Condition for Explosion by Impact of a Planar, Self-sustained Detonation

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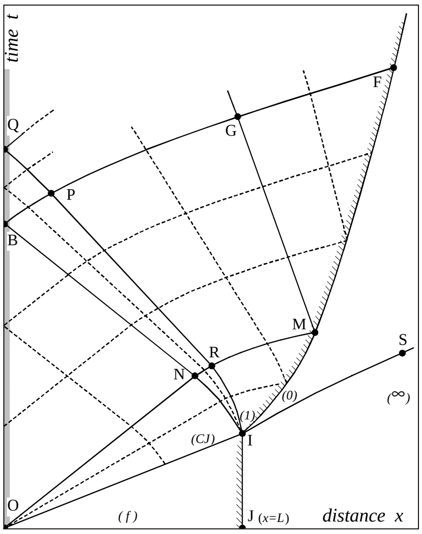
Abstract

We study the induction of an explosion in a homogeneous reactive substance solicited by the impact of a planar, self-sustained detonation. We obtain the explosion time and a condition for ignition as a constraint on the length of the detonating donor charge.

1 Introduction

1.1. The shock-to detonation process (SDT) in homogeneous explosives has been identified in such impact experiments as those by Campbell et al. [1] in liquid nitromethane, or by Meyer and Oppenheim [2] in gaseous H_2-O_2 mixtures. In these experiments, a shock-induced thermal explosion first occurs in the close vicinity of the impactor, a so-called superdetonation then builds very rapidly in the shock-compressed material, and, after the superdetonation catches up with the shock, the relaxation towards the normal self-sustained detonation regime takes place. The understanding of the SDT process is an important safety issue. In previous publications [3],[4], we have presented an approach for studying the explosion stage of the SDT process. This approach can be applied to various dynamical conditions for generating the shock. This model identifies a criterion for explosion that prescribes a bounded induction time. We have demonstrated that this criterion expresses the predominance of the effective heat-production rate over the volumetric-expansion loss rate at the beginning of the chemical transformation. As a matter of fact, the necessity of this predominance had already been postulated by Dremin for a particular case of chemical decomposition law e.g., [5]. The induction properties and the explosion criterion are determined by the initial values (i.e., at the shock) of the variables and of their material derivatives. The determinations of the former and the latter represent particular Riemann and Cauchy problems, respectively. The intermediates to the obtention of their solutions are the determinations of the shock velocity and acceleration, which depend on the considered problem. Thus, for a shock with prescribed dynamics (i.e., velocity, acceleration and curvature), we have expressed the criterion as a constraint on the normal shock velocity D_n, the normal shock acceleration $\delta D_n/\delta t$, and the total shock curvature C, and, in the case where the shock is generated by the impact of a piston with prescribed speed, acceleration and curvature, we have determined, first, the velocity and the acceleration of the shock at the time of impact and, then, expressed the criterion as a constraint on the piston speed, acceleration and total curvature [3], [4]. We have validated these results, in particular the explosion criterion, by means of direct numerical simulations of impacts of uniformly decelerating planar pistons.

1.2. We summarize here one part of a study devoted to the one-dimensional planar modeling of the configurations associated with shocks generated by the expansion of the products of constant-velocity detonations. The present paper addresses the particular case of the self-sustained (CJ) detonation [6]. The detonation is initiated at time $t = 0$, at the fixed end $x = 0$ of a charge with length $x = L$, hereafter referred to as the donor. The mixture to be ignited, hereafter referred to as the target, is adjacent to the donor. We assume that the transient phenomena induced by the build-up of the self-sustained detonation or by the thickness of the detonation chemical-reaction zone have negligible characteristic times compared to the run time of the detonation in the donor, or to the induction time in the target. We also assume planar processes, and compressible perfect fluids in adiabatic evolution, initially homogeneous and at rest. In such conditions, the donor detonation can be modeled as a totally reactive discontinuity followed by a self-similar flow of its products [7],[8],[9]. In the configuration considered in the present analysis, the impact of the donor detonation at time $t = t_I$ induces a shock in the target mixture, and an expansion that goes up the self-similar flow of the donor detonation products (**figure 1**). The column of products thus acts on the shocked medium as a compressible piston, in a way similar to the case studied in [10]. The dynamics of the donor products-shocked target interface, in particular its acceleration, depends on the length of the donor charge, on the initial conditions in the donor and target charges, and on the physical properties of the two explosives. Our objective is to determine the minimal length of the donor charge, L_{cr}, that induces sufficiently large an interface acceleration for generating the explosion in the target (§3). The notations are the same as in [3],[4] and [6] ; most are introduced in the text or detailed in the figures and at the end of this abstract.



