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Direct Initiation of Gaseous Detonations

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Abstract: A theoretical analysis of the direct initiation of gaseous detonations by an energy source has been published recently, the results are recalled here. Nonlinear curvature effects are proved to be essential mechanisms controlling the critical condition. These effects are first studied in a quasi-steady (q-s) state approximation valid for a characteristic time scale much larger than the reaction time scale. Two branches of q-s solutions are exhibited with a C-shaped curve and a critical radius below which generalised Chapman-Jouguet (CJ) solutions cannot exist. At ordinary conditions this critical radius is much larger than the thickness of the plane CJ detonation front (typically 300 to 500 times larger). Direct numerical simulations show that the upper branch of q-s solutions, acts as an attractor of the unsteady blast waves originating from a sufficiently strong energy source. The criterion of initiation derived here works to a good approximation and exhibits the huge numerical factor ($10^6 - 10^8$) which is observed in the experimental data of the critical energy source and which was not explained up to now. Transient may induce additional failure mechanisms close to the critical condition.

1. INTRODUCTION

Direct initiation of gaseous detonation by an energy source is an old problem which has been reviewed by Lee in 1977 and 1984 [1], [2]. For a subcritical level of the total energy of the igniter $E_s$, $E_s < E_c$, the shock wave decays continuously, the reaction front separates from the inert shock, and a premixed flame is finally ignited. With an energy larger than the critical value $E_c$, $E_s > E_c$, the shock wave and the reaction layer remain always coupled; the strong overdriven detonation originating from the source relaxes to a CJ detonation wave propagating at a constant velocity, $D_{CJ}$. The onset of this CJ detonation occurs at a distance from the point source increasing with the energy of the igniter $E_s$, $R^*(E_s) = (E_s/\rho_0 Q)^{1/3}$, where $Q$ is the heat release per unit mass. A critical radius $R_C = R^*(E_c)$ has been identified experimentally at the critical condition. No CJ detonation can be observed with a front radius $R_s$ smaller than $R_C$ which is about twenty times larger than the cell spacing size which is itself ten to fifty times larger than the thickness of the reaction zone of a planar detonation (see Desbordes [3]). The existing theoretical models for the critical conditions were essentially phenomenological. Zeldovich et al. [4] provided the first criterion: a successful initiation occurs when the time necessary for the blast wave to decay to the level of the leading shock of a planar CJ detonation is larger than the chemical induction time $\tau_i$ at the Neuman spike of a CJ detonation. The kinetics data available at that time were too inaccurate for providing a meaningful experimental check of this criterion. The corresponding critical conditions are wrong by many orders of magnitude indeed. They may be estimated from the self-similar solution of Taylor [5] and Sedov [6] for strong adiabatic blast waves generated by an instantaneous deposition of energy at a point.
\[
E_s = k_j (j+3)/2 \]^{j+1} \rho_0 D^{j+3} \tau^{j+1} \iff E_s = k_j \rho_0 D^2 R_s^{j+1} \tag{1}
\]
where \( j = 0, 1, 2 \) in the planar, cylindrical and spherical geometry respectively, \( \rho_0 \) is the gas density of the initial mixture, \( D \) and \( R_s \) are the shock velocity and the radius of the shock wave at any instant of time \( \tau \), \( E_s \) is the energy of the point source and \( k_j \) is a dimensionless constant of order unity. The critical energy and radius are evaluated from (1) by replacing \( D \) by \( D_{\text{CJ}} \) and \( \tau \) by \( \tau_{\text{i}} \). This criterion yields a critical radius of the same order of magnitude as the thickness of the detonation \( R_c = l_{\text{CJ}} = D_{\text{CJ}} \tau_{\text{i}} \), in contradiction with the experiments of Desbordes [3] \( R_c = 300 l_{\text{CJ}} \). When the relation \( R_c = l_{\text{CJ}} \) is used, the critical energy obtained from (1), \( E_c = \rho_0 D_{\text{CJ}}^2 l_{\text{CJ}}^{j+1} \), is roughly speaking the chemical energy available in a sphere of radius the detonation thickness (for a large Mach number, \( D_{\text{CJ}}^2 = 2(\gamma^2-1)Q \)). As shown later by Edwards et al. [7] who used accurate data for \( l_{\text{CJ}} \), the natural energy scale \( \rho_0 D_{\text{CJ}}^2 l_{\text{CJ}}^{j+1} \) is much smaller than the experimental data of critical energy for a detonation initiation by many orders of magnitude \( 10^6 \). Other phenomenological criteria have been derived later in a similar way but by replacing \( l_{\text{CJ}} \) by much larger length scales as theses obtained from measurements of cell sizes or critical tube diameters, see Lee [1-2]. The best phenomenological fits have been obtained with a "magic ratio" 13/4 the cell size. Correlations with the cell size seem fortuitous; the initiation conditions are the same for mixtures in which detonation fronts have no cell structure, as is more likely the case for warm hydrogen mixtures encountered in safety problems of some nuclear plans.

