

$$\to \begin{cases} 0 & \text{for } \frac{1}{2} < n < 1 \\ -\,\text{constant} & \text{for } n = \frac{1}{2} \\ -\infty & \text{for } 0 < n < \frac{1}{2} \end{cases} \qquad \text{as } \xi \to \xi_{\text{CJ}} . \tag{25c}$$

Moreover, since the reaction profile lies on the Rayleigh line $\frac{\mathsf{d}}{\mathsf{d}\xi} P_h = -m^2 \frac{\mathsf{d}}{\mathsf{d}\xi} V_h$, and the pressure has a similar behavior at the end of the reaction; *i.e.*,

$$\frac{\mathsf{d}}{\mathsf{d}\xi} P_h\big(\lambda(\xi)\big) \to \begin{cases} 0 & \text{for } \frac{1}{2} < n < 1 \\ \text{constant} & \text{for } n = \frac{1}{2} \\ \infty & \text{for } 0 < n < \frac{1}{2} \end{cases} \qquad \text{as } \xi \to \xi_{\text{CJ}} . \tag{26}$$

Next we derive Eq. (24) based on the expansion of the CJ isentrope of the products EOS to second order in $(V_{\text{CJ}} - V)/V_{\text{CJ}}$

$$P_{\text{CJ}}(V) = P_{\text{CJ}} + (\rho c^2)_{\text{CJ}} \big[(1 - V/V_{\text{CJ}}) + \mathcal{G}_{\text{CJ}} \cdot (1 - V/V_{\text{CJ}})^2\big] \ , \tag{27a}$$

$$e_{\text{CJ}}(V) = e_{\text{CJ}} + P_{\text{CJ}} \cdot (V_{\text{CJ}} - V) + \tfrac{1}{2}\, c_{\text{CJ}}^2 \cdot (1 - V/V_{\text{CJ}})^2 \ . \tag{27b}$$

Due to the tangency condition at the CJ state, Eq. (3), and the Hugoniot equation (2), the partially burned detonation state on the Rayleigh line is given by

$$P_h(V) = P_{\text{CJ}} + (\rho c)^2 (1 - V/V_{\text{CJ}}) \ , \tag{28a}$$

$$e_h(V) = e_{\text{CJ}} + P_{\text{CJ}} \cdot (V_{\text{CJ}} - V) + \tfrac{1}{2}\, c_{\text{CJ}}^2 \cdot (1 - V/V_{\text{CJ}})^2 \ . \tag{28b}$$

We note that to second order $e_{\text{CJ}}(V) = e_h(V)$.

For a fixed λ, the pressure can be expanded based on the product EOS

$$P(V, e, \lambda) = P(V, e, 1) - (1-\lambda)\, \rho\, c^2\, \sigma \ . \tag{29}$$

To second order in $(V_{\text{CJ}} - V)/V_{\text{CJ}}$, we require

$$P_h(V) = P_{\text{CJ}}(V) - (1-\lambda)\, \rho\, c^2\, \sigma \ . \tag{30}$$

Substituting Eq. (28a) and Eq. (27a) into Eq. (29) gives

$$\sigma \cdot (1-\lambda) = \mathcal{G}_{\text{CJ}} \cdot (1 - V/V_{\text{CJ}})^2 \ . \tag{31}$$

Hence $1 - V/V_{\text{CJ}} = (\sigma/\mathcal{G})_{\text{CJ}} (1-\lambda)^{1/2}$, which is the desired result, Eq. (24).

Fine points

Three common tacit assumptions on the EOS have been used in the previous sections:

1. The EOS for fixed λ is convex; *i.e.*, for an isentrope, $P(V)$ is a convex function. This guarantees that shock waves are compressive and that on the subsonic branch of the detonation locus the pressure is monotonically increasing with the wave speed, and hence the slope of the Rayleigh line.

