## Ignition between a Shock and a Contact Surface with Arbitrary Reflection Coefficient

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The generic problem of ignition between a shock and a material surface with arbitrary acoustic reflection coefficient encompasses many relevant situations. This includes obviously the piston-initiated ignition problem, studied by Blythe and Crighton (1989) assuming high activation energy and a specific heat ratio  $\gamma$  close to unity. But this generic problem describes also other interesting scenarios such as hot spot formation between a shock and a contact surface after shock collision (Short and Dold 1996), reignition following failure in propagation of galloping detonations (Bauwens et al. 1998), and, last but not least, hot spot formation ahead of a flame, which is relevant to DDT. The results show existence of two families of ignition mechanisms, with a weak mechanism when the temperature is higher in the interval between shock and contact surface, and a stronger mechanism when, for instance ahead of a flame, the temperature behind the contact surface is higher.

At a piston face, the pressure reflection coefficient  $F_C$  equals 1. At a contact surface across which the temperature ratio equals  $\theta$ ,  $F_C$  is given by

$$F_{\rm C} = -\frac{\sqrt{\theta - 1}}{\sqrt{\theta} + 1} \tag{1}$$

Thus, the piston face is effectively equivalent to  $\theta = 0$ . For a contact surface resulting from shock collision, studied numerically by Short and Dold (1996), in the Newtonian limit the temperature ratio  $\theta$  across the contact surface approaches 1, so that the reflection coefficient  $F_C$  approaches 0. Finally,  $F_C$  is negative in the reignition problem and also in the case of hot spot formation between a flame and its precursor shock, when  $\theta > 1$ . Effectively, all these scenarios are encompassed in a study generalizing Blythe and Crighton's (1989) for arbitrary reflection coefficients at the material surface, or equivalently, considering an arbitrary  $\theta$ , and their results will be recovered when setting  $\theta = 0$ .

Although in the current study, the problem is formulated starting ab-initio with a two-parameter expansion in the inverse dimensionless activation energy  $\beta$  and in  $\gamma - 1$ , with  $\beta \ll \gamma - 1 \ll 1$ , the solution effectively proceeds as in Blythe and Crighton (1989). The frame of reference x is attached to the contact surface, with the shock moving away in the direction of negative x; x and t are the outer space and time coordinates based upon the slow chemical time. To order  $1/\beta$ , the problem is described by the Clarke equations. Furthermore, in the Newtonian limit, the energy equation is decoupled from momentum and continuity, because the contribution due to flow-induced pressure fluctuations to the energy balance is then negligible compared with the internal energy. This results in ignition occurring at the contact surface x = 0 for  $t \rightarrow 1/q$ , with q representing the dimensionless heat release parameter.

Following the approach of Blythe and Crighton (1989), the inner hot spot solution, near the contact surface, is obtained using a local time  $\tau = -(\gamma - 1) \log (1 - qt)$  and a centered space variable  $\chi = qx/(1 - qt)$ . Since x is negative in the solution domain, so is  $\chi$ . The local order  $\beta/(\gamma - 1)$  solution is spatially uniform with temperature equal to  $\tau$ . The order  $\beta$  temperature T<sup>\*</sup> is given by

$$T^* = -\log \left[ 1 + F(\tau) \chi \right] + 2\tau T_{11}$$
(2)

in which  $T_{11}$  is the (constant) temperature correction of order  $\gamma - 1$  downstream of the shock, that appears because of the formulation based upon the two-parameter expansion. The integration constant  $F(\tau)$  is determined by the

requirement that the solution to next order in  $\gamma - 1$  must be regular, with bounded derivative at the contact surface,  $\chi = 0$ . This results in Eq. (3), in which  $\theta$  now appears:

$$\frac{\mathrm{d}F}{\mathrm{d}\tau} = \frac{1}{\sqrt{\theta} + 1} \frac{F - \sqrt{\theta}}{F - 1},\tag{3}$$

with an initial condition that results from matching the inner result at  $\tau = 0$ , given by Eq (4), in which M is the shock Mach number:

$$f(0) = -M \tag{4}$$

As expected, for  $\theta = 0$ , the same result obtained by Blythe and Crighton (1989) is recovered; in that case, F remains negative at all times and  $F \to 0$  for  $t \to \infty$ . As a result, since  $\chi \le 0$ ,  $-\log [1 + F(\tau)\chi]$  remains finite, negative, and approaches zero at all values of  $\chi$  as  $\tau \to \infty$ , when the order  $\beta/(\gamma - 1)$  solution finally blows up at the piston face.