In a recent theoretical work [8] we have shown that the critical conditions for a direct initiation of a gaseous detonations by a point source are governed by a nonlinear curvature effect presenting some analogies with a quenching phenomenon. The main steps of this analysis are briefly reported at this conference. The point source approximation is valid when the characteristic size of the igniter is much smaller than \( R_c \) and when the deposition time of energy is much smaller than the induction time \( \tau_{\text{i}} \). Then, when multi-dimensional effects such as those governing the cell structures, are neglected, a successful initiation may be viewed as a transition between two self-similar regimes:

i) At early times, the total heat released by the chemical reactions is negligibly small compared to \( E_s \), the self-similar solution of Taylor and Sedov for strong adiabatic blast waves hold.

ii) At sufficiently long times after a successful initiation, \( E_s \) becomes negligibly small compared to the energy released by the chemical reactions. And, in the case of a stable detonation, the solution is well approximated by the self-sustained wave of Zeldovich [9] and Taylor [10] constituted by a smooth detonation front expanding at a constant CJ velocity and followed by a self-similar rarefaction wave.

Numerical solutions of a "detonation-wave model" were carried out by Korobeinikov [12] to describe such a transition in the limit of an infinitely fast chemical rate (\( \tau_{\text{i}} \to 0 \)). The detonation front was considered as a discontinuity with Rankine-Hugoniot jump conditions. No critical condition of initiation is observed in this work; the onset of the CJ detonation occurs in spherical geometry at \( \Delta(V_0) = (1.3 E_s/\rho_0 Q)^{1/3} \) for a specific heat ratio of 1.3, whatever be \( E_s \). This shows clearly that the physical mechanisms governing the critical conditions are associated with those involved inside the inner detonation structure and characterised by a finite chemical time (length) scale \( \tau_{\text{i}} \) (detonation thickness \( l_i = \tau_{\text{i}} D_{\text{CJ}} \)). The interesting question to answer is how such small effects may induce so strong effects as those responsible for critical conditions which involve a so large critical radius, typically 300 the CJ detonation thickness ? As for flames quenching [13-14], the answer lies on an amplification by a large sensitivity to temperature of the reaction rate. A small curvature of the detonation front may have a drastic effect upon the inner structure of the detonation wave in a way similar to quenching of planar detonations by momentum losses which was described by Zeldovich [15] for representing detonations propagating in rough tubes. A difficulty for solving analytically the initiation problem is its strong unsteady character. It turns out that a quasi-steady approximation of the detonation structure allows to capture the essential physical mechanisms.
2. THE BASIC EQUATIONS

When the molecular transport are neglected and when the chemical reaction is modelled by an exothermic irreversible one-step reaction, the unsteady and one-dimensional conservation equations are

\[ \frac{\partial p}{\partial t} + \frac{\partial (pu)}{\partial r} + \frac{j}{r} (pu) = 0 \]  (2.1a)

\[ \frac{\partial (pu)}{\partial t} + \frac{\partial (pu^2 + p)}{\partial r} + \frac{j}{r} (pu^2) = 0 \]  (2.1b)

\[ \frac{\partial E}{\partial t} + \frac{\partial [(E + p)u]}{\partial r} + \frac{j}{r} (E + p)u = 0 \]  (2.1c)

\[ \frac{\partial (\rho y)}{\partial t} + \frac{\partial (\rho uy)}{\partial r} + \frac{j}{r} (\rho uy) = - \rho \omega \]  (2.1d)

