



Calhoun: The NPS Institutional Archive

DSpace Repository

Faculty and Researchers

Faculty and Researchers' Publications

1983

A Method of Calculation of the Critical Energy for Direct Initiation of Unconfined Detonation

Eidelman, Shmuel

Gordon and Breach Science Publishers

Eidelman, Shmuel (1983) A Method of Calculation of the Critical Energy for Direct Initiation of Unconfined Detonation, Combustion Science and Technology, 30:1-6, 133-144, DOI: 10.1080/00102208308923616 http://hdl.handle.net/10945/68428

This publication is a work of the U.S. Government as defined in Title 17, United States Code, Section 101. Copyright protection is not available for this work in the United States.

Downloaded from NPS Archive: Calhoun



Calhoun is the Naval Postgraduate School's public access digital repository for research materials and institutional publications created by the NPS community. Calhoun is named for Professor of Mathematics Guy K. Calhoun, NPS's first appointed -- and published -- scholarly author.

> Dudley Knox Library / Naval Postgraduate School 411 Dyer Road / 1 University Circle Monterey, California USA 93943

http://www.nps.edu/library

A Method of Calculation of the Critical Energy for Direct Initiation of Unconfined Detonation

SHMUEL EIDELMAN Research Associate, Department of Aeronautics, Naval Postgraduate School, Monterey, CA 93940

(Received August 5, 1981; in final form June 25, 1982)

Abstract—A simple method is developed which allows the calculation of the minimum energy of direct initiation of unconfined detonations with cylindrical and spherical symmetry. The method uses the detonability limit data for planar detonations, and the data on reaction zone length for computation of the critical energy of initiation. The results are verified by comparison with available experimental data and by numerical simulation of the full governing equations.

I INTRODUCTION

The lack of well-founded closed theory led to experimental studies for the wide range of the initiation conditions (Matsui and Lee, 1979; Lee and Matsui, 1977) and to full-scale experiments, to study the threshold for the direct spherical (Bull *et al.*, 1976, 1978; Atkinson *et al.*, 1980) and planar (Benedick, 1979) detonations in gaseous mixtures.

First research to define the limits of detonation phenomena was conducted using shock tube technique. In this case the initiating shock and the detonation wave had the planar symmetry (Schelkin and Troshin, 1964). The shock tube technique is a well-established experimental technique, where the initial condition of the mixture, the initiating energy and the detonation wave parameters could be measured with high accuracy relatively easily. But the initiation limits obtained in shock tubes are not applicable to the more interesting cases of unconfined spherical and cylindrical detonations.

The present work, on the basis of the developed model of direct initiation of unconfined detonations, explores the method of calculation of the critical energy of direct initiation. The developed method allows the calculation of the critical energy of direct initiation of unconfined spherical detonation in combustible mixture using the shock tube data of the detonability limits for the same mixture.

II THE MATHEMATICAL MODEL

The direct initiation of an unconfined, self-sustained detonation wave can occur under certain specific conditions. One of the main conditions is the generation of a supersonic compression front of sufficient strength to initiate fast exothermal reactions in the medium. The energy released in these exothermal reactions must be sufficient to compensate for the energy density lost through hydrodynamic expansion and for the work done on the surrounding medium.

Let us assume that both these conditions have been met at a great distance from the initiation region and that the self-sustained detonation wave is propagating with a constant velocity through the combustible medium. It is obvious that if the detonation

wave is distant enough from the initiation region, its parameters are not dependent on the symmetry of the wave or on the reaction zone length. Moreover, its parameters could be found with very good accuracy using Chapman-Jouguet's theory, which does not consider any one of these factors. On the other hand, if the initiation source produces in its vicinity a supersonic compression front of sufficient strength to initiate fast exothermal reactions, this is not a sufficient condition for direct initiation of the self-sustained detonation wave. The experimentally determined, minimum critical energy needed for direct initiation varies by three or more orders of magnitude for different fuels and for initiation sources of different geometry. The initiation energy is larger than that required to produce the supersonic compression front necessary for initiation of fast chemical reactions in the medium.

