Temperature Profiles and their Influence on the ZND Detonation Structure

Luc Bauwens[1] and D. Scott Stewart[2]

[1]Dept. of Mechanical and Manufacturing Engineering
University of Calgary, Calgary AB T2N 1N4, Canada
bauwens@ucalgary.ca

[2]Dept. of Theoretical and Applied Mechanics,
University of Illinois, Urbana-Champaign, U.S.A.
dss@uiuc.edu

1 Introduction

High activation energies usually lead to a detonation structure made up of a shock followed by a subsonic deflagration structure that includes a long induction zone in which temperature changes are of the order of the inverse activation energy, and finally a narrow zone of intense reaction. But it has been known at least since Kassoy and Clarke [1] that, in a subsonic stream of reactive mixture delivered at a fixed origin, this deflagration structure cannot exist, if the Mach number is above $1/\sqrt{\gamma}$ at the origin. On the other hand, it is clear that ZND solutions exist for arbitrary heat release models and arbitrary Mach numbers above the Chapman-Jouguet value, and that similar underdriven steady solutions also exist under the same conditions up the the sonic point (which appears then at incomplete reaction).

This apparent contradiction is addressed in detail; it is found that a number of structures are theoretically possible, including, in addition to the zone of intense reaction, which is thin at high activation energies, either an induction zone, or a completion zone, or both.

2 Formulation

The study considers the initial value problem describing steady, one-dimensional ZND detonations in a reactive mixture with ideal gas behavior. The dimensionless problem results from scaling $\tilde{x}$ by $\tilde{L}$, a measure of the reaction length yet to be precisely defined, velocities $\tilde{U}$, including $\tilde{D}$, the velocity upstream of the shock, by the Chapman-Jouguet value $\tilde{D}_{cj}$, time by $\tilde{L}/\tilde{D}_{cj}$, pressure by $\tilde{\rho}_0\tilde{D}_{cj}^2$, density by $\tilde{\rho}_0$ and energy and also the heat release $\tilde{Q}$ by $\tilde{D}_{cj}^2$, and the reaction rate r by $\tilde{D}_{cj}/\tilde{L}$, yielding the dimensionless initial value problem (1):

$$\frac{d(\rho u)}{dx} = 0, \quad \frac{d(\rho u^2)}{dx} + \frac{dp}{dx} = 0, \quad \frac{d}{dx}\left[\rho u\left(e + \frac{p}{\rho} + \frac{1}{2}u^2\right)\right] = 0, \quad u\frac{d\lambda}{dx} = r(\lambda, p/\rho) \tag{1}$$

with

$$e(p, \rho, \lambda) = \frac{1}{\gamma - 1}\frac{p}{\rho} - q\lambda \tag{2}$$

with initial values at x = 0 obtained from Rankine-Hugoniot conditions across the leading shock, for upstream velocity D, unit density and a pressure equal to δ/γ. The independent parameters are the overdrive D, γ, and either δ, which equals the inverse of the Chapman-Jouguet Mach number squared, or the heat release q. Indeed, q and δ are related by:

$$q = \frac{(1-\delta)^2}{2(\gamma^2 - 1)} \tag{3}$$

The strong shock limit $\delta = 0$ yields a finite maximum value for q; the pressure ratio across the shock $\rightarrow \infty$, and the pressure upstream of the shock vanishes. The limit $\delta = 1$ corresponds to small heat release.

Eqs. (1) to (3) are valid for arbitrary rate law. For Arrhenius kinetics, writing $\theta = \tilde{E}^0/\tilde{D}_{cj}^2$ and $T = p/\rho$,

$$r = \frac{\tilde{k}\tilde{L}}{\tilde{D}_{cj}}(1-\lambda)^\nu exp\left(-\frac{\theta}{T}\right) \tag{4}$$

In Erpenbeck's scaling, denoted by the subscript E, the overdrive $f = D^2$. Dimensionless heat release and activation energy are related to the parameters used here by:

$$q_E = \gamma q/\delta = \frac{\gamma q}{1 - \sqrt{2(\gamma^2-1)q}}, \quad \theta_E = \theta\gamma/\delta \tag{5}$$

3 Structure

The solution in the reaction zone, taking λ as the independent variable, is obtained integrating Eqs. (1) from 0 to a generic location x, with

$$x(\lambda) = \int_0^\lambda \frac{U d\bar{\lambda}}{r} \tag{6}$$

The complete solution is readily found. On the subsonic branch,

$$\frac{1}{\rho} = \frac{\gamma D^2 + \delta - \sqrt{\Delta}}{(\gamma+1)D^2}, \quad U = \frac{\gamma D^2 + \delta - \sqrt{\Delta}}{(\gamma+1)D}, \quad p = \frac{\gamma D^2 + \delta + \gamma\sqrt{\Delta}}{\gamma(\gamma+1)},$$
$$T = \frac{(\gamma D^2 + \delta)^2 + (\gamma-1)(\gamma D^2+\delta)\sqrt{\Delta} - \gamma\Delta}{\gamma(\gamma+1)^2 D^2}, \quad M^2 = \frac{\gamma D^2 + \delta - \sqrt{\Delta}}{\gamma D^2 + \delta + \gamma\sqrt{\Delta}} \tag{7}$$

in which

$$\Delta = (D^2 - \delta)^2 - (1-\delta)^2 D^2 \lambda \tag{8}$$

Values at the shock are readily found setting λ to zero.