with \( j = 0, 1 \) and \( 2 \) in the planar, cylindrical and spherical geometry and with \( p = \rho \Gamma \) for a polytropic gas. In these equations \( p, \rho, T, E \) and \( y \) are respectively the pressure, density, temperature, specific energy and reactant mass fraction. These variables have been dimensionless by reference to the preshock state; \( p/p_0 \rightarrow \rho, \rho/\rho_0 \rightarrow \rho, T/T_0 \rightarrow \Gamma, E/E_0 \rightarrow E \). The velocity is denoted \( u \) after non-dimensionalization through division by \( c_0 \sqrt{\gamma} \) where \( c_0 \) is the sound speed at the preshock state and \( \gamma \) is the specific heat ratio. The non-dimensional time and space variables \( t \) and \( r \) are based on the chemical induction time \( \tau_{ICJ} \) of the planar CJ detonation and on the reference length scale \( (\tau_{ICJ} c_0) / \sqrt{\gamma} \) which is typically of the same order of magnitude as the thickness of the detonation front. When the reaction is governed by an Arrhenius law, the reduced chemical reaction rate takes the following form,

\[ \omega = y \frac{B \tau_{ICJ}}{E_a} e^{-E_a/T} \]  (2.1g)

where \( B \) is the frequency factor and \( E_a \) the reduced activation energy. And the reference time scale is defined by

\[ \tau_{ICJ} = \frac{T_{NCJ}^2}{B (\gamma - 1) Q E_a - e^{E_a/T_{NCJ}}} \]  (2.2)

where \( T_{NCJ} \) is the reduced temperature at the Neumann spike of the planar CJ detonation and \( Q \) the reduced heat release parameter, \( Q/(C_p-C_v)T_0 \rightarrow Q \). In the moving frame attached to the shock, Eqs.(2.1a-d) can be written as

\[ \frac{\partial p}{\partial \tau} + \frac{\partial (pv)}{\partial \xi} + \frac{j}{R_s - \xi} \rho (D - v) = 0 \]  (2.3a)

\[ \frac{\partial (pv)}{\partial \tau} + \frac{\partial (pv^2 + p)}{\partial \xi} + \frac{j}{R_s - \xi} \rho (D - v)v - \rho \frac{dD}{d\tau} = 0 \]  (2.3b)

\[ \frac{\partial h}{\partial \tau} + v \frac{\partial h}{\partial \xi} - \frac{1}{R_s - \xi} \frac{\partial p}{\partial \tau} = 0 \]  (2.3c)

\[ \frac{\partial y}{\partial \tau} + v \frac{\partial y}{\partial \xi} = - \omega \]  (2.3d)

with reduced space and time coordinates.
\[ \xi = \frac{D}{R_s} - \frac{D}{t}, \quad \tau = t \] (2.4a)

\[ R_s = \int_0^1 D(t') \, dt' \] (2.4b)

where \( D \) and \( R_s \) are respectively the velocity and the position of the shock at any instant of time \( t \), \( v = D - u \) is the flow velocity relative to the leading shock wave, and the total enthalpy is

\[ h = \frac{T}{\gamma - 1} + \frac{1}{2} v^2 + \frac{y}{1 - \gamma} Q \] (2.5)

Three types of term appear in (2.3): i) unsteady terms, ii) three conserved scalars in plane and steady detonations \((p v, p v^2 + p, h)\), iii) curvature terms.

3 NONLINEAR CURVATURE EFFECT

In the study of detonation structures with a radius of front curvature much larger than the detonation thickness, \( R_s \gg 1 \), \( \xi \) may be neglected in \((R_s - \xi)\). The reference time scale which has been used is of the same order of magnitude as the intrinsic reaction time characterising the internal detonation structure. In the quasi-steady state approximation when the characteristic time of evolution is much longer than this reaction time, unsteady terms may be neglected. Then, in the framework of such multiple scales assumptions, the governing equations for the structure of a curved detonation reduce at the leading order to the following system of first order ordinary differential equations,

\[ \frac{d(pv)}{d\xi} = - \frac{j}{R_s} \rho(D - v) \] (3.1a)

\[ \frac{d(pv^2 + p)}{d\xi} = - \frac{j}{R_s} \rho(D - v)v \] (3.1b)

\[ \frac{dh}{d\xi} = 0 \] (3.1c)

\[ \frac{dv}{d\xi} = - \omega \] (3.1d)