Why, in most cases, is the achievement of the necessary conditions for initiation not sufficient for the formation of the self-sustained detonation wave? This question leads to the concept that in most cases the energy of combustion required for self-sustained detonation waves is a function of the distance from the initiation source.

Figure 1 shows the pressure distribution behind the front of a typical detonation wave. The region behind the wave front is divided into two zones. Zone I lies from the radius r=0 up to the Chapman-Jouguet point. Zone II is beteen the Chapman-Jouguet point and the front of the detonation wave. Let us estimate the energy which is contained in each of these zones.



FIGURE 1

We now consider the self-sustained detonation wave. Its parameters and the structure of the wave shown in Figure 1 do not change over time. If the kinetic energy of Zone I is neglected (because the mass velocity of the gas is very low in this region) and the average pressure is taken equal to $1.25 \times P$ (see Figure 1), then the energy of Zone I:

$$E_{\rm I} = \frac{1}{\nu} \sigma_{\nu} S \left(\frac{1.25 P}{\gamma - 1} \right) r_1^{\nu} \tag{1}$$

where $\nu = 1, 2, 3$ for planar, cylindrical and spherical symmetries.

$$\sigma_{\nu} = 2 (\nu - 1)\pi + (\nu - 2) (\nu - 3)$$

S = 1[m^(3-\nu)]—dimensional coefficient

The kinetic energy of Zone II should be considered. Let us assume it to be the average between the kinetic energy at the shock front and the kinetic energy at the Chapman-Jouguet plane. Let us also assume that the pressure in Zone II is equal to the average of the pressure immediately behind the shock front and at the Chapman-Jouguet plane. These assumptions yield an approximate value of $2.5 \times P$. Zone II energy then will be:

$$E_{\rm II} = \frac{1}{\nu} \sigma_{\nu} S\left(\frac{2.5 P}{(\gamma - 1)} + \frac{\rho_{cJ} V_{cJ}^2 + \rho_{sh} V_{sh}^2}{4}\right) (r_2^{\nu} - r_1^{\nu}) \tag{2}$$

where ρ_{CJ} , V_{CJ} -density and the mass velocity of the gas at the Chapman-Jouguet point. ρ_{sh} , V_{sh} -density and the mass velocity of the gas immediately behind the shock front.

The accurate calculation of the energy of Zones I and II using the numerical code simulating the full governing equation (Eidelman and Burcat, 1981), shows that Eqs. (1) and (2) approximate these values with 10–15 percent accuracy.

Let us now calculate the energy increment of Zone I, when the wave radius increases by Δr :

$$\Delta E_{\rm I} = 2S \, \frac{1.25 \, P}{(\gamma - 1)} \, \Delta r, \quad \text{for } \nu = 1 \tag{3a}$$

$$\Delta E_{\rm I} = \pi S \frac{1.25 P}{(\gamma - 1)} (2\Delta r r_1 + \Delta r^2), \text{ for } \nu = 2$$
(3b)

$$\Delta E_{\rm I} = \frac{4}{3} \pi \frac{1.25 P}{(\gamma - 1)} (3r_1^2 \Delta r + 3r_1 \Delta r^2 + \Delta r^3), \quad \text{for } \nu = 3 \tag{3c}$$

The energy increment of Zone II when the detonation wave radius increases by Δr will be:

$$\Delta E_{II} = 0, \quad \text{for } \nu = 1 \tag{4a}$$

$$\Delta E_{II} = \pi SA(2\Delta r r_2 - 2\Delta r r_1), \text{ for } \nu = 2$$
(4b)

$$\Delta E_{II} = 4/3\pi A[3\Delta r^2 (r_2 - r_1) + 3\Delta r(r_2^2 - r_1^2)] \text{ for } \nu = 3$$
(4c)

where

$$A = \left(\frac{2.5 P}{\gamma - 1} + \frac{\rho_{cJ} V_{cJ}^2 + \rho_{sh} V_{sh}^2}{4}\right)$$