2. On the shock locus we assume $-\mathsf{d}P_h/\mathsf{d}V > 0$. This implies that

$$1 - \tfrac{1}{2}\Gamma \cdot (V_0 - V)/V > 0 \tag{32}$$

in the domain of interest; see for example [Menikoff & Plohr, 1989].

3. $\Gamma > 0$. This implies isentropes in the (V, P)-plane do not cross. Hence, the thermodynamic phase space can be parameterized by V and P.

With these assumptions we now prove: If the thermicity $\sigma > 0$ then the partly burned detonation loci do not cross.
The detonation locus corresponds to the zero level set of the Hugoniot function

$$h(V, e, \lambda) = e - e_0 - \tfrac{1}{2}\big[P(V, e, \lambda) + P_0\big](V_0 - V) \ . \tag{33}$$

For fixed V, the differential of h is

$$\mathsf{d}h = \big[1 - \tfrac{1}{2}(\partial_e P)_{V,\lambda}(V_0 - V)\big]\mathsf{d}e - \tfrac{1}{2}(\partial_\lambda P)_{V,e}(V_0 - V)\mathsf{d}\lambda \ . \tag{34}$$

The energy on the detonation loci is a function $e_h(V, \lambda)$. For fixed V, the derivative with respect to λ is

$$\frac{\partial e_h}{\partial \lambda}\big(V, \lambda\big) = -\frac{(\partial_\lambda h)_{V,e}}{(\partial_e h)_{V,\lambda}} = \frac{\frac{1}{2}(\partial_\lambda P)_{V,e}(V_0 - V)}{1 - \frac{1}{2}\Gamma \cdot (V_0 - V)/V} \ . \tag{35}$$

Then from the EOS, the derivative of the pressure on the detonation loci is given by

$$\begin{aligned} \frac{\partial P_h}{\partial \lambda}\big(V, \lambda\big) &= (\partial_e P)_{V,\lambda}\frac{\mathsf{d}e_h}{\mathsf{d}\lambda} + (\partial_\lambda P)_{V,e} \\ &= \frac{(\partial_\lambda P)_{V,e}}{1 - \frac{1}{2}\Gamma \cdot (V_0 - V)/V_0} \end{aligned} \tag{36}$$

The numerator is proportional to the thermicity, and positive by assumption. The denominator is positive by assumption 2 above. Hence, $\mathsf{d}P_h/\mathsf{d}\lambda > 0$, and P_h is monotonically increasing with λ for fixed V. Therefore, the loci with different λ do not cross.

A corollary is that the wave speed at the sonic point of a partly burned detonation locus, $D_{\rm CJ}(\lambda)$, is monotonically increasing with λ. It can be proved as follows. Let $V_1 = V_{\rm CJ}(\lambda_1)$. For $\lambda < \lambda_1$, $P_h(V_1, \lambda) < P_h(V_1, \lambda_1)$. Consequently, the slope of the Rayleigh line is lower, and hence

$$D_{\rm CJ}(\lambda) \le D_h(V_1, \lambda) < D_h(V_1, \lambda_1) = D_{\rm CJ}(\lambda_1)\ . \tag{37}$$

Since the choice of λ_1 is arbitrary, $D_{\rm CJ}(\lambda)$ must be monotonically increasing. This implies the Rayleigh line through the CJ state crosses the strong branch of all partly burned detonation loci.

Uniqueness of the sonic point on the partly burned detonation loci can be proved by adapting the proof of the Bethe-Wendroff theorem in [Menikoff & Plohr, 1989].

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References

W. Fickett and W. C. Davis, **Detonation**, Univ. of Calif. press, 1979.

R. Menikoff, *"Deflagration Wave Profiles,"* technical report 2012, Los Alamos National Lab, LA-UR-12-20353. http://dx.doi.org/10.2172/1038128

R. Menikoff and B. J. Plohr, *"The Riemann problem for fluid flow of real materials,"* Revs. Mod. Phys., 61 (1989) pp.175–130.