This quasi-steady approximation is meaningful whenever the unsteady terms are smaller than the perturbative curvature effects. The additional curvature term on the r.h.s. of (3.1a-b) are to be considered as perturbations, \( R_s \gg 1 \). When they are omitted, eqs.(3.1a-c) reduce to the ordinary conservative system describing planar detonations. But even small, the curvature terms change the phase portrait. After elimination of \( p \) and \( \rho \), eqs.(3.1a-d) may be written in the following form, suitable for the analysis of the detonation structure in the phase space \( v^2 - y \) [15],

\[ \frac{dv}{dy} = - \frac{\psi(y,v,D)}{\omega(y,v,D)} \frac{v(y,v,D)}{\phi(y,v,D)} \] (3.2a)

with \( \psi \equiv \left(\frac{\gamma - 1}{c^2} Q \omega \right) - \frac{j}{R_s} (D - v) \) and \( \phi \equiv 1 - \frac{v^2}{c^2} \) (3.2b)

where \( \omega \), the reduced reaction rate (2.1g), \( c \), the reduced local sound speed, and the reduced temperature \( T \) are expressed in terms of \( y, v, D \) by the total enthalpy conservation as

\[ c^2 = \gamma T = \gamma + (\gamma - 1) \left[ \frac{1}{2} (D^2 - v^2) + (1 - \gamma) Q \right] \] (3.2c)

3.1 Weak curvature effects

System of equations (3.2a-c) has been used with a reaction rate \( \omega \) represented by a regular function, to study the detonation structure in slightly divergent flows [16] or with weak curvature effects of the front.
For a given value of $R_s$, there is a one-parameter family of solutions labelled by $D$. A marginal solution corresponding to a local minimum of $D$, called "generalised CJ solution" and referred by $D_+(R_s)$ in this paper, has been pointed out, with a sonic condition $v = c$ occurring at $y = y^* > 0$, before the completion of the reaction. This marginal solution is qualitatively different from the CJ solution of the plane case, the condition $v = c$ corresponds to saddle point in the phase space $v^2 - y$, $\psi = 0$, $\varphi = 0$ but $dv^2/dy \neq \infty$ while in the plane case $v = c$ at $y = 0$ with $dv^2/dy = \infty$. Solutions exist for larger detonation velocities, $D > D_+$, and they all correspond to overdriven detonations with a subsonic flow ($v < c$) everywhere ($0 \leq y \leq 1$). The trajectory of the marginal solution, $D = D_+$, passes through the saddle critical point ($y = y^*$) into the supersonic region and, as a consequence, this solution is qualitatively different from all the overdriven ones, the flow is subsonic in a first part behind the shock wave, $1 \geq y > y^*$, and supersonic in the last part of the combustion process $y^* > y \geq 0$. For slightly smaller detonation velocities, $D < D_+$, the sonic condition $v = c$ corresponds to a turning point $(dv^2/dy = \infty)$ which appears at $y > 0$ as in the plane case for $D < D_{CJ}$, and no solution exists any longer because $y = 0$ cannot be attained. The relation between $D$ and $R_s$, referred below as $(D(R_s))$, has been obtained from the marginal solution $D_+[17]$.

Our analysis [8] shows that there exists indeed another branch of marginal solutions $D_+(R_s)$ ($D < D_+$) with solutions for $D < D_-$. Due to nonlinear effects the $D(R_s)$ curve has a C-shaped form with a critical radius $R_c$. An analytical solution of $(3.1a-c)$ has been obtained in ref [8] for describing the nonlinear curvature effects in the framework of a square-wave model yielding a nonlinear relation for $D(R_s)$. For $R_s > R_c$, the velocity spectrum of quasi steady detonations is unbounded but presents two extrema. One, $D_+$, is a local minimum and the other $D_-$ a local maximum, with a forbidden band $[D_-, D_+]$. An analytical expression for the critical radius $R_c$ below which no generalised CJ solution exists, is obtained. When compared with numerical solutions of $(3.1a-c)$ for an Arrhenius law, these analytical results show a good accuracy. They yield also an analytical determination of the critical energy of direct initiation. These results are briefly recalled below.

### 3.2 Square-wave model

The square-wave model is defined in a phenomenological way as follows. The chemical reaction is assumed to proceed in two sequential steps. The heat is released during a reaction time $\tau_1$ after a time delay called the induction time $\tau_1$. The square-wave model corresponds to the limit $\tau_2 / \tau_1 \to 0$. The reaction rate $\omega$ becomes singular, and the heat release is localised within a thin exothermic layer considered as a discontinuity following the shock wave at a distance $l_1$ defined as

$$l_1 = v_N \tau_1,$$

where by definition of the reference length scale used in $(2.1a-d)$, $l_{CJ} = O(1)$. The induction time is highly sensitive to the temperature fluctuations of the shocked gas just downstream the shock wave, $\delta T_N$. Let $\beta$ be the large nondimensional reduced activation energy, $(\delta \tau_1 / \delta T_N)$, with $\beta >> 1$, then,