At the large distance from the initiation source the reaction zone length is negligible comparative to the detonation wave radius. This means that the energy of Zone II is negligible compared to the energy of Zone I, which leads to the conclusion that if the detonation wave is distant enough from the initiation region, its parameters are not dependent on the symmetry of the wave or on the reaction zone length, and its parameters could be found with very good accuracy using the Chapman-Jouguet theory.

On the other hand, in the vicinity of the initiating source, the energy of Zone II and Zone I is of the same order of magnitude. This means that the energy of Zone II and the peculiarities of the flow in Zone II should affect the evolution of the detonation wave in the vicinity of the initiating source.

To be able to compare the energy required for a self-sustained detonation wave at the large and small distances from the initiation source, let us now calculate the limit of the ratio between the total energy behind the detonation wave and the energy of the Zone I, when $\Delta r \rightarrow 0$:

$$F_1(r_1, L) = \lim_{\Delta r \to 0} \frac{\Delta E_1 + \Delta E_{11}}{\Delta E_1} = 1, \text{ for } \nu = 1$$
(5a)

$$F_2(r_1, L) = \lim_{\Delta r \to 0} \frac{\Delta E_1 + \Delta E_{11}}{\Delta E_1} = 1 + \frac{A(\gamma - 1)}{P \, 1.25} \, \frac{L}{r_1}, \quad \text{for } \nu = 2 \tag{5b}$$

$$F_{3}(r_{1},L) = \lim_{\Delta r \to 0} \frac{\Delta E_{I} + \Delta E_{II}}{\Delta E_{I}} = 1 + \frac{A(\gamma - 1)}{P \, 1.25} \left(\frac{2L}{r_{1}} + \frac{L^{2}}{r_{1}^{2}}\right), \text{ for } \nu = 3$$
(5c)

where $L = r_2 - r_1$, the reaction zone length.

We conclude from Eqs. (5a), (5b) and (5c) that at the large distance from the initiating source $(r_1 \rightarrow \infty)$, the energy requirement for self-sustained detonation wave is not dependent on the symmetry of the flow nor on the peculiarities of the flow in Zone II.

On the other hand, in the vicinity of the initiation source or during the initiation process, the energy and the peculiarities of the flow in Zone II are very important. Equations (5a), (5b) and (5c) show that in the vicinity of the initiation source the energy requirements for the self-sustained detonation wave vary according to the symmetry of initiation.

In the case of planar symmetry, the energy requirement is not dependent on the distance from the initiating source and the length of the reaction zone. For this reason the direct initiation of the planar detonation must be the easiest to attain. We will use this peculiarity of the planar detonation in calculation of the critical energy of initiation for spherical case.

In the cases of cylindrical and spherical symmetry, as Eqs. (5b) and (5c) show, the energy required for self-sustained detonation is a function of the radius r_1 and the reaction zone length L. In these cases, according to Eqs. (5b) and (5c), in the region close to the initiation source the values of F_2 and F_3 can be considerably larger than 1. For example, if L=1 cm, $r_1=10 \text{ cm}$ and $[A(\gamma+1)/P \ 1.25]=2$ (which is a minimum

.

.

estimate not taking into account the kinetic energy of the gas), then $F_3=1.42$. This means that to support the self-sustained detonation wave at the constant level, the energy released from the medium at the radius 10 cm must be 42 per cent larger than what is required at a very large distance from the source. If the density of the chemical energy, which can be released in the detonation process, is constant, the propagating detonation wave will have an *energetic deficit* which decreases when the radius of the wave increases. For this reason, when the detonation wave is initiated by a spherical or cylindrical source with the energy close to critical, it has a region of decay. If this decay does not bring to an end rapid combustion in the reaction zone, the detonation wave, after reaching its minimum value, is gradually accelerated towards the Chapman-Jouguet detonation velocity of the mixture. This behavior of the detonation wave was observed experimentally by Bar-Or *et al.* (1980) for cylindrical symmetry and by Bull *et al.* (1978) for spherical symmetry.

