

TAM Report No. 1043

UILU-ENG-2004-6004

ISSN 0073-5264

**TAM**  
Theoretical and Applied Mechanics  
University of Illinois at Urbana-Champaign

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March 2004

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## Abstract

In this work we discuss the application of an evolution equation that we have developed for the dynamics of a slowly evolving weakly-curved detonation to a problem of direct detonation initiation. Despite the relative simplicity of the theory, it successfully explains basic features of the initiation process which are observed in experiments and numerical simulations. Moreover, the theory allows one to calculate initiation energies based on the explosive chemical and thermodynamic properties only, without having to invoke significant modeling assumptions. The evolution equation exhibits the competing effects of the exothermic heat release, curvature, and shock acceleration. The detonation dynamics during the initiation depends on the relative strength of the heat release and flow divergence, resulting in successful initiation of self-sustained detonation if the heat release is sufficiently stronger than divergence or in failure if otherwise. Using global kinetic data from Caltech detonation database, which are derived from detailed chemical calculations, we have calculated critical initiation energies of spherical detonation for hydrogen-oxygen, hydrogen-air, and ethylene-air mixtures at various equivalence ratios and found a very good agreement with recent experimental data.

## 1 Introduction

The problem of detonation initiation in gases is of great practical importance, particularly because of related safety issues. Understanding the critical conditions delineating initiation and failure by a given energy source is a major problem that has challenged researchers for decades. Although many qualitative features of the underlying mechanisms are well known, sufficiently accurate quantitative theories and measurements have been difficult to achieve. One of the main mechanisms by which a gaseous detonation can be initiated is referred to as a direct initiation. In this case detonation is initiated by a strong localized source, for example, a high-explosive charge, electric spark, an exploding wire, etc., all of which produce a blast wave that propagates into the surrounding explosive gas and, if sufficiently strong, can trigger a detonation wave in the gas. The main quantity of interest is the critical energy of the initiating source. Current understanding in the area is such that critical energies experimentally determined by different researchers can disagree by orders of magnitude. Most existing models of direct initiation require major empirical inputs to fit the experimental data. A theory that would be able to explain the essential mechanism involved in the direct initiation and to predict the critical energy based only on thermodynamic and chemical properties of an explosive mixture has been absent. This work presents such a theory based on an analysis of reactive Euler equations in the asymptotic limit of small shock curvature (measured on the steady reaction-zone length) and slow time evolution (measured on the reaction time scale of the steady detonation).

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In both experiments and numerical simulations, a successful direct initiation process is observed to proceed as follows. The shock speed of an initial strong blast wave decays to speeds below the Chapman-Jouguet (CJ) speed,  $D_{CJ}$ , of the gaseous explosive, reaches a certain minimum speed and subsequently accelerates to  $D_{CJ}$  and propagates at that level, often exhibiting a pulsating character after ignition. There exists an extensive literature on experimental investigations and modeling of the direct initiation that attempt to characterize the observed dynamics. For a recent review and further references the reader is referred to [1]. All currently proposed models are based on the idea first proposed in Zel'dovich, Kogarko, and Simonov's 1957 work, [2], on blast initiation of spherical detonation. That influential work proposed that the time required for the initial blast-wave speed to decay to  $D_{CJ}$  has to be proportional to the induction period  $\tau_i$  of the explosive gas. From this idea one can derive that the critical energy  $E_c$  is proportional to  $\tau_i^3$ , or equivalently to reaction zone thickness cubed,  $l_{rz}^3$ . In a number of works since 1957, this correlation has been made to agree with experiment by invoking variety of assumptions, most notably by Lee and coworkers, (see references in [1]), and by Vasiliev and his colleagues, (see [3] and references therein). Essentially, the modeling assumptions involve various other relevant length scales, such as the detonation cell size, critical diameter, etc., that replace the reaction zone length in the expression for the critical energy. In addition, because of the experimental observation that the detonation proceeds through a phase of sub-CJ speeds, it is often suggested that the shock speed used in the critical energy calculations be some empirically determined sub-CJ velocity rather than the CJ velocity.

Two other models should be mentioned, namely the one by He and Clavin [5, 6] and by Eckett et al. [4]. He and Clavin, [5, 6], build their theory based on the theoretical observation that the quasi-steady solution of a curved detonation has a C-shaped form in the space of the shock speed  $D$  and shock radius  $R$  (an observation that dates back at least to Tsuge and coworkers in the early 70's, see the review by Stewart [7]). The  $D - R$  curve was derived using a square-wave model of the detonation reaction zone. They used the upper turning point of the quasi-steady detonation speed  $D$ , curvature  $\kappa$  response curve, to define the critical conditions for detonation initiation. They assumed that failure occurs due to the loss of the quasi-steady solution below the turning point. They did not consider the possibility that unsteady effects (such as the shock acceleration  $\dot{D}$  that we consider in this work) can affect the critical conditions. As Lee and Higgins emphasize in [1], unsteady effects in direct initiation can be significant and the curvature considerations alone are insufficient for accurate prediction of the critical energy. Eckett et al. [4] demonstrated that unsteady processes play a very important role in the direct initiation and affect the critical energies significantly. Eckett, Quirk, and Shepherd's model that accounts for unsteadiness shows much better agreement with experiments than can be obtained based on the model of He and Clavin, the latter overpredicting the critical energies by three orders of magnitude. In the present theory we show that with the inclusion of the shock acceleration term from rational analysis that derives the detonation evolution equation that results in  $\dot{D} - D - \kappa$  relation results in critical conditions for initiation that differ from the quasi-steady theory significantly and result in much better agreement with experiment.