$$l_1 / l_{CJ} = \exp \{- \beta (T_N - T_{NCJ})/T_{NCJ} \} \text{ valid for } \beta >> 1,$$

where subscripts $N$ and CJ denote the state at the shock and the planar CJ case respectively. Relation (3.3b) may be obtained from an Arrhenius law at the leading order of an asymptotic expansion in the limit $\beta \to \infty$ (see Appendix of ref. [8]). This simplified model is sufficient to pick up the essential phenomena as well as the right orders of magnitude. Such a singular model is known from a long time to introduce spurious singularities when it is used for describing the intrinsic dynamics of a detonation front which develops on a characteristic time scale $\tau_1$ [18-19]. These problems, including the nonlinear dynamics of galloping detonations, have been very recently solved also analytically [20-21]. However the square-wave model has been proved already to be very powerful to describe critical conditions associated with quasi-steady mechanisms developing on a time scale longer than $\tau_1$ and which are stressed by a high sensitivity of the induction time [22]. When the attention is focused on cases where $\beta >> 1$ and $R_s = O(1)$, the curvature terms in the r.h.s. of $(3.1a-b)$ being small, of the same order of magnitude as $1/\beta$, the variations of the
shocked gas temperature from its value in the planar case are also small, $\delta T_N/T_N = O(1/\beta)$. But strong nonlinear effects are included at the leading order of the limit $\beta \to \infty$; according to the high sensitivity to $T_N$ in (3.3), one has $(\delta T_N/T_N) = O(1)$ and $(\delta v/v) = O(1)$. In the square-wave model, the thickness of the reaction zone is negligible and the curvature effects modify only the induction zone which does not consume the reactant, $\gamma = 1$. The $1/R_s$ terms being negligible in the thin exothermic zone, this last one is described in the phase plane by the same equations as in the planar case, but with a different initial condition at $y = 1$, $v^2 = v_N^2(D)$ resulting from the curvature induced modifications across the induction zone. As for the planar case, the marginal solutions of the square wave model may be obtained directly from the conservation laws across the detonation structure without investigating the phase space. These conservation laws are readily obtained by a $\xi$-integration of (3.1a-c) across the detonation structure and may be written in a dimensionless form as:

\[ p_b v_b = D - D \Gamma_1 \]  
\[ (\rho_b v_b^2 + p_b) = (D^2 + 1) - D^2 \Gamma_2 \]  
\[ (\gamma / (\gamma - 1)) p_b / \rho_b + (1/2) v_b^2 = \gamma / (\gamma - 1) + (1/2) D^2 + Q \]

where the subscript $b$ denotes the burned gases ($y = 0$). The source terms of (3.4a-b), defined as

\[ \Gamma_1 = \frac{1}{D} \int_0^1 \rho (D - v) \, d\xi \]  
\[ \Gamma_2 = \frac{1}{D^2} \int_0^1 \rho (D - v) \, v \, d\xi \]

represent the curvature induced modifications of mass and momentum fluxes across the detonation structure. They are both small perturbation terms; when they are neglected, (3.4a-c) reduce to the ordinary Hugoniot relations. Using $1/R_s = O(1/\beta)$, the leading order of $\Gamma_1$ and $\Gamma_2$ in the asymptotic limit $\beta \to \infty$ can be easily computed from (3.5a-b) with the square wave model by using the values at the Neumann spike of the CJ solution for $D$, $v$ and $p$.

\[ \Gamma_1 = \frac{j \, (\rho_{NCJ} - 1)}{R_s} = O(1) \]  
\[ \Gamma_2 = j \, (1 - \frac{1}{\rho_{NCJ}}) \frac{1}{R_s} = \frac{1}{\rho_{NCJ}} \Gamma_1 \]

where the thickness of the induction zone is given by (3.3) and may be expressed in terms of the modification of detonation velocity $(D - D_{CJ})/D_{CJ}$ by using the Hugoniot relation of the leading shock in the fresh mixture,

\[ \frac{T_N - T_{NCJ}}{T_{NCJ}} = - \frac{2}{1 + D_{CJ}^2 \gamma / (\gamma - 1)} \frac{D - D_{CJ}}{D_{CJ}} = -2 \frac{D - D_{CJ}}{D_{CJ}} \]

where the last approximation is valid for a sufficiently strong shock wave, $(\gamma - 1)D_{CJ}^2 \gg 1$, yielding according to (3.3),

\[ \frac{l_i}{l_{NCJ}} \approx \exp \{ - 2\beta \frac{D - D_{CJ}}{D_{CJ}} \} \]