Mitrofanov *et al.* (1979), Eidelman and Burcat (1980), and Eidelman and Sichel (1981) all have simulated detonation wave decay and acceleration in two-phase medium. In these works (Eidelman and Burcat, 1980; Eidelman and Sichel, 1981) the value of the detonation wave parameters of the minimum point were found to be inversely dependent on the reaction zone length, which is in qualitative agreement with Eq. (5c), where increase of the reaction zone length leads to increase of the energetic deficit; in other words decrease of the detonation wave.

III TEST OF THE MODEL OF ENERGETIC DEFICIT

When a detonation wave is initiated in a two-phase medium the energetic deficit should be greater than that of the gaseous phase detonation, because the reaction zone length is usually larger in the former than in the latter. Numerical modeling of spherical two-phase detonation, initiation, and propagation shows decay of the detonation wave to the minimum value point. In some cases the pressure immediately behind the shock front during the initiation period is half that of the Chapman-Jouguet detonation wave (Eidelman and Burcat, 1980; Eidelman and Sichel, 1981).

A series of numerical simulations were carried out to test qualitatively and quantitatively the model of energetic deficit. The detailed exposition of the direct initiation problem including the basic assumptions and the mathematical model has been presented previously (Eidelman and Burcat, 1980). The details of the numerical solution and the algorithm for the calculations are also published (Eidelman and Burcat, 1981). The mathematical model and method of numerical solution, therefore, are only described briefly below. The conservation equations governing the flow are written separately in Eulerian form for the solid or liquid fuel and the gaseous oxidizer. In this study the equations for the one-dimensional case with spherical symmetry were used. The conservation equations of the gaseous and condensed phases are interconnected through source terms on the right-hand side of the equations, which describe the mass, momentum, and energy exchange between phases. The fuel particles or droplets are considered to behave as a continuous medium composed of noninteracting spheres whose size is equal to the average size of the particles or droplets in the cloud. It is assumed that chemical reactions occur only in the gas phase, and that the burning rate of the condensed phase fuel is determined by the rate of evaporation. A combined evaporation and shattering model was used to reproduce the reaction zone lengths observed in experiments. The initial distribution of gas dynamic parameters behind the shock wave was calculated using the similar

solution for the deposition of a finite amount of explosive energy as described previously (Burcat *et al.*, 1978). This "starting solution" introduces the initiating charge into the model.

The Flux Corrected Transport (FCT) method was used for numerical solution of the problem (Eidelman and Burcat, 1981). This method is particularly well suited to problems with complex shock waves since the numerical diffusion generated by this method is the lowest among presently known algorithms.

The general error of the code was determined by applying it to the model problem of the propagation of a blast wave from a strong point explosion without counterpressure. Comparing the numerical to the exact analytical solution it was found that the phase error was less than 2 percent and the amplitude error was less than 3 percent.

For the numerical simulation two kinds of combustible media were chosen:

a) Stoichiometric mixture of oxygen and decane droplets with diameter 120 μ .

b) Stoichiometric mixture of oxygen and decane droplets with diameter 300 μ .

The reaction zone length for these mixtures differs by approximately one order of magnitude during the initiation process. This difference allows us to evaluate the influence of this parameter on the model of energetic deficit.

For each of these mixtures, three kinds of the numerical simulations were performed :

I) Initiation and propagation of a planar detonation wave.

II) Initiation and propagation of a spherical detonation wave.

III) Initiation and propagation of a spherical detonation wave with compensation for energetic deficit.