The present work is an application of a more general, rational theory of self-sustained detonation waves that is developed in [8]. Essentially, the theory treats a self-sustained detonation wave as a structure containing an embedded sonic surface, that serves as an information boundary, isolating the reaction zone behind the lead shock from acoustic perturbations in the far field. The theory generalizes classical notion of a sonic locus in a detonation wave (in steady planar CJ detonation) to unsteady and multi-dimensional detonation waves in explosives with general constitutive description. Particularly, here we apply a simple version of the theory that retains leading contributions from chemical reaction, flow divergence (curvature  $\kappa$ ), and shock acceleration  $\dot{D}$  and uses ideal-gas equation of state. A simple evolution equation is derived that is shown to reproduce the essential physical processes involved in detonation initiation. With the help of the strong-blast wave solution and global description of the chemical heat-release rate, the theory is capable of predicting the critical initiation energy from the thermo-chemical properties of the explosive only. We calculate the

critical energies for a number of explosive mixtures and show that the agreement is remarkably good for most of the mixture compositions considered. It should also be noted that the present theory does not involve the notion of a critical radius, which is a major departure from all previous work. Instead, it is shown that appropriate criticality is based on a critical  $D_s(R)$  ignition curve which we call *ignition separatrix* that separates solutions with initial conditions that lead to ignition from those that lead to failure.

In section 2, we start with a general discussion of the evolution equation that predicts the ignition and failure phenomenon. Section 3 contains the detailed discussion of the solutions of the evolution equation and calculations of the critical energies for several explosive mixtures with comparison against experimental data. Section 4 contains concluding remarks.

## 2 The evolution equation

The basis of the present theory of direct initiation is a general theory of weakly-curved and slowly-varying detonations that are self-sustained and are assumed to contain an embedded sonic locus within the post-shock flow, that is developed in [8, 9, 10]. Specifically, we consider a simplified version of the theory that retains leading order unsteady and shock curvature terms, and obtain an evolution equation in the form of a functional relationship between shock speed  $D$ , its acceleration  $\dot{D}$ , and curvature  $\kappa$ . When applied to spherically (or cylindrically) expanding detonations, the evolution equation is a relatively simple second order ordinary differential equation. Nevertheless, solutions of the equation exhibit basic physical characteristics of the initiation process that are observed in experiments and numerical simulations. Most importantly for the present purpose, it contains the critical behavior of solutions, such that depending on the initial condition, the long-time attractor is either a stable Chapman-Jouguet detonation (in which case we have successful initiation) or an essentially inert decaying shock whose final speed is that of an acoustic disturbance in the unreacted mixture (in which case we have initiation failure).

Here, we summarize the basic ideas of the analysis behind the evolution equation, and refer the reader for a detailed discussion of the theory to [8, 9]. The starting point is the system of reactive Euler equations in which general unsteady terms and leading-order curvature terms have been retained. In addition, one has the Rankine-Hugoniot conditions at the shock. With only these conditions, the system is not closed and requires that some conditions in the far field of the reaction zone be satisfied for determination of the shock speed, a situation analogous to classical Chapman-Jouguet analysis, but complicated by unsteadiness and multi-dimensionality. Such conditions have been derived in [8, 10], and are called speed relation (analog of local sonicity requirement) and compatibility condition (essentially a generalization of the equation for the Riemann invariant on forward-facing characteristics). These equations form a closed system of equations that allow for a solution that includes the detonation speed and the location of the sonic locus.

The reactive Euler equations, written in the shock-attached frame, that retain the general unsteady terms and leading-order curvature terms are

$$M_n = -\rho_t - \kappa\rho(U + D), \quad (1)$$

$$P_n = -M_t - \rho\dot{D} - \kappa\rho U(U + D), \quad (2)$$

$$H_n = -\frac{H_t}{U} - \dot{D} + \frac{p_t}{\rho U}, \quad (3)$$

$$\lambda_t + U\lambda_n = \omega, \quad (4)$$

where conserved variables are introduced,  $M = \rho U$ ,  $P = p + \rho U^2$ ,  $H = e + p/\rho + U^2/2 - \lambda Q$  as mass flux, momentum flux, and total enthalpy, respectively. The primitive variables are density  $\rho$ , pressure  $p$ , particle velocity relative to the shock  $U$ ,  $e$  is the internal energy ( $e = p/\rho/(\gamma - 1)$ ) in the case of an ideal

gas),  $Q$  is the heat of reaction, and reaction progress variable  $\lambda$  is such that  $\lambda = 0$  at the shock and  $\lambda = 1$  at the end of the reaction zone. The reaction rate  $\omega = \omega(p, \rho, \lambda)$  is assumed general for now since the basic analysis does not require that it has a specific form. Subscripts  $t$  and  $n$  indicate time- and space differentiation, respectively. Total time derivative will be indicated by a dot over a symbol. The shock is located at  $n = 0$  and the reaction zone extend to  $n < 0$ .