According to (3.6a-c),

\[ \delta \Gamma_{1,2} = \frac{\delta D}{D_{CJ}} (2\beta \Gamma_{1,2}) \]

then, a variation around the marginal solution of (3.4a-c) which is defined by an extremum condition $\delta D = 0$, confirms that such a solution is still determined in curved fronts by the same sonic condition in the burned gases as in the plane case: $v_b = c_b = (\gamma p_b / \rho_b)^{1/2}$. Then, introducing $v_b = (\gamma p_b / \rho_b)^{1/2}$ in (3.4a-c), a
perturbative analysis around the planar CJ detonation yields the curvature-induced modification of the detonation velocity \( \Delta \text{D}_{\text{DCJ}} \) as a linear function of \( \Gamma_1 = O(1/\beta) \) and \( \Gamma_2 = O(1/\beta) \),

\[
\left\{ - \frac{2}{\gamma^2} \frac{\gamma (\gamma+1) + (\gamma^2-1) Q}{1 + \Delta^2_{\text{DCJ}}} \left( \frac{\Delta \text{D}_{\text{CJ}}}{\Delta^2_{\text{CJ}}} \right) + \frac{2}{\Delta^2_{\text{CJ}}} \right\} \Delta \text{D}_{\text{DCJ}} = (1 + \frac{1}{\Delta^2_{\text{CJ}}}) \Gamma_1 - \Gamma_2 
\]

which, by using a nonlinear expression obtained for \( \Gamma_1 \) from (3.6a-c),

\[
\Gamma_1 = j \left( \rho_{\text{NCJ}} - 1 \right) \frac{\Delta^2_{\text{CJ}}}{R_s} \exp \left\{ -2 \beta \frac{\Delta \text{D}_{\text{DCJ}}}{\Delta^2_{\text{CJ}}} \right\} 
\]

provides a nonlinear equation for the velocity \( \Delta \text{D} \) of the marginal detonations,

\[
(2\beta \frac{\Delta \text{D}_{\text{CJ}} - \Delta \text{D}_{\text{DCJ}}}{\Delta^2_{\text{CJ}}} \exp \left\{ -2\beta \frac{\Delta \text{D}_{\text{DCJ}} - \Delta \text{D}_{\text{CJ}}}{\Delta^2_{\text{CJ}}} \right\} = \frac{8j}{1 - \gamma^2} \left( \frac{\rho_{\text{NCJ}} - 1}{\Delta^2_{\text{CJ}}} \right) \beta \frac{\Delta^2_{\text{CJ}}}{R_s} 
\]

where the simplified forms of the coefficients corresponding to a strong detonations, \( (\gamma-1)^2 \Delta^2_{\text{CJ}} > 1 \), have been used for simplicity, \( \Delta^2_{\text{DCJ}} = \frac{2(\gamma^2-1)Q}{(\rho_{\text{NCJ}} - 1)^2/R_{\text{NCJ}}} = \frac{4(\gamma^2 - 1)}{1} \). Eq.(3.8) yields a nonlinear velocity-radius relation, \( \Delta \text{D}(R_s) \), valid in the distinguished limit \( \beta \rightarrow \infty \), \( \beta \frac{\Delta^2_{\text{CJ}}}{R_s} = O(1) \), \( \beta (\Delta \text{D}_{\text{CJ}} - \Delta \text{D})/\Delta^2_{\text{CJ}} = O(1) \), corresponding to a relatively small curvature intensity. This result exhibits a critical radius \( R_c \)

\[
\frac{R_c}{\Delta^2_{\text{CJ}}} = \frac{8 e j}{1 - \gamma^2} \beta 
\]

below which no solution exits, and a critical detonation velocity \( \Delta \text{D}_c \) given by

\[
\frac{\Delta \text{D}_{\text{CJ}} - \Delta \text{D}_c}{\Delta^2_{\text{CJ}}} = \frac{1}{2\beta} 
\]