In this case the energy released behind the shock front was assumed to follow Eq. (5c). That means that compensation for the energetic deficit in the initiation region was done by artificially increasing the thermal effect of the chemical reaction per unit mass of fuel according to Eq. (5c).

The results of these simulations are presented in Figure 2, which plots detonation wave velocity versus shock radius. In cases of spherical symmetry the energy of the igniting explosion was equal to 156,000 J, while in cases of planar symmetry the corresponding value was $3 \times 10^6 \text{ J/m}^2$. The velocity of the Chapman-Jouguet detonation was calculated for a stoichiometric gaseous mixture of deeane and oxygen using the Gordon and McBride (1971) program. The calculated Chapman-Jouguet value is noted on the velocity scale of Figure 2.

Figure 2 reveals quite clearly that, in cases of planar detonation, the initiation process proceeds without a significant region of decay. Beyond 0.6 m graphs 1 and 2 coincide, regardless of differences in the reaction zone length (2 cm for Case 1 and 6 cm for Case 2). The velocity of the detonation wave for Case 1 is equal to the Chapman–Jouguet detonation velocity of the mixture at a distance of 0.2 m from the initiating source. In Case 2 the C–J velocity is reached at a distance of 0.6 m. After initiation the wave decay is up to 5 percent below the C–J velocity value. This can be explained by the energetic deficit caused by changes in the detonation wave structure, which are not considered in Eqs. (5a), (5b) and (5c) and which are larger in Case 2 because of the greater reaction zone length.

In Cases 5 and 6 spherical detonation was initiated in mixtures "a" and "b". In accordance with the significant energetic deficit predicted by Eq. (5c), the detonation wave decayed far below the C-J velocity. After reaching its minimum value the detonation wave accelerated slowly.



The decay is much greater in Case 6, because the reaction zone length is larger. This is in accordance with Eq. (5c), which holds that reaction zone length and energetic deficit are directly proportional to one another.

In Cases 3 and 4 the energetic deficit of the spherical detonation initiation process was compensated for in accordance with Eq. (5c). Figure 2 reveals that the energy released in accordance to Eq. (5c) completely compensated for the energetic deficit of the initiation process. The detonation wave in these cases does not decay below 5 percent of the C–J velocity and steady-state detonation with the velocities close to the C–J velocity value are achieved at a distance of 0.3–0.4 m from the initiation source.

In the process of testing the energetic deficit model, the energy of Zones I and II was calculated. In the case of planar detonation, the energy of Zone II is constant beyond radius 0.25 m for Case 1, and 0.5 m for Case 2, which is consistent with Eq. (5a).

In Cases 3 and 4, when the energetic deficit was artificially compensated for, the actual ratio of the energies of Zone II and I differed by only 5-13 percent from those predicted by Eq. (5c).

Thus, Eq. (5c) gives a very good approximation of the energetic deficit of the initiation process in cases of spherical detonation.

IV CALCULATION OF THE ENERGY FOR DIRECT INITIATION, USING THE ENERGETIC DEFICIT MODEL

For direct initiation of the self-sustained detonation wave, the energetic deficit of the initiation process of spherical and cylindrical detonations is usually compensated for by increasing the igniting source energy. The increase in the energy released by the igniting source, increases the radius of the region of the overdriven detonation wave. This permits initiation of a self-sustained detonation wave beyond the radius where the energetic deficit given by Eqs. (5b) and (5c) is small and does not result in the complete decay of the detonation wave.

The determination of the threshold for the direct initiation of the self-sustained detonation is of significant applied interest. Equations (5a), (5b) and (5c) allow the calculation of the critical energy for direct initiation of the spherical and cylindrical detonations if the detonation thresholds for planar case are known. As we noted before, Eqs. (5a), (5b) and (5c) show that the planar detonation is easiest to obtain, because in planar case the propagating detonation wave does not have the energetic deficit in the region of the initiation source. For this reason the case of the planar detonations.