We rescale the state variables with respect to the initial state by using the ambient pressure  $p_a$ , density  $\rho_a$ , and  $u_a = \sqrt{p_a/\rho_a}$  for velocity. The spatial variable is scaled with respect to the half-reaction length,  $l_{1/2}$ , and time as  $l_{1/2}/u_a$ . All governing equations retain their form.

The following conditions must be satisfied at the sonic locus (denoted by subscript  $*$ ),

$$\dot{n}_* = c_* + U_*, \quad (5)$$

$$\dot{p}_* + \rho_* c_* \dot{u}_* + \kappa \rho_* c_*^2 u_* = (\gamma - 1) Q \rho_* \omega_*, \quad (6)$$

where  $\gamma$  is the ratio of specific heats,  $c$  is the sound speed. Equation 5 is the equation of the forward characteristics, which reflects the fact that the sonic locus in general is a characteristic surface, and Eq. 6 is the form of equation for the  $J_+$  Riemann invariant that must hold on  $C_+$  characteristics; the dot in this equation indicates time-differentiation on this limiting  $C_+$  characteristic. Two equations, Eq. 5 and Eq. 6, are the necessary closure equations that allow one to determine the lead shock speed  $D(t)$  and the sonic locus  $n_*(t)$ . To obtain the evolution equation one has to integrate the Euler equations from the shock to the sonic locus and substitute the result in the sonic conditions.

Now we look for solutions that have slow time evolution, that is the time-derivatives in Euler equation can be considered small in addition to small curvature assumption, that is we assume

$$\kappa = o(1), \quad \frac{\partial}{\partial t} = o(1). \quad (7)$$

In our scales, small curvature means that the length of the reaction zone is much smaller than the radius of shock curvature. Small time derivative means that the dynamical processes of interest take place on time scales long compared to the half-reaction time. We should note that these are two essentially *independent* assumptions and one does not necessarily has to relate them (that is choose a distinguished limit) explicitly in order to proceed with derivations in a consistent manner. For a numerical example illustrating the time scales involved, consider the case of a stoichiometric hydrogen-oxygen mixture for which a detailed calculation of the dynamics is given below. The length of the reaction zone and the detonation speed for the mixture are roughly  $l_{rz} \approx 0.04 \text{ mm}$  and  $D_{CJ} \approx 2800 \text{ m/s}$ , which gives the reaction time scale  $t_{rz} \sim 0.1 \mu\text{s}$ , while the initiation dynamics takes place over time scales of at least  $100 \cdot t_{rz} \approx 10 \mu\text{s}$  (see figure 3). As far as the curvature is concerned, for the same mixture we have  $\kappa < 0.01$  even near the upper turning point (see figure 1).

With the above assumptions and after some algebra, we find that the speed relation, Eq. 5 reduces to the following equation,

$$1 + F - \lambda_* + \kappa f + \dot{D}g = 0, \quad (8)$$

where

$$F = (D^2 - D_{CJ}^2) \frac{D^2 D_{CJ}^2 - \gamma^2}{D^2 (D_{CJ}^2 - \gamma)^2}, \quad (9)$$

and  $D_{CJ}$  is the CJ speed given by

$$D_{CJ} = \sqrt{\gamma + q} + \sqrt{q}, \quad \text{where} \quad q = \frac{\gamma^2 - 1}{2} Q.$$

One can see that for  $D < D_{CJ}$ ,  $F$  is negative; it is also easy to show that  $F \geq -1$  for any  $D$  with  $F = -1$  only if  $D = \sqrt{\gamma}$ , the ambient sound speed. Functions  $f$  and  $g$  are explicit nonlinear functions of  $D$  (see Appendix) that depend on certain integrals over the reaction zone. Notice also that because  $0 \leq \lambda_* \leq 1$ , the speed relation 8 is not always satisfied which puts constraints on the possible dynamics (e.g. the sonic locus may be absent if  $D > D_{CJ}$ ).