OI	: CJ detonation (discontinuity)
OIN	: Taylor-Zel'dovich (TZ) self-similar flow
ONB	: constant-state domain
ONM	: tail of the action of the TZ flow
I	: impact point
IS	: shock generated in the target
IMF	: interface between the donor and the target
INB	: head of the expansion generated at the impact
BF	: head of the expansion after reflection

Figure 1. Space (x)-Time (t) diagram

2 Initial Dynamics of the Shock and of the Interface

Our analysis requires to first determining the initial speed, u, and acceleration, du/dt, of the material interface at point I, immediately after impact (**figure 1**). To summarize, the determinations of the velocity D of the shock generated in the target, of the speed u, and of the thermodynamical states at the impact point I are based on the homo-entropy of the flow in the donor products and on the requirement that the pressure p and the material speed u are continuous across the material interface IM. This classical calculation, as well as the properties of the CJ state and of the following self-similar flow of the CJ detonation products, are recalled in [6]-§2.1 and §2.2 (solution to the Riemann problem). The determinations of the acceleration $\delta D/\delta t$ of the shock and of the interface du/dt immediately after impact are based upon a perturbation analysis about the impact point I. Its main ingredients are (i) the self-similarity of the donor flow before impact, (ii) the derivation of a compatibility relationship between the material derivatives of the pressure and of the material speed in the donor products in the expanded state (1), and (iii) the requirement that, because of the continuity in u and p across the material interface IM, these derivatives are equal to the material derivatives of u and p in the target, respectively. This calculation is detailed in [4] and [6]-§2.3 and §2.4 (solution to the Cauchy problem). The initial (i.e., at point I) acceleration of the interface is thus obtained as a function of the donor-charge length $L = D_{CJ}\, t_I$:

$$\left(\frac{du}{dt}\right)_1 = \left(\frac{du}{dt}\right)_{0I} = -D_I \frac{2mM_0 \frac{v_0}{v_\infty}\sigma_0 w_0 + \left(1+2M_0^2+\Omega\right)\frac{D_{CJ}}{D_I}\Psi_{CJ1}/t_I}{\left(1+2M_0^2+\Omega\right)+mM_0\left(3+\Omega\right)}, \quad m = \frac{(c/v)_0}{(c/v)_1}, \tag{1}$$

The quantity m is the ratio of the acoustic impedances (c/v) of the shocked target (0) and of the expanded donor products (1), and the quantity Ψ_{CJ1} is a function of the states CJ and 1 of the donor products that is determined from the solution to the Riemann problem, as any other state function involved in this work.

3 Condition for Explosion and Discussion

3.1. We have shown in [3] and [4] that the induction time τ of the adiabatic explosion can be defined as the reciprocal of the initial rate of change of the reaction rate w along the material trajectories, e.g. (2a), if the latter rate is a sufficiently convex state function. Such is the case for most of homogeneous explosives, indeed well represented by the Arrhenius law (2b), which, at the dominant order, leads to the induction time (2c). As a matter of fact, the ratio T_a/T_0 of the activation temperature to the shock temperature is usually a large number, typically $O(10)$. If the shock is generated by a planar piston with prescribed speed u and acceleration du/dt, the induction time (2c) can be re-written as (2df) [3], [4]. The groupings $\tau_{\pi o}$ and τ_p (2gh) can be interpreted, respectively, as the induction times of the transformation induced by a shock generated by a planar constant-speed piston and of the isobaric transformation issuing from the same thermodynamical state (i.e., 0):