Returning to the general case, Eq. (3) is readily solved implicitly, yielding:

$$\tau = (1 + \sqrt{\theta})(F + M) - (1 - \theta)\log\frac{\sqrt{\theta} - F}{\sqrt{\theta} + M}$$
(5)



<u>Fig. 1</u>:  $F(\tau)$  vs.  $\tau$ , from top to bottom, for  $\theta = 0, 0.2, 0.4, 0.8, 1, 1.2, 2.0$  and 10.0

<u>Fig. 2</u>: Motion of the front in the  $\chi_0 - \tau$  plane, (if  $\sqrt{\theta} > \sqrt{1+q} - \sqrt{q}$ , this solution is only valid for  $\chi_0 < \chi_{CJ}$ )

This solution is shown on Fig. 1 for various values of  $\theta$ . The behavior of the solution is markedly different depending upon whether  $\theta$  is less or more than 1, as shown on Fig. 1. In all cases, the solution starts at the initial condition F(0) = -M. The solution increases, reaching a zero value and becoming positive at the time  $\tau^* = \tau(0)$ , which depends upon M and  $\theta$ , and is given by Eq. (6). For  $0 < \theta < 1$ , a solution exists at all times  $0 \le \tau < \infty$ , with  $F(\tau) \rightarrow \sqrt{\theta}$  as  $\tau \rightarrow \infty$ . However, if  $\theta > 1$ , then Eq. (3) admits a solution only for  $0 \le \tau < \tau^{**}$ , with  $\tau^{**} = \tau(1) > \tau^*$ , with  $F \rightarrow 1$  and  $\frac{dF}{d\tau} \rightarrow \infty$ , as  $\tau \rightarrow \tau^{**}$ , at which point our magnitude assumptions are no longer valid since  $\frac{dF}{d\tau} >> F/\tau$  in the neighborhood of  $\tau$ . Equation (7) gives  $\tau^{**}$  as a function of M and  $\theta$ .

$$\tau^* = (1 + \sqrt{\theta}) M - (1 - \theta) \log \frac{\sqrt{\theta}}{\sqrt{\theta} + M}$$
(6)

$$\tau^{**} = (1 + \sqrt{\theta})(1 + M) - (1 - \theta) \log \frac{\sqrt{\theta} - 1}{\sqrt{\theta} + M}$$
(7)

In all cases, the solution remains similar to Blythe and Crighton's (1989) until  $\tau$  reaches  $\tau^*$  corresponding to F = 0 at which time the temperature correction  $-\log [1 + F(\tau)\chi]$  develops a singularity for  $\chi \to -\infty$ . The singularity subsequently moves, initially at infinite speed, in the direction toward the contact surface located at the origin  $\chi = 0$ . Physically, this describes a constant volume ignition occurring at  $\chi \to -\infty$ . In the original frame of reference, ignition occurs at t = t\* given by:

$$t^* = \frac{1}{q} \left( 1 - \exp \frac{-(1 + \sqrt{\theta})M + (1 - \theta)\log \frac{\sqrt{\theta}}{\sqrt{\theta} + M}}{\gamma - 1} \right)$$
(8)

As it moves, for  $\tau > \tau^*$ , the singularity is instantaneously located at  $\chi_0 = -1/F(\tau)$ , shown on Fig. 2. Thus, starting from  $\chi_0 = -\infty$  at  $\tau^*$ , the singularity moves toward the contact surface located at the origin, at a speed that decreases from its initial infinite value. Obviously, the solution characterized by Eq. (2) is now only valid in the region ahead of the front, i.e. for  $\chi > \chi_0 = -1/F(\tau)$ . Furthermore, as it decreases, the speed of the front as given (up to a correction of order  $\gamma - 1$ ) by  $-\chi_0 = 1/F(\tau)$  will either reach the speed of sound 1 at  $\tau^{**}$  if  $\theta > 1$  or, if  $\theta < 1$ , the value  $1/\sqrt{\theta}$  as  $\tau \to \infty$ . But in the former case, and, if  $\sqrt{\theta} > \sqrt{1 + q} - \sqrt{q} < 1$ , in the latter case also, these final values are below the Chapman-Jouguet speed  $-\chi_{CJ} = 1/[\sqrt{1 + q} - \sqrt{q}]$ , which the front would actually reach at the finite time  $\tau = \tau_{CJ} < \tau^{**}$ .

In order to be valid, the solution found, with a front located at  $\chi_0$ , requires a consistent solution for the reaction zone, which is situated in the region where  $\chi < \chi_0$ . The structure of the reaction zone moving supersonically toward the contact surface can be determined using a nonlinear scaling similar to Kassoy and Clarke's (1985):

$$\chi = \chi_0(\tau) - H(T) \exp\{\frac{1}{\beta}T - [1 + (\gamma - 1)T_{11}]/\beta + \tau/(\gamma - 1)\}$$
(9)