The compatibility condition, Eq. 6, can be shown to result in the following equation,

$$\dot{D} = a_1 Q \omega_* - a_2 \kappa, \quad (10)$$

where again,  $a_1$  and  $a_2$  are explicit nonlinear functions of  $D$  and are given in Appendix. By eliminating  $\lambda_*$ , which is the reaction progress variable at the sonic locus, from Eqs. 8 and 10, one obtains a single evolution equation, relating  $\dot{D}$ ,  $D$ , and  $\kappa$ . By setting  $\dot{D} = 0$  in the evolution equation, one obtains the quasi-steady  $D - \kappa$  relation,  $a_1 Q \omega_* = a_2 \kappa$ . The evolution equation holds generally for two-dimensional detonations, but we specify the equation for spherically expanding detonations for the purpose of analyzing the direct initiation problem. We also assume a one-step Arrhenius reaction rate  $\omega = k(1 - \lambda)^v \exp(-E/pv)$  with simple-depletion,  $v = 1$ , where pre-exponent  $k$  is fixed by the scaling choice, and  $E$  is the activation energy. We emphasize that the activation energy is not assumed large, in fact it can be arbitrary. The only assumptions on which the present theory is based are that of small curvature and slow evolution. It is a fully non-linear theory since  $D$  can deviate from  $D_{CJ}$  by  $O(1)$  amount, that is  $D$  does not have to be close to  $D_{CJ}$ .

### 3 Direct initiation of spherical detonation and comparison with experiment

We calculate critical energies for hydrogen-oxygen, hydrogen-air, and ethylene-air mixtures at various equivalence ratios. All global reaction parameters used in this work, that is activation energy  $E$ , heat release  $Q$ , and specific heat ratio  $\gamma$ , are based on the data available at Caltech, [11], which have been derived from detailed chemical calculations for real mixtures. Both activation energies  $E$  and heat releases  $Q$ , which depend on the equivalence ratio  $\phi$ , are taken exactly the same as in the database, but the constant specific heat ratio  $\gamma$  has been chosen so that the post-shock temperature for CJ detonation matches the detailed calculations. Although some of the detonation properties, such as the detonation Mach number or CJ pressure differ somewhat from the detailed calculations, still this is a sensible choice because it retains the overall energetics and state sensitivity of the heat release rate near the shock. Similar parameter assignments were used by Eckett et al. [4].

Next we show how to calculate the critical energy for one of the mixtures, namely stoichiometric hydrogen-oxygen, which has the following parameters:  $\gamma = 1.258$ ,  $E = 38.25$ , and  $Q = 40.5$ . Consider the quasi-steady response, that is  $D - \kappa$  dependence obtained by setting  $\dot{D} = 0$  in Eqs. 8 and 10. Figure 1 shows the dependence with a characteristic turning point and two branches, a stable upper one and unstable bottom one. The stability properties of the two branches will be demonstrated by solving the full equation that retains  $\dot{D}$  term. We point out one important feature of the curve, that is the fact that the bottom branch seems to terminate at  $\kappa = 0$ . But in fact, as in [12] a second turning point always exists at a very small curvature (in figure 1, at a curvature  $\kappa'_c < 10^{-8}$ ) and another stable branch extends to large  $\kappa$  at smaller shock speeds  $D$ , close to  $c_a$ , the ambient sound speed in the unreacted explosive. As an example clearly demonstrating the lower turning point, figure 2 shows theoretically computed  $D - \kappa$  response curve for  $\gamma = 1.258$ ,  $Q = 40.5$ , and a lower value of the activation energy,  $E = 10$ . Thus, the full  $D - \kappa$  curve has a Z-shape. The existence of the second turning point is a property of the one-step Arrhenius model and can have implications for the detonation reignition after apparent failure. Strictly speaking, because of the second turning point, once a decaying transient-wave speed passes through the second turning point at  $R$  large, the shock acceleration  $\dot{D}$  becomes positive and reignition is possible. But how serious is this unphysical feature of the one-step kinetics? From figure 1 one finds that for the stoichiometric hydrogen-oxygen mixture, reignition

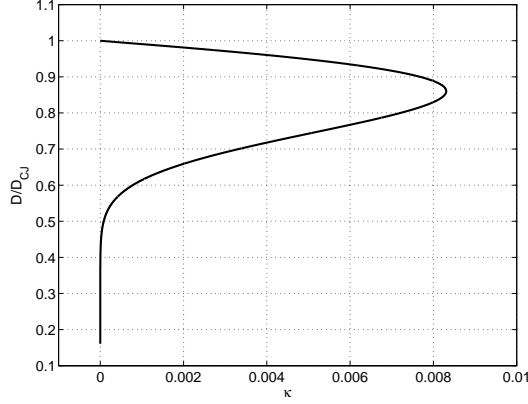


Figure 1: Theoretical  $D - \kappa$  curves for stoichiometric hydrogen-oxygen,  $\gamma = 1.258$ ,  $E = 38.25$ , and  $Q = 40.5$ .