$$\tau = 1/\left(\frac{1}{w}\frac{dw}{dt}\right)_0, \quad w = t_c^{-1}F(1-y)^a \exp\left(\frac{-T_a}{T}\right) \quad \Rightarrow \quad \tau = \frac{T_0}{T_a}/\left(\frac{1}{T}\frac{dT}{dt}\right)_0 + ..., \qquad \text{(2ac)}$$

$$\frac{\tau_\pi}{\tau_{\pi o}} = \left(1 - \frac{\Delta_\pi}{\Delta_{\pi\,\inf}}\right)^{-1}, \quad \Delta_\pi = \frac{\tau_{\pi o}}{u_0}\left(\frac{du}{dt}\right)_0, \quad \Delta_{\pi\,\inf} = -\frac{T_0}{T_a}\frac{1+2M_0^2+\Omega}{g_0 M_0^2(\frac{v_\infty}{v_0}-1)(3+\Omega)}, \qquad \text{(2df)}$$

$$\frac{\tau_{\pi o}}{\tau_p} = \frac{1+2M_0^2+\Omega}{1+2\theta_0 M_0^2+\Omega}, \quad \tau_p = \frac{T_0}{T_a}\left(\frac{C_pT}{Q_{pT}}\right)_0 \frac{t_c}{F_0}\exp\left(\frac{T_a}{T_0}\right) \equiv \frac{T_0}{T_a}\left(\frac{\theta-1}{g\sigma w}\right)_0. \qquad \text{(2gh)}$$

3.2. The induction time for the transformation induced by the shock generated by the impact of a CJ detonation issuing from a rigid wall is thus obtained by substituting the material speed and the acceleration of the interface (1) at point I (i.e., the associated shock state, cf. [6]-§2.2) for the arbitrary speed and acceleration in (2e). Some arrangements thus lead to the expression (3a). The ignition can occur if and only if the induction time τ_π is bounded, so if $\tau_\pi < \infty$ or $\Delta_\pi > \Delta_{\pi\,\inf}$, cf. (2df), or $L > L_{\min}$, cf. (3a). The minimal charge length is thus given by the grouping $L_{\min}$ (3b):

$$\frac{\tau_\pi}{\tau_{\inf}} = \left(1 - \frac{L_{\min}}{L}\right)^{-1}, \quad L_{\min} = \lambda\,\ell_{\inf}, \quad \ell_{\inf} = (D_I - u_0)\,\tau_{\inf}, \quad L = D_{CJ}\,t_I \qquad \text{(3ad)}$$

$$\frac{\tau_{\inf}}{\tau_p} = \frac{(1+2M_0^2+\Omega) + mM_0(3+\Omega)}{(1+2\theta_0 M_0^2+\Omega) + mM_0(3+\Omega)}, \quad \lambda = \frac{T_a}{T_0}\frac{g_0(3+\Omega)(D_{CJ}/c_0)^2\,\Psi_{CJ1}}{(1+2M_0^2+\Omega)+mM_0(3+\Omega)}. \qquad \text{(3ef)}$$