The key difference with Kassoy and Clarke (1985) is that here,  $\tau$  appears as a parameter, and that the location  $\chi_0(\tau) = -1/F(\tau)$  is no longer a constant. In effect, the structure of the reaction zone is quasi-steady, and a solution is found to exist only for propagation speeds at least equal to the Chapman-Jouguet value. Furthermore, at the CJ speed, a discontinuity appears in the solution at the back end of the reaction zone where T = 1 + q, which it crosses, indicating that the initial shockless supersonic weak detonation evolves into a strong CJ wave. Thus, if  $\sqrt{\theta} < \sqrt{1 + q} - \sqrt{q}$ , this solution describes a weak shockless detonation wave which slows down from an initially infinite speed at  $\tau = \tau^*$ , and reaches the contact surface at a speed approaching  $\sqrt{\theta}$  which remains larger than the CJ speed  $-\chi_{CJ}$  as  $\tau \rightarrow \infty$ . But if  $\sqrt{\theta} > \sqrt{1 + q} - \sqrt{q} < 1$ , then, as it decreases, the speed of the weak detonation reaches the Chapman-Jouguet value  $-\chi_{CJ} = 1/[\sqrt{1 + q} - \sqrt{q}]$  before hitting the contact surface, at a finite  $\tau = \tau_{CJ}$ . The speed of the front cannot drop below the CJ value, and instead a shock appears and the wave proceeds then at the constant CJ speed, as a strong detonation wave.

But if  $\theta > 1$ , the solution given by Eq. (2) in the region between the CJ wave and the contact surface only exists while  $\tau < \tau^{**}$ . As  $\tau \to \tau^{**}$ ,  $F \to 1$  and  $\frac{dF}{d\tau} \to \infty$ . A faster time scale is thus required, corresponding to very fast chemistry in the zone between the CJ wave and the contact surface, ahead of the CJ wave, and since at that time scale, the flow is effectively frozen, a homogeneous thermal explosion occurs at t\*\* given by Eq. (10) for  $\chi_{CJ} < \chi < 0$ , i.e., in the interval x\*\* < x < 0, with x\*\* given by Eq. (11).

$$t^{**} = \frac{1}{q} \left( 1 - \exp \frac{-(1 + \sqrt{\theta})(1 + M) + (1 - \theta) \log \frac{\sqrt{\theta} - 1}{\sqrt{\theta} + M}}{\gamma - 1} \right)$$
(10)

$$x^{**} = -\frac{1}{q} \frac{1}{\sqrt{1+q} - \sqrt{q}} \exp \frac{-(1+\sqrt{\theta})(1+M) + (1-\theta)\log \frac{\sqrt{\theta} - 1}{\sqrt{\theta} + M}}{\gamma - 1}$$
(11)

This describes a much stronger and qualitatively different ignition mechanism for  $\theta > 1$ , when the temperature jump across the contact surface corresponds to the case of a flame or reignition. In particular, the rate of energy release is then much larger.

Finally, in the Newtonian limit, ignition following collision between shocks (Short and Dold 1996) is described by  $\theta = 1$ . In that case, the requirements that resulted in Eq. (3) are somewhat different:

$$\frac{\mathrm{dF}}{\mathrm{d\tau}} = \frac{1}{\sqrt{\theta} + 1} \qquad \text{or } \mathbf{F} = 1 \tag{12a,b}$$

This is consistent with the limit behavior of the solutions above shown on Fig. 1, both for  $\theta < 1$  and  $\theta > 1$ . When  $\theta$  approaches 1 from below, the solution approaches the linear behavior of Eq. (12a) until F becomes close to 1, at which point it becomes constant. When  $\theta$  is larger than 1, the solution ends at F = 1.

In summary, depending upon the value of the temperature ratio  $\theta$  across the contact surface, the analysis yields various scenarios, as follows:

- Only for θ = 0, i.e., the piston-driven case of Blythe and Crighton (1989), does the hot spot appear at the piston face for t = 1/q (τ = τ\* → ∞). But in all other cases (θ > 0), τ\* is finite and ignition occurs somewhat earlier, at t = t\* and χ → -∞, i. e., at a distance from the piston face that is small compared with the distance between shock and contact surface;
- After ignition, for 0 < θ < [√1 + q √q]<sup>2</sup> < 1, a weak detonation wave moves supersonically toward the contact surface, slowing down until its speed approaches a value 1/√θ still faster than the CJ speed as it approaches the contact surface as t → 1/q (i.e. τ → ∞);</li>
- For  $[\sqrt{1+q} \sqrt{q}]^2 < \theta < 1$ , the supersonic weak detonation moving toward the contact surface slows down, reaches the CJ value at which point a shock forms and a strong CJ wave proceeds toward the contact surface, which it reaches as  $t \to 1/q$  ( $\tau \to \infty$ );
- For θ > 1, the weak detonation moves supersonically toward the contact surface, slows down, reaching the CJ speed and continuing as a strong CJ wave until the unburnt mixture that separates it from the contact surface explodes at constant volume at t = t\*\*, somewhat before t reaches 1/q, i.e., before the CJ wave reaches the contact surface.

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