If the discriminant reaches zero for a value $\lambda^* < 1$, i.e., for

$$\lambda^* = \frac{(D^2 - \delta)^2}{D^2(1-\delta)^2} \tag{9}$$

then the wave is underdriven. The stationary solution ends at a sonic point before the reaction is complete, and at this end point,

$$\frac{1}{\rho^*} = \frac{\gamma D^2 + \delta}{(\gamma+1)D^2}, \quad U^* = \frac{\gamma D^2 + \delta}{(\gamma+1)D}, \quad p^* = \frac{\gamma D^2 + \delta}{\gamma(\gamma+1)}, \quad T^* = \frac{(\gamma D^2 + \delta)^2}{\gamma(\gamma+1)^2 D^2} \tag{10}$$

And $M^{*2} = 1$ thus the double root is sonic.

On the other hand, for overdriven waves, when $\lambda = 1$, combustion is complete and then, for the CJ case, $r = 0$ implies $\lambda_{cj} = 1$. Thus the conditions at the end of the reaction zone are by setting Δ equal to:

$$\Delta^* = (D^2 + \delta^2)(D^2 - 1) \tag{11}$$

4 Scenarios and boundaries

The detailed structure yields the evolution in the reaction zone, taking λ as the independent parameter. But using the local Mach number as the independent variable

$$\frac{dT}{d\lambda} = \frac{q(\gamma-1)}{\gamma}\frac{1-\gamma M^2}{1-M^2}, \frac{d(u^2)}{d\lambda} = q(\gamma-1)\frac{2M^2}{1-M^2}, \frac{d(M^2)}{d\lambda} = \frac{q(\gamma-1)}{\gamma T}\frac{M^2(1+\gamma M^2)}{1-M^2} \tag{12}$$

As in any one-dimensional flow with heat addition, temperature peaks when the local Mach number reaches $1/\sqrt{\gamma}$. Below that threshold, the Mach number increases with λ, and temperature increases along the particle path. But beyond that value, temperature decreases until either the sonic point or the point where $\lambda = 1$ is reached. And for sufficiently large δ still < 1, hence sufficiently small heat release, the Mach number M_s immediately behind the shock is above that threshold, for moderate overdrives. Since the CJ wave ends at a sonic point, its necessarily includes a region where the Mach number is above $1/\sqrt{\gamma}$.

If the activation energy is relatively high, even small temperature changes strongly affect the reaction times and lengths and an increasing temperature produces an induction zone much longer than the region of intense reaction. But if the temperature decreases, the final temperature results in time and length scales much longer than the earlier part of the process, hence no induction zone.

Four different regions can be identified in the (D^2, δ) plane, corresponding to different reaction zone structures:

(1) Temperature increases monotonically until the reaction is complete and the Mach number at the point of complete reaction is below $1/\sqrt{\gamma}$. CJ waves do not fit within this description since the Mach number reaches 1.

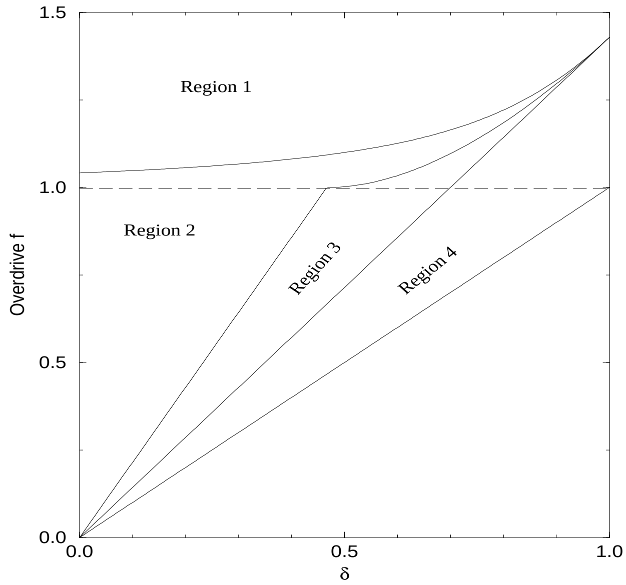

Figure 1: Scenarios and boundaries [Overdrive $f = (D/D_{CJ})^2$]

(2) The temperature increases from its initial value T_s, reaches a maximum and then decreases, but the final value $T^* > T_s$. Strong CJ waves belong in this scenario.