For \( R_s > R_c \) (3.8) yields two branches of solutions \( \Delta \text{D}_+(R_s) > \Delta \text{D}_{\text{CJ}}(R_s) \). The physical one is the upper one which reaches the CJ planar solution from below when \( R_s \rightarrow \infty \), \( \Delta \text{D}_+(R_s) \rightarrow \Delta \text{D}_{\text{CJ}} \). The second branch of solution \( \Delta \text{D}_-(R_s) \) is not physical: in the limit \( R_s \rightarrow \infty \) one gets \( \beta \frac{\Delta \text{D}_{\text{CJ}} - \Delta \text{D}}{\Delta^2_{\text{CJ}}} \rightarrow \infty \) which does not correspond to the domain of validity of (3.8), \( \beta (\Delta \text{D}_{\text{CJ}} - \Delta \text{D})/\Delta^2_{\text{CJ}} = O(1) \) for \( \beta \rightarrow \infty \). We will discuss later the nature of this second branch of solutions. The critical condition (3.9a-b) is within the validity domain of the limit \( \beta \rightarrow \infty \). For weak curvature effects, \( \beta \frac{\Delta^2_{\text{CJ}}}{R_s} \rightarrow 0 \), one gets the following linear relation for the upper branch,

\[
(\Delta \text{D}_{\text{CJ}} - \Delta \text{D}_+)(\Delta \text{D}_{\text{CJ}}) = 4 \gamma^2 (\gamma^2 - 1) j \left( \frac{\Delta^2_{\text{CJ}}}{R_s} \right) 
\]

which corresponds to a linear result obtained in the particular case of a one-step first-order reaction governed by an Arrhenius law at the limit of an infinitely large activation energy [17]. Finally, notice that the numerical factor in the r.h.s. of (3.9a) which is of order unity in the asymptotic limit \( \beta \rightarrow \infty \) and which controls the numerical value of the critical radius, is a larger number \( 8 e j (1 - \gamma^2) = 90 \) for \( \gamma = 1.4 \) and \( j = 2 \) (spherical detonation). Thus, for ordinary values of the reduced activation energy based on the temperature at the Neumann spike, \( \beta = E_{\text{NCJ}}/T_{\text{NCJ}} = 5 \) to 10, the critical radius is 400 to 900 times larger than the detonation thickness while the corresponding relative modification of the detonation velocity (3.9b) is small, \( 10^{-1} \) to \( 5 \times 10^{-2} \). Thus, the origin of the large value of \( R_c/\Delta^2_{\text{CJ}} \) is clearly exhibited by the analytical results of the square wave model. These results are confirmed by those obtained by a numerical integration in the phase space of (3.1-2) with an Arrhenius law [8]. The critical value is well approximated by (3.9a). For a given \( R_s \) larger than the critical value \( R_c \) there are two trajectories corresponding to two different marginal detonation velocities \( \Delta \text{D}_+ \) and \( \Delta \text{D}_- \). The trajectories associated with intermediate velocities of detonation, \( \Delta \text{D}_- < \Delta \text{D} < \Delta \text{D}_+ \), are the only one for which there is no solution linking the initial state \( y = 1 \) to the final one \( y = 0 \); a turning point appears at \( y > 0 \). The set of solutions corresponds to two disconnected
ranges of detonation velocities, an upper one \((D_+, +\infty)\) with a lower bound \(D_+\) (local minimum) and another one with an upper bound \(D_-.\) In solutions corresponding to \(D > D_+\) or \(D < D_-\) the flow behind the leading shock is subsonic everywhere relatively to the shock. The marginal solutions \(D_+\) and \(D_-\) are the only ones presenting a sonic condition in the burned gases. When \(R_s\) decreases \(D_+\) decreases while \(D_-\) increases so that the two trajectories of the marginal solutions \((D_+, D_-)\) in the phase space \(v^2 - y\) become closer and closer and collapse at \(R_s = R_c\) (see fig. 1). When \(R_s < R_c\) there is no more local extrema, a solution does exist for every value of \(D\) and the flow behind the leading shock is subsonic everywhere. Similar results with same order of magnitude as predicted by the square-wave model are also obtained with a complex chemistry for H2-O2 mixtures [23].