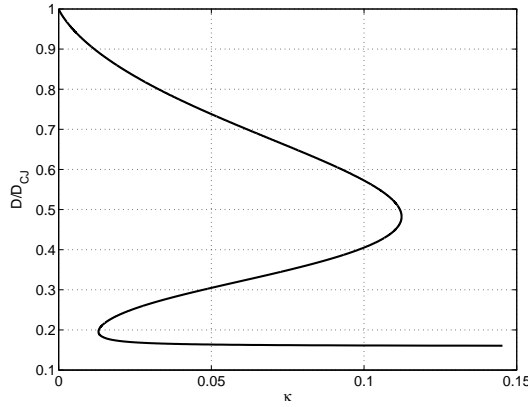


Figure 2: Theoretical  $D - \kappa$  curve at  $\gamma = 1.258$ ,  $E = 10$ , and  $Q = 40.5$  showing both turning points.

at the second turning point is achieved only somewhere at  $R > 10^8$ . In dimensional terms, with the steady reaction zone length of the mixture  $l_{rz} = 0.043 \text{ mm}$ , the lower turning point is located farther than 4 kilometers away from the center, and would not be encountered in practice. In general, the location of the second turning point depends strongly on the activation energy, but real mixtures have sufficiently large activation energies so that the lower turning point is often irrelevant.

Next consider the full evolution equation obtained by substituting  $\lambda_* = 1 + F + \kappa f + \dot{D}g$  from Eq. 8 into Eq. 10,

$$\dot{D} = a_1 Q k (1 - \lambda_*) \exp\left(-\frac{\gamma E}{c_*^2}\right) - a_2 \kappa, \quad (11)$$

where  $c_*^2 = [(\gamma + 1)/\gamma]^2 D^2 / (1 + D^2)^2$ . We write Eq. 11 as a second-order ordinary differential equation in the shock radius  $R = 2/\kappa$  using  $D = \dot{R}$  and  $\dot{D} = \ddot{R}$ . Our goal is to obtain the solution of equation 11 subject to various initial conditions,  $\dot{R}(0) = D_0$  and  $R(0) = R_0$ . Figure 3 shows the computed results. Shown are the quasi-steady  $D - R$  curve (i.e. with  $\dot{D} = 0$ ) and a series of  $D - R$  curves representing solutions of Eq. 11 starting from different initial conditions. An important feature is that solutions with large  $D_0$  (sufficiently strong initiation source) suffer an initial drop in velocity, pass through a minimum and then  $D$  increases and asymptotically approaches  $D_{CJ}$  as  $R \rightarrow \infty$ . But solutions corresponding to initial conditions with low

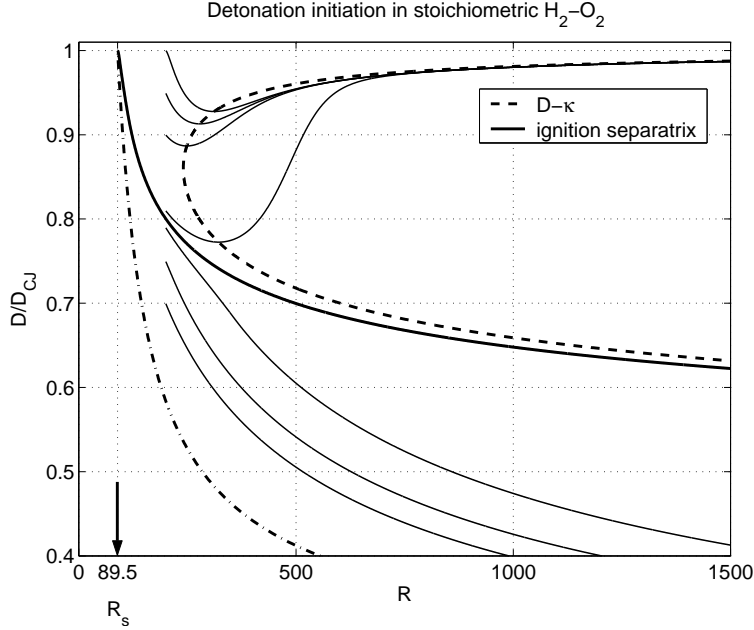


Figure 3: Ignition and failure for a hydrogen-oxygen at  $\phi = 1$ . Thin solid lines are solutions of Eq. 11 for different initial conditions:  $R_0 = 200$  and  $D_0/D_{CJ} = 1.0, 0.95, 0.9, 0.81, 0.79, 0.75$ , and  $0.7$  from top to bottom. Dash-dot line is the reactive blast wave solution at critical energy  $E_c = 1.48 \cdot 10^8$  and radius  $R_s = 89.5$ .

$D_0$  (weak initiation source) decay with  $R$  and never recover. This critical behavior is strikingly similar to what is observed in experiments and numerical simulations of detonation initiation by a strong blast. Thick solid curve in the figure separates states that lead to ignition from those that lead to failure and is designated as the “ignition separatrix”. The separatrix is found by solving the governing evolution equation, Eq. 11, backward in time starting from an initial condition just below the unstable branch of the quasi-steady  $D - R$  curve at a very large distance. Typically we took the initial point at  $R = 10^4 - 10^5$ , although much smaller or larger distances can be taken with very little effect on the curve for small  $R$ , i.e. they all essentially collapse on the same curve as  $R$  decreases. This just demonstrates extreme sensitivity of the dynamics on the initial conditions near the ignition separatrix.