A small run of the donor detonation $\ell(t) = D_{CJ}\,t$, in particular a small donor length $L = \ell(t_I) = D_{CJ}\,t_I$, induces large derivatives behind the detonation front, thus, for example, stiffer profiles. Because of the self-similarity of the flow in the OIN domain of the donor-detonation products (**figure 1**), any derivative of this flow is indeed inversely proportional to the time, thus to the detonation run $\ell(t)$ (e.g., $\partial u/\partial t = -u'(\xi)\,\xi/t, \partial u/\partial x = u'(\xi)/\ell$, with $\xi = x/D_{CJ}t$ the similarity variable, cf. [6]-§2.1), as well as immediately after impact (e.g., (1)). Thus, the shorter the donor length, the larger the interface deceleration, cf. (1), and, consequently, the longer the explosion time. Conversely, a long run of the donor detonation induces small derivatives, so that in the limit of an infinite run, the influence of the donor-charge length on the derivatives behind the shock generated by the impact, in particular on the explosion time, becomes negligible compared to that of the chemical kinetics. This implies that, in the limits of infinite t_I (or L), the above expressions become identical to the planar restrictions of the expressions obtained in our study of cylindrical and spherical shock tubes presented in [10]. For instance, $\tau_{\inf}$ (3e) is identical to τ_{CP0} [10]-(4d).

3.3. We have specialized the above results to the case of donor and target explosives each modeled as an ideal mixture of two ideal gases with distinct physical properties, the reactants and the combustion products [4]. The results presented in **figure 2** are relative to the simplified situation where the donor and the target have constant and identical physical properties, except for theirs heats of reaction Q_f and Q_∞. In the chosen range of initial-pressure ratio p_f/p_∞, the time $\tau_{\inf}$ (3e) is sligthly smaller than the isobaric time τ_p (because here $\theta = \gamma = 1.25$ is closed to 1, cf. (3e)), and the Mach number of the shock transmitted in the target varies by 30% (cf. [6]-**figure 2a**). The normalized minimal length λ (3f) varies by more than 50% with the initial-pressure ratio p_f/p_∞ and by about 30% with that of the heat of reaction Q_f/Q_∞ (**figure 2a**). From a quantitative standpoint, by setting $t_c = 10^{-10}$ s and

$m_{mol.f,\infty} = 30$ g.mol^{-1}, we find, with $T_a/T_* = 67.57$ and $\gamma_{f,\infty,b,z} = 1.25$, that the minimal length $L_{\min}$ (3b) decreases from 15.8 m to 9.6 mm if $Q_{f*}/Q_{\infty*} = 5/4$, and from 1.9 m to 2.3 mm if $Q_{f*}/Q_{\infty*} = 3/2$, when the initial-pressure ratio increases from 1 to 3. Insofar as the other control parameters have lesser influence, our analysis thus generates realistic orders of magnitude and also reproduces the experimental trends according to which ignition is favored by a donor explosive that has high initial pressure p_f and large heat of reaction Q_f.