In order to calculate the minimum initiation energy using the energetic deficit model one needs to define how much energy should be released by the source of the initiation to compensate for the energetic deficit. Therefore, a new concept—*Minimum Compensation Energy*—should be introduced. Here we will define this concept in order to present an unambiguous method of calculation of the minimum energy for direct initiation of the unconfined spherical or cylindrical detonations.

Minimum compensation energy is the minimum additional energy needed to be released in the process of direct initiation of spherical or cylindrical detonations in order to compensate for the energetic deficit up to the level of the planar detonation wave at the detonation limits. This energy extends the radius of the overdriven detonation to the point where the energetic deficit given by Eqs. (5b) and 5c) will be at least equal to the deficit of the energy at the lean detonability limit, determined experimentally by the shock tube technique, comparing with the stoichiometric concentration for the same combustible mixture. In this instance the energetic deficit in the cases of cylindrical or spherical detonations will not lead to the complete decay of the detonation wave. The detonation wave after *reaching* its minimum in the vicinity of the initiation source will reinforce itself up to the steady-state detonation.

The minimum compensation energy can be calculated using Eqs. (5a), (5b) and (5c). For cylindrical symmetry it is given by:

$$E_{c2} = 2\pi \int_{r_0}^{r_c} [F_2(r_1, L) - F_1] Q r_1 dr_1 = 2\pi \int_{r_0}^{r_c} \frac{A(\gamma - 1)L Q}{P 1.25} dr_1$$
(6a)

For spherical symmetry it will be:

$$E_{c3} = 4\pi \int_{r_0}^{r_c} [F_3(r_1, L) + F_1] Q r_1^2 dr_1$$

= $4\pi \int_{r_0}^{r_c} \frac{A(\gamma - 1)}{P 1.25} \left(\frac{2L}{r_1} + \frac{L^2}{r_1^2}\right) Q r_1^2 dr_1$ (6b)

- where E_{c2} , E_{c3} —minimum compensation energy for cylindrical and spherical symmetry respectively;
 - r_0 initiating source radius;
 - r_c —minimum compensation radius;
 - Q —heat release per unit volume for the stoichiometric mixture.

It is assumed that the detonation wave parameters do not change during the initiation process the minimum compensation energy can be simply calculated:

$$E_{c2} = 2\pi \frac{A(\gamma - 1)}{P \, 1.25} \, Q \, L(r_c - r_0) \tag{7a}$$

$$E_{c3} = 4\pi \frac{A(\gamma - 1)}{P \ 1.25} Q[L(r_c^2 r_{-0}^2) + L^2(r_c - r_0)]$$
(7b)

The minimum energy of the direct initiation can be determined from:

$$E_{\min} = E_{ct} + E_0 \tag{8}$$

where i = 2, 3 for cylindrical and spherical symmetry respectively;

 E_0 — energy release behind the radius r_0 .

The value of r_0 must be larger than the reaction zone length L. The energy E_0 must be of sufficient magnitude to generate a supersonic compression front sufficiently strong to initiate fast exothermal reactions in the medium. Shock tube data on the initiation of the detonation waves obtained by the bursting diaphragm or other planar initiation source could be used to determine this condition. With this information the minimum value of E_0 in Eq. (8) can be found.

The value of E_{ct} can be determined if the minimum compensation radius r_c is known. According to our definition, the energetic deficit radius r_c from the initiation source is small and a self-sustained detonation wave can propagate in the mixture beginning from the radius r_c regardless of the energetic deficit.

V RESULTS

In order to calculate the minimum energy of initiation using the method presented in this article, one needs to know the detonability limits of the combustible mixture. We will use the data obtained recently by Borisov and Loban (1977) for different hydrocarbon-air mixtures.