A feature observed in experiments and simulations, but not reproduced by this theory is the appearance of pulsations during and subsequent to the successful initiation phase. A theory that retains higher-order terms, similar to what is found in [13], is required for their prediction, but it is important that the present simplified theory contains the essential physics of the phenomenon, required to delineate criticality.

It is interesting to interpret the solution in the successful initiation case in terms of the form of the evolution equation, Eq. 11. Equation 11 is the dynamical law governing the shock evolution with acceleration  $\dot{D}$  and two “forcing” terms, one positive due to the heat release,  $a_1 Q \omega_*$ , and one negative due to the flow divergence,  $-a_2 \kappa$ . Clearly, the heat release tends to accelerate the shock, while the flow divergence takes away the energy from the shock and tends to decelerate it. At the early stage of the initiation process, that is at small radii, the curvature term is stronger than the heat release term and the shock decelerates. But eventually, the increasing heat release balances the curvature term (corresponds to the minimum on  $D(R)$  curve) and then becomes much stronger than the curvature term, resulting in initiation. During further evolution, the heat release term starts to decrease because the sonic point moves closer to the end of the reaction zone and  $\lambda_* \rightarrow 1$ , as can be seen from the speed relation, Eq. 8. As a result, at large  $R$ , both “forcing” terms



diminish to zero, and one obtains a steady solution  $D = D_{CJ}$  at  $R \rightarrow \infty$ . The heat release “force” is proportional to  $Q$  and depends on the activation energy as  $\exp(-\gamma E/c_*^2)$ . Both of these dependencies have simple physical consequences on the dynamics of initiation. The heat release  $Q$  plays a role of the “strength” of the “force” and the greater  $Q$ , the sooner the initiation takes place. The exponent serves as an energy barrier that delays the initiation process. These effects can be demonstrated by direct solution of Eq. 11, which shows that increasing  $Q$  leads to the shift of the quasi-steady  $D - R$  curve toward smaller  $R$  and hence the initiation occurs at shorter distances from the origin. On the other hand, increasing activation energy  $E$  has the opposite effect, delaying the initiation till the lead shock propagates to larger distances.

Since we have obtained the criticality condition in terms of the initial conditions (that is  $D_0$  and  $R_0$ ) relative to the ignition separatrix, it is important to describe how the initial state is created, and in particular, we relate the initial conditions to a strong point-blast wave solution. Strictly speaking, one has to match the strong-blast wave solution which is valid at  $R \rightarrow 0$  with our theoretical solution that holds at  $D < D_{CJ}$  by means of an intermediate solution that is valid at  $D > D_{CJ}$  and  $R = O(1)$ . Here we adopt a simple matching procedure that connects reactive blast wave solution with the solution of the evolution equation 11 at the point on the ignition separatrix at  $D = D_{CJ}$ , which corresponds to smallest radius on the separatrix, that we denote as  $R_s$ . The reason for this choice is that the blast wave solution is most accurate at smaller radii. Clearly, any point on the ignition separatrix at  $D < D_{CJ}$  can be chosen, but one has to have a blast wave solution that is sufficiently accurate to reproduce the reactive shock wave at such small speeds. With our choice, given the blast wave solution as  $D(R, E_{bw})$  with source energy  $E_{bw}$ , and letting the solution pass through  $D_{CJ}, R_s$ , we can estimate the critical energy  $E_c = E_{bw}$ . We use the Taylor-Sedov-Korobeinikov blast wave solution, [14, 15, 17, 4],

$$E_{bw} = A_j \left( \frac{j+3}{2} \right)^2 \rho_0 D_{bw}^2 R^{j+1} \exp\left(-\frac{B_j Q}{D_{bw}^2}\right), \quad (12)$$

which accounts for the leading-order asymptotic effect of the chemical reaction on the strong blast dynamics ( $j = 0, 1, 2$  correspond to planar, cylindrical, and spherical symmetry, respectively). In the case of a spherical detonation, the constants  $A_2$  and  $B_2$  are functions of  $\gamma$  that can be calculated by the following formulas, given in Korobeinikov, [16, 17], which we reproduce here for the sake of completeness,

$$A_2 = 0.31246 (\gamma - 1)^{-1.1409 - 0.11735 \log_{10}(\gamma - 1)}, \quad (13)$$

$$B_2 = 4.1263 (\gamma - 1)^{1.253 + 0.14936 \log_{10}(\gamma - 1)}. \quad (14)$$

Figure 3 shows the blast wave solution for the critical initiation energy as a dash-dot line.

Following the procedure described above, we have calculated the critical energies for hydrogen-oxygen, hydrogen-air, and ethylene-air mixtures for a range of equivalence ratios, and compared the predictions with recent experimental data. The detonation database at Caltech, [11], was used as a source of the experimental data. The results are shown in Figs. 4-6. Excellent agreement is found for hydrogen-oxygen, especially near the stoichiometry. Except for lean mixtures, hydrogen-air also shows very close agreement with experiment. From detailed chemical calculations, the two lean compositions of hydrogen-air with very large initiation energies, have reaction zone thicknesses of 91.3 and 2.3 mm and very large activation energies. Initiation energy is quite sensitive to both of these parameters and possible errors could be amplified by orders of magnitude. As for the ethylene-air mixtures, the present theory overpredicts the critical energies by about an order of magnitude, although the overall shape of the curve is reproduced very well.