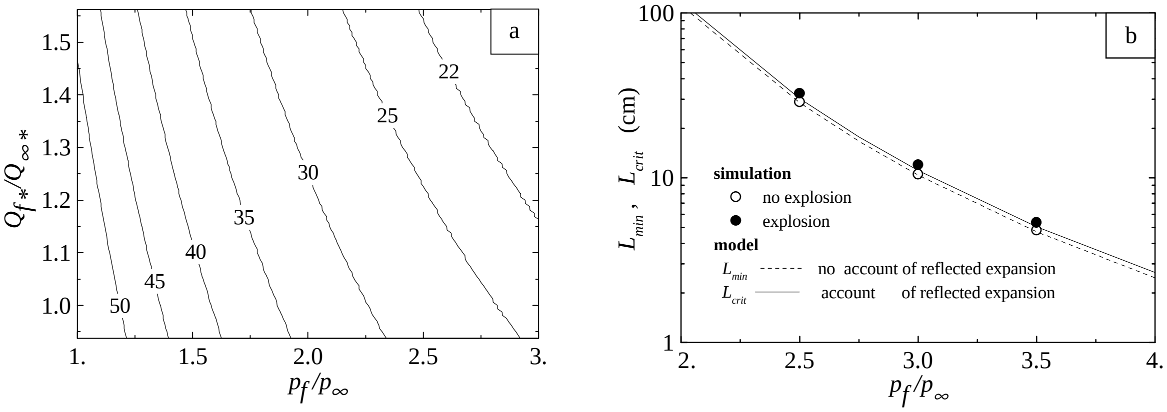


Figure 2. -a. Level lines of the normalized minimal length of the donor charge λ (8f) as function of the ratios of the initial pressures and of the heats of reaction of the donor and target explosives ($\gamma_{f,\infty,b,z} = 1.25, Q_{\infty*}/RT_* = 40, T_a/T_* = 67.57, T_f = T_\infty = T_*$). **-b.** Minimal and critical lengths $L_{\min}$ (3b) and L_{crit} (cf. §3.4) as functions of the ratio of the initial pressure in the donor and in the target ($\gamma_{f,\infty,b,z} = 1.25, Q_{\infty*}/RT_* = 48.43, Q_{f*}/Q_{\infty*} = 1, T_a/T_* = 67.57, T_f = T_\infty = T_* = 298$ K$, t_c = 10^{-10}$ s and $m_{mol.f,\infty} = 30$ g.mol^{-1}, $p_\infty = 1$ bar).

3.4. We emphasize that, depending on which constraint is prescribed to the magnitude of the induction time τ_π (3a), various critical lengths for the donor-charge can be obtained. In our opinion, the most significant constraint is that τ_π should be smaller than the time interval $t_F - t_I \equiv t_{IF}$ (**figure 1**). This interval separates the time of departure of the head IB of the expansion fan from the impact point I, and the time t_F when, after having been reflected at point B on the $x = 0$ rigid wall, it reaches the interface at point F. Beyond time t_F, the expansion induces an additional deceleration of the interface that prevents explosion. The calculation of the time interval t_{IF} does not offer any particular difficulty but is too long to be presented here. To summarize, it is based on classical properties of homo-entropic flows [7] and on some compatibility requirements accounting for the change in the interface deceleration at point M, with respect to its value (1) at point I. As a matter of fact, point M is the limit beyond which the dynamics of the interface is no longer influenced only by the self-similar flow behind the CJ detonation front, and the conditions ahead of the interface, but, also, by the conditions at the rigid wall. This calculation is a local analysis about point M, and, in some aspects, presents some similarities with the determinations of the solutions to the Riemann and Cauchy problems at point I. The constraint $\tau_\pi \leqslant t_{IM}$ thus yields a minimal (critical) donor-charge length L_{crit} that turns out to be only slightly larger than the minimal length $L_{\min}$ (3b) obtained by prescribing to the induction time τ_π to remain finite. This is shown in **figure 2b**, which also compares the minimal length $L_{\min}$ and the critical length L_{crit} (dashed and solid lines, respectively) to the critical length obtained from our direct numerical simulations (symbols) by means of a Lagrangian code. A good agreement is obtained, which however requires a good representation of the self-similar flow in the donor charge before impact and a sufficient accuracy in the target after impact, that is at least 2000 computational cells in between the shock and the interface at the time of explosion.

3.5. We have summarized one part of a study devoted to the ignition of homogeneous explosives by means of shocks generated by the impact of constant-velocity detonations. The present work addresses the case of the self-sustained (CJ) detonation originating from a rigid wall. Other configurations are CJ detonations originating from a free boundary or from constant-speed pistons, and overdriven detonations. The conditions that we have discussed here are necessary conditions for obtaining an explosion. They must not be mistaken with the conditions that lead to the formation of a detonation in the target explosive. The determination of the latter requires a different type of analysis that we are currently conducting. As for the explosion condition, the trends and the orders of magnitude obtained for the case of explosives modeled as ideal gases agree qualitatively with the experimental observations and quantitatively with our numerical simulations but additional work is necessary to confirm the predictive ability of our model.