![Diagram](image.png)

**Fig. 1** Numerical results of the initiation of spherical detonations. The front velocity is plotted as a function of the front radius and is compared with the corresponding marginal solutions for a reactive mixture characterised by \(\gamma = 1.4, \beta = 5.33, Q = 12.5\) and for four values of the nondimensional source energy \(E_s/(\rho_0 D_{CJ}^2 (CJ)^3)\):

1.) 3.30x10^7, 2.) 5.69x10^7, 3.) 1.34x10^8, 4.) 2.64x10^8

4. DIRECT INITIATION

The selection mechanism of the CJ solution is worth recalling at this stage (see for example Landau and Lifchitz, [11]). Faster detonations waves are associated with a subsonic flow in the referential frame of the leading shock. Thus, the shock intensity is continuously weakened (down to CJ) by the rarefaction wave which has a leading weak discontinuity travelling at a sonic velocity relatively to the burned gases. This damping effect is screened only at the marginal CJ regime of propagation by a sonic condition of the flow at the end of the chemical reaction. Following the same idea, a selection mechanism may be predicted in the presence of curvature effects. Due to the rarefaction wave in the burned gas of an expanding overdriven detonation \((D(t) > D_+)\) which are initially generated by a point source explosion, the upper branch \(D_+\) of marginal solutions (minimum velocity) is naturally selected from above. The shock velocity of the solutions of the other set \((D < D_-)\) is continuously decreased; the marginal \(D_-\) solution (local maximum) can never be
selected. Thus the upper branch of marginal solutions $D_+$ is predicted to act as an attractor for the unsteady blast waves generated by a sufficiently strong energy source. But this $D_+$ branch is not always caught; in such circumstances the detonation wave dies out. Consider the direct initiation of a detonation by an energy source $E_s$. As discussed in the introduction, the initial stages correspond to the self-similar solution of a strong adiabatic blast wave (1.1) which is represented by a curve in the $D-R_s$ plane,

$$E_s = k_j \rho_0 R_s^{j+1} D^2.$$  \hfill (4.1)

Ignition failures may be predicted for source energies $E_s$ for which the $D-R_s$ curve do not cross the upper branch $D_+$ (see case 1 in Fig. 1). Successful initiations are expected in the opposite case (see case 3 and 4 in Fig. 1). As a result, a critical energy $E_c$ may be evaluated from (4.1) by replacing $R_s$ by $R_c$ and $D$ by $D_c ( = D_{CJ})$, yielding the following approximate criterion when (3.9a-b) is used,

$$\frac{8ej\beta}{1 - 1/\gamma^2} \frac{j+1}{i_{CJ}^2} \rho_0 D_c^2 R_c^{j+1}$$  \hfill (4.2)

Equation (4.2) defines the critical energy which exhibits a huge factor $(R_c i_{CJ}^2)^{j+1} = (8ej\beta 2/(\gamma^2 - 1) j+1$ with an order of magnitude ranging from $10^7$ to $10^9$ in the spherical case. The numerical simulations of a direct detonation initiation by an energy source confirm these predictions [8] [23]. Solutions corresponding to four values of the energy source are shown in figure 1 where the two branches of marginal quasi-steady solutions, $D_+$ and $D_-$, are also plotted for comparison.

5 DISCUSSION OF THE RESULTS

The results presented in this paper show clearly that the criterion for a direct detonation initiation by an energy source in cylindrical and spherical geometry is directly controlled by nonlinear curvature effects of the detonation front, at least in the range of parameters where the planar detonation is not strongly unstable. Considering the unsteady effects one must first discuss the validity of the quasi-steady state approximation used in (3.1a-d). The characteristic evolution rate on the $D_+$ branch, $1/t_e = dD_+/dR_s$, is given far enough from the turning point by (3.9c), yielding $1/t_e = 4j^2/(\gamma^2 - 1) (i_{CJ}/R_s)^2 (D_{CJ}/i_{CJ})$. The neglected unsteady terms $\partial/\partial \tau$ in (3.1a-d), are effectively of the following order in the large radius expansion $\tau t_e = O(i_{CJ}/R_s)^2$. Such an approximation does not hold close to the critical point where $dD_+/dR_s \to \infty$ but this does not change the final results because the divergence affects only a small vicinity of the critical point. More important are the unsteady effects related to the intrinsic dynamics of detonations (see ref. [20-21] for recent theoretical results). The detonation is known to become unstable for a sufficiently high activation energy and the instability mechanism is reinforced when approaching the critical point. Another problem is the dynamics of the selection mechanism of the $D_+$ branch which is unknown. The corresponding unsteady effects are enlightened by a comparative numerical study of the ignition problem in planar geometry. For the same set of parameters the critical size is much smaller than the critical radius in spherical geometry. This points out that the curvature effects are dominant in spherical and cylindrical geometries. Good order of magnitudes are obtained with our simple theory. But the unsteady effects cannot be ignored for an accurate prediction of the critical conditions and more specially for strongly unstable detonations. The multidimensional effects remain an open question.

REFERENCES