(3) The temperature increases from its initial value T_s, reaches a maximum and then decreases to a final value $T^* < T_s$. The initial increase then results in an induction zone followed by a zone of intense reaction, but the time scale associated with the sonic point is now larger than the induction time, so that the induction length is now of smaller magnitude than the overall reaction length, now controlled by the final temperature;

(4) If the temperature behind the shock is large enough, the temperature is monotonically decreasing throughout the reaction zone, and so is the reaction rate. The zone of intense reaction, much thinner than the completion zone that follows, is then situated immediately behind the shock. For $D^2 = 1$, $\lambda^* = 1$, while for $D^2 = \delta$, $\lambda^* = 0$.

For given γ, the two independent parameters are the overdrive D^2, and either δ or q. The crucial boundaries in the (D^2, δ) plane, shown on Fig. 1, are:

The locus $dT/d\lambda = 0$ at $\lambda = 1$ separates Region 1 from Region 2. From Eq. (7d), for $\delta = 0$, this curve starts at a value of D^2 slightly above 1, given by

$$D_0^2 = \frac{4}{(3-\gamma)(\gamma+1)} \tag{13}$$

at $\delta = 0$ and intersects the previous curve at $\delta = 1$. This line is entirely contained in the overdriven domain; indeed, at a sonic point, from Eq. (7d), $dT/d\lambda \to \infty$.

The curve $dT/d\lambda = 0$ at $\lambda = 0$ separates Regions 3 and 4. Again, from Eq. (7d), this locus is a straight line on the D^2 vs. δ plot:

$$D^2 = \frac{\delta(3\gamma - 1)}{\gamma(3-\gamma)} \tag{14}$$

For D^2 above that value, the temperature is increasing with λ, behind the shock, while it is decreasing for lower values. For γ above 3, the temperature gradient at the shock becomes negative. This is consistent with the inert Rankine-Hugoniot relations, which show that the minimum value of the shock Mach number is the value for an infinite incident Mach number,

$$M_s^2 \to \frac{\gamma - 1}{2\gamma} \tag{15}$$

which is above $1/\gamma$ for $\gamma > 3$, so that then $dT/d\lambda < 0$ at the shock.

Finally, the locus $T_s = T^*$ separates Regions 2 and 3. From the solution above, it is found that, comparing the value at the shock with the value at the sonic point.

$$D^2 = \frac{\delta(2\gamma - 1)}{\gamma(2 - \gamma)} \tag{16}$$

But this solution is only valid for D^2 up to 1, since for higher values, there no longer is a sonic point and instead, T^* corresponds to the point where $\lambda = 1$. Then, equality between these temperatures yields

$$[(\gamma - 2)\gamma D^2 + \delta(2\gamma - 1)]^2 = \gamma^2(D^2 - \delta^2)(D^2 - 1) \tag{17}$$

This equation for D^2 has no roots in the interval $\delta^2 < D^2 < 1$. Also, the double root $D = 1$ is obtained for $\delta = (2 - \gamma)\gamma/(2\gamma - 1)$. Indeed, for $D^2 = 1$, the r.h.s. is zero, yielding this double root in δ for the l.h.s., thus intersecting the curve $T_s = T^*$, as it should, at $D^2 = 1$. Furthermore, the branch on the left of that intersection is spurious.

Fig. 1, for $\gamma = 1.4$, is typical of the range $1 < \gamma < 2$. In region 1, above the locus where $dT/d\lambda = 0$ at $\lambda = 1$, temperature increases monotonically in the reaction zone. In region 2, below that curve but above the curves $T_s = T^*$ (for $D^2 > 1$) or $T_s = T^*$ (for $D^2 < 1$), temperature initially increases, reaches a maximum (when the local Mach number equals $1/\sqrt{\gamma}$, and then decreases, reaching a final value still above T_s. In region 3, below these lines but still above the locus where $dT/d\lambda = 0$ at $\lambda = 0$, i.e., at the shock, the temperature increases to a maximum and decreses, reching a final value lower than the shock value. Finally, below that latter curve, in Region 4, temperature is a monotonically decreasing function of λ and x. For $\gamma < 2$, all three last scenarios affect the CJ regime $D^2 = 1$.

However, for increasing values of γ, the point on $D^2 = 1$ where $T_s = T^* = T^*$ moves left, and for $\gamma = 2$, it reaches the value $\delta = 0$ so that the part of Region 2 below $D^2 = 1$ disappears. Finally, for $\gamma > 3$, the point on $\delta = 1$ where $dT/d\lambda = 0$ at the shock reaches the limit $D^2 \to \infty$. Region 4 now occupies the entire parameter space and T is now unconditionally monotonically decreasing.

Finally, details will be shown for the various scenarios, in the high activation energy limit. These results will be applied to quasi-steady oscillations of near-CJ detonation.

References

[1] Kassoy, D.R. & Clarke, J.F., The structure of a high-speed deflagration with a finite origin, *J. Fluid Mech.*, 1985, V. 150, pp. 253 - 280.