References

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Nomenclature

− indices f and b : reactants and products of the donor; f also defines the initial state in the donor.
− indices ∞ and z : reactants and products of the target; ∞ also defines the initial state in the target.
− indices CJ and 1 : products of the donor immediately behind the detonation and after expansion at I.
− index 0 : state behind the shock generated in the target.
− indices p or π ($\pi 0$) : isobaric or variable (constant) piston-speed transformations.
− index $*$: thermodynamical reference , e.g., $p_* = 1$ bar, $T_* = 298$ K.
− $p, T, y; v$ and e : pressure, temperature, extent of chemical decomposition; specific volume and internal energy.
− $g = v/\left(\frac{\partial e}{\partial p}\right)_{vy}, c = \sqrt{v^2(p + (\frac{\partial e}{\partial v})_{py})/\left(\frac{\partial e}{\partial p}\right)_{vy}}, \sigma = \frac{-v}{c^2}\left(\frac{\partial e}{\partial y}\right)_{pv}/\left(\frac{\partial e}{\partial p}\right)_{vy}, Q_{pv} = -\left(\frac{\partial e}{\partial y}\right)_{vy}$: Gruneisen coefficient, frozen sound speed, thermicity coefficient, specific heat released at v and p.
− $C_v = \left(\frac{\partial e}{\partial T}\right)_{vy}, C_p = \left(\frac{\partial h}{\partial T}\right)_{py}$; $Q_{vT} = -\left(\frac{\partial e}{\partial y}\right)_{vT}, Q_{pT} = -\left(\frac{\partial h}{\partial y}\right)_{pT}$: heat capacities at constant v, at constant p, specific heats released at v and T, at p and T ($h = e + pv$ (specific enthalpy). With the dimensionless coefficients $\gamma = C_p/C_v$, $\omega = Q_{pT}/Q_{vT}$ and $\theta = \gamma/\omega$, one obtains the identities $Q_{pT}/C_pT = g\sigma/(\theta - 1)$ and $Q_{vT}/C_vT = g\sigma\theta/(\theta - 1)$.
− $x, t, u, d./dt = \partial./\partial t + u\ \partial./\partial x, ^{\pm} d./dt = \partial./\partial t + (u \pm c)\ \partial./\partial x$: distance, time, material speed and derivatives, acoustic derivatives (i.e., characteristics).
− $de/dt = -p\,dv/dt$, $de = Tds - pdv - Ady$: First Principle of Thermodynamics for adiabatic evolutions of perfect fluids, Gibbs' identity (s specific entropy , A chemical affinity).
− $D, \delta D/\delta t$: discontinuity velocity and acceleration.
− $M_{CJ} = D_{CJ}/c_f, M_\infty = D/c_\infty, M_0 = (D - u_0)/c_0, \Omega$: Mach numbers of the detonation, of the shock in the target and of the flow at this shock, ratio of the slopes of the Rayleigh-Michelson line and of the Hugoniot curve. We recall the identity $\Omega = (1 - g_0(\frac{v_\infty}{v_0} - 1)/2)/(M_0^{-2} - g_0(\frac{v_\infty}{v_0} - 1)/2)$.
− $F, t_c, a, T_a, r = R/m_{mol}$: arbitrary state function (less sensitive than the exponential in (7b)), intrinsic chemical time, reaction, effective activation temperature , ratio of the perfect-gas constant (8.3149 J mol^{-1}K^{-1}) and of the molar mass of the fluid.
− $Q_{f(\infty)} = h_{f(\infty)}\left(T_{f(\infty)}, p_{f(\infty)}\right) - h_{b(\infty)}\left(T_{f(\infty)}, p_{f(\infty)}\right)$: heat of reaction of the donor (of the target).
− For the ideal gas with a constant molar mass : $pv = rT$, $Q_{pv} = Q_{vT}$, $\omega = 1$, $\theta = \gamma =$ const., $g = \gamma - 1$, $\Omega = M_\infty^{-2}$. The strong shock limit corresponds to $\Omega = 0$.
− $w = dy/dt, \theta(\theta - 1)^{-1}\sigma w, v^{-1}dv/dt$: reaction rate , e.g., the Arrhenius law (2b), effective heat-production rate associated with (2b), volumetric-expansion rate, i.e., adiabatic-loss rate.