For example, let us calculate the minimum energy required for direct initiation of the spherical detonation wave in a propane/air mixture. To calculate the value of E_{c3} from the Eq. (6b) we should know the minimum compensation radius r_c for this mixture. According to our definition of the minimum compensation energy, at the radius r_c the energetic deficit given by Eq. (5c) should be equal to the deficit of the energy at the lean detonability limit of propane/air comparing with the stoichiometric propane/air mixture. For the propane/air, the lean detonability limit is $\lambda=0.64$ (Borisov and Loban, 1977) [where $\lambda=(fuel\divair)/(fuel\divair)$ stoichiometric]. The energetic deficit of this mixture, compared with the stoichiometric propane/air

mixture, will be $1 - \lambda = 0.36$. Now the r_c value can be calculated from Eq. (5c):

$$\frac{A(\gamma-1)}{P\cdot 1.25} \left(\frac{2L}{r_c} + \frac{L^2}{r_c^2}\right) = 0.36 \tag{9}$$

 $[A(\gamma+1)/P \cdot 1.25] \simeq 2$, if we neglect the kinetic energy of the gas in Zone II (see Figure 1). The reaction zone length of this mixture for the Chapman-Jouguet detonation, according to Burcat *et al.* (1971) ignition delay data is $L \simeq 0.03$ m. Then, solving Eq. (9), we arrive at:

$$r_c = 0.354$$
m.

If $r_0 = L = 0.03$ m, E_{c3} can be calculated from Eq. (7b):

$$E_{c3}\simeq 0.38\times10^6$$
 j

To generate a supersonic compression front which will have a velocity of 2000 m/sec (maximum velocity of the detonation wave in this mixture is 1815 m/sec; see Borisov and Loban, 1977) at the distance of $r_0=0.03$ m from the point initiation source one will need:

$$E_0 = 0.351 \times 10^3 \text{ j}$$

Now the minimum energy of the initiation can be calculated using the Eq. (8):

$$E_{\min} = E_{c3} + E_0 \simeq 0.38035 \times 10^{6} \text{ j}$$

The experimentally found minimum of the initiation energy in the propane/air mixture is $E_{ex}=0.388 \times 10^6$ j (Bull *et al.*, 1978), which is very close to the calculated value.

In Table I we presented the values of the minimum energy of the initiation calculated for the conditions of spherical and cylindrical detonations using the model of energetic deficit along with the data experimentally obtained by Bull *et al.*, 1978. Because of the lack of the experimental data required for calculation we were able to calculate the minimum energy of the initiation for only four fuel/air mixtures. The theoretically obtained values of the E_{\min} in spherical cases are very close to the values determined by Bull *et al.* (1978). Unfortunately, we did not find the experimental data to compare with calculated minimum energy of initiation for cylindrical detonations.

VI DISCUSSION AND CONCLUSIONS

The model developed here verifies that the process of direct initiation of the detonation wave differs significantly for planar, spherical, or cylindrical detonations. The energy requirements for the self-sustained detonation wave in the planar case does not change in the medium surrounding the initiator. In spherical and cylindrical detonation the energy requirement for the self-sustained detonation wave is a function of the distance from the initiator and reaction zone length.

In this study the mathematical expressions representing the energetic deficit of the initiation process were found. By a series of numerical experiments it was shown that compensation for the energetic deficit in accordance with the analytically determined function resulted in the spherical and planar initiation processes to evolve similarly.

Mixtures	Fuel stoichiometry λ	Spherical detonation Emin (J)	Cylindrical detonation E _{min} (J/m)	Experimental values for spherical detonation E_{ex} (J)	Reaction zone length L (M)
C ₃ H ₈ /air	1.0	0.38 × 10 ⁶	0.196 × 10 ⁸	0.388 × 10°	0.03
C ₂ H ₀ /air	1.0	0.123×10^{6}	0.93 × 105	0.194 × 10 ⁶	0.025
C₂H₄/air	1.0	0.14×10^{5}	0.21×10^{5}	0.72×10^{5}	0.012
C4H10/air	1.0	$0.21 imes 10^{6}$	0.132×10 ⁶	0.388×10^{6}	0.025