Figures 4-6 also show a comparison with predictions based on He & Clavin’s theory [5]. To calculate

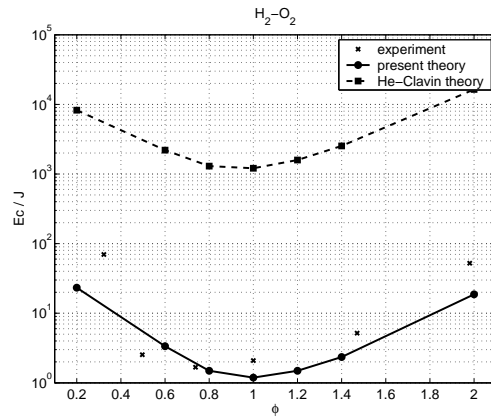


Figure 4: Comparison of theoretical and experimental, [18], critical energies for hydrogen-oxygen mixtures.

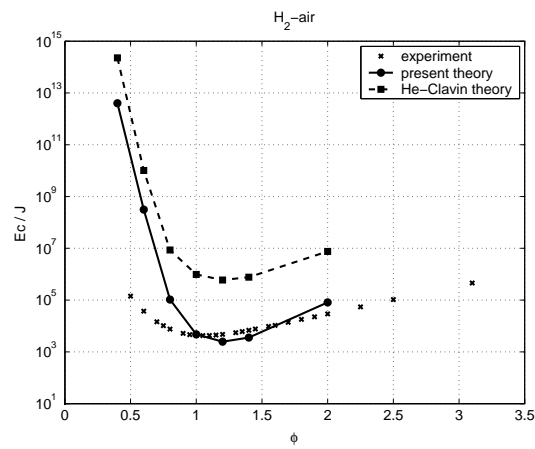


Figure 5: Comparison of theoretical and experimental, [19], critical energies for hydrogen-air mixtures.

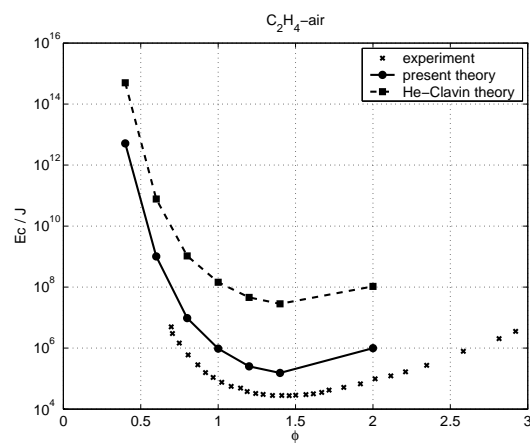


Figure 6: Comparison of theoretical and experimental, [19], critical energies for ethylene-air mixtures.

the dimensionless critical energy we use

$$E_c = A_j \left( \frac{j+3}{2} \right)^2 \rho_0 D_c^2 R_c^{j+1}, \quad (15)$$

where

$$D_c = D_{CJ} \left( 1 - \frac{1}{2\vartheta} \right), \quad R_c = \frac{8e j \gamma^2}{\gamma^2 - 1} \quad (16)$$

are the critical speed and critical radius at the quasi-steady turning point as predicted by the square-wave model of He & Clavin [5],  $\vartheta = ET_a/T_s$  is the post-shock temperature-scaled activation energy. As all comparisons show, the theory based on the quasi-steady turning point overestimates the experimental critical energy by about 3 orders of magnitude, as was also pointed out by Eckett et al. [4]. For numerical comparison, consider the stoichiometric hydrogen-oxygen, for which we have:  $\gamma = 1.258$ ,  $Q = 40.5$ ,  $E = 38.25$ ,  $D_{CJ} = 7.0478$ ,  $R_s = 89.5$ ,  $l_{rz} = 0.043 \text{ mm}$ ,  $\vartheta = 6.386$ ,  $A_2 = 1.3349$ ,  $B_2 = 0.8512$ . Then we find that the present theory predicts  $E_c = 1.192 J$ , He and Clavin's theory gives  $E_c^{HC} = 1.213 \cdot 10^3 J$ , while the experimental result is  $E_c^{exp} = 2.092 J$ . Overprediction of the critical energies seems to be a general feature of a theory that defines the criticality by the upper turning point of the quasi-steady  $D - \kappa$  curve, which apparently has to do with the actual onset of unsteady self-sustained detonation at radii much below the quasi-steady critical radius. That higher-order unsteady contributions can change the critical conditions significantly compared to the quasi-steady theory was first demonstrated by Eckett et al. [4] in a combined numerical-analytical study. Their simulations and the present theory are in agreement in that the critical conditions occur well before the quasi-steady critical radius is reached. In view of the sensitivity of the critical energy to the radius ( $E_c \sim R^3$ ), accurate prediction of the ignition separatrix is extremely important.

Considering numerous uncertainties and sources of error involved in both experiment and kinetic data used for theoretical predictions (for more detailed discussion of these issues, see [4]), and that the theory does not rely on any fitting adjustments, the agreement can be considered quite satisfactory to excellent. It is also possible that higher order corrections to the evolution equation that account for oscillatory or cellular dynamics similar to that observed in experiments and simulations, may adjust the critical initiation conditions, but that is a subject for future analysis, as are the demands for more precise experimental measurements and precise constitutive descriptions.

We make a final remark regarding the constitutive description on which the present study is based. Theories and models based on one-step Arrhenius kinetics have been criticized over recent years because of the unphysical feature essentially associated with the lower turning point on the  $D - \kappa$  curve, namely that such kinetics predicts that reignition occurs after an initial decay, given detonation is allowed to run sufficiently far. In the absence of a satisfactory theory, even an extreme call has been made that the one-step model "...should be abandoned in favor of more complex chemistry...", [1]. While, undoubtedly, studies of the role played by more complex chemistry are important, it is also clear that the single-step kinetics has tremendous power in predicting not only qualitative aspects, but as can be seen from this work, even sensitive quantitative aspects of direct initiation. The problem of delayed reignition behavior is essentially absent in the systems that we have considered here, because the second turning point is located at unrealistically large distances from the origin. The most important features here are the upper turning point and the ignition separatrix. In the context of a corresponding evolution equation derived from the full reactive Euler equations, they define criticality and allow connection to an external initiating point-blast source in a theory of direct initiation.

## 4 Conclusions

In this paper we have presented a simplified version of a general theory developed by us in [8, 9, 10] and applied it to the problem of initiation of spherical detonation by a strong blast wave. We have shown that the evolution equation of the theory exhibits ignition/extinction phenomenon and that it predicts an ignition separatrix which is a curve in the plane of the shock speed vs the shock radius such that any initial condition above the separatrix leads to ignition while that below it leads to failure. A major strength of the present theory is that it does not involve any empirical input, besides the constitutive description of the explosive gas. By using a global kinetic description derived from detailed chemical calculations, we calculated critical initiation energies for hydrogen-oxygen, hydrogen-air, and ethylene-air, and found close agreement with recent experimental data.

## Acknowledgments

The authors would like to thank Brad Wescott for his original work on comparison of the present theory with direct numerical simulations of detonation diffraction. This work was financially supported by U.S. Air Force Office of Scientific Research under contracts F49620-00-1-0005 and F49620-03-1-0048, Program Manager Dr. Arje Nachman. D.S.S. was also supported by the U.S. Air Force Research Laboratory Munitions Directorate, Eglin AFB, under contract F8630-00-1-0002, and by the U.S. Department of Energy, Los Alamos National Laboratory, DOE/LANL 3223501019Z.

## Appendix: Functions in the evolution equation

The following functions are used in the evolution equation 11:

$$a_1 = \frac{\gamma+1}{\gamma} \frac{(\gamma^2-1)D^3}{(1+D^2)(\gamma+3D^2)}, \quad a_2 = \frac{\gamma}{\gamma+1} \frac{(1+D^2)(D^2-\gamma)}{\gamma+3D^2}, \quad (17)$$

$$b = \frac{D(D_{CJ}^2 - \gamma)}{\gamma D_{CJ}(1+D^2)}, \quad f(D) = \frac{2}{b^2} \left[ n_{0*} - I_0 + \frac{D^2}{1+D^2} (n_{0*} - J_0) \right], \quad (18)$$

$$g(D) = \frac{2}{b^2} \left[ \frac{1 + (2 - 1/\gamma^2)D^2}{(1+D^2)^2} (n_{0*} - I_0) + \frac{hD}{2(1+D^2)^2} S_1 - \frac{1}{D} I_1 \right], \quad (19)$$

$$n_{0*} = -D \int_0^{1+F} \frac{d\lambda_0}{\rho_0 \omega_0}, \quad I_0 = -D \int_0^{1+F} \frac{d\lambda_0}{\omega_0}, \quad J_0 = -D \int_0^{1+F} \frac{d\lambda_0}{\rho_0^2 \omega_0}, \quad (20)$$

$$I_1 = -D \int_0^{1+F} \frac{\partial \rho_0}{\partial D} \frac{d\lambda_0}{\rho_0 \omega_0}, \quad S_1 = -D \int_0^{1+F} \frac{\partial p_0}{\partial D} \frac{d\lambda_0}{\rho_0 \omega_0}, \quad (21)$$

$$\rho_0 = \frac{\gamma+1}{\gamma} \frac{D^2}{1+D^2} \frac{1}{1-\delta_0}, \quad p_0 = \frac{1+D^2}{\gamma+1} (1+\gamma\delta_0), \quad \delta_0 = b\sqrt{1+F-\lambda_0}. \quad (22)$$

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