TABLE I

In this study the method of calculation of the minimum energy of direct initiation of detonation wave is presented. This method is based on the model of the energetic deficit of the initiation process and allows one to apply the shock-tube data on the detonability limits for calculation of the minimum energy of initiation of the spherical and cylindrical detonations. The calculated values of the detonation threshold in Table I are in good agreement with the experiment. More experimental shock-tube data is required for calculation of the detonation threshold for the wider range of the combustible mixtures. Shock-tube experiments directed on the evaluation of the detonability limits and reaction zone length should be performed in order to improve the accuracy of the calculation.

On the base of the model developed here a qualitative conclusion can be made:

If, for the planar case in a particular combustible mixture, the detonation cannot be obtained, according to the Eqs. (5b) and (5c) in the cases of cylindrical and spherical symmetry to initiate the detonation process should be even harder. This fact alone leads to a very valuable conclusion for the estimation of the detonation hazard: The detonability limits and the critical initiation energy data obtained for the planar case could serve as a safe lower limit for the cases of cylindrical and spherical detonations.

The fact that it is much easier to initiate the detonation waves in the case of planar symmetry than cylindrical or spherical was noted by a number of experimentalists (Benedick, 1979), but lack of systematic theoretical explanation did not allow the formulation of a general conclusion about the greater sensitivity to detonation of the cases with planar symmetry.

In addition it should be noted that for the same reasons, the direct initiation by planar source should be easier than by cylindrical or spherical. That means that an accidental explosion of the planar source in a combustible medium should be more hazardous than the explosion of spherical or cylindrical source.

ACKNOWLEDGEMENT

The author gratefully acknowledges Professor M. Sichel for several stimulating discussions, and Dr. R. Tank for careful reading of the manuscript and helpful comments. Part of this work was accomplished while the author held an NRC Research Associateship.

REFERENCES

Atkinson, R., Bull, D. C., and Schuff, P. J. (1980). Initiation of spherical detonation in hydrogen/ air. Comb. and Flame 39, 287.

Bar-Or, R., Sichel, M., and Nicholls, J. A. (1980). The propagation of cylindrical detonations in monodisperse sprays. *Eighteenth Symposium (International) on Combustion*, Waterloo, Ontario. Benedick, W. B. (1979). High-explosive initiation of methane-air detonations. *Comb. and Flame* 35, 89.

Borisov, A. A., and Loban, S. A. (1977). Detonation limits of hydrocarbon-air mixtures in tubes. Fiz. Gor. i Vzryva 13, 129.

Bull, D. C., Elsworth, J. E., Hooper, G., and Quinn, C. P. (1976). A study of spherical detonation in mixture of methane and oxygen diluted by nitrogen. J. Phys. D: Applied Phys. 9.

Bull, D. C., Elsworth, J. E., and Hooper, G. (1978). Initiation of spherical detonation in hydrocarbon/air mixtures. Acta Astronautica 5, 997.

Burcat, A., Eidelman, S., and Manheimer-Timnat, Y. (1978). The evolution of a shock wave generated by a point explosion in a combustible medium, *Symp. of High Dynamic Pressures* (*H.D.P.*), Paris, p. 347.

Burcat, A., Scheller, K., and Lifshitz, A. (1971). Shock tube investigation of comparative ignition delay times for C_1 - C_5 alkanes. Comb. and Flame 16, 29.

Eidelman, S., and Burcat, A. (1980). Evolution of a detonation wave in a cloud of fuel droplets. Part I. Influence of igniting explosion. *AIAA Journal* 18, 1103.

Eidelman, S., and Burcat, A. (1981). Numerical solution of a non-steady blast wave propagation in two-phase ("separated flow") reactive medium. J. Comput. Physics 39, 456.

Eidelman, S., and Sichel, M. (1981). The structure of the detonation waves in multi-phase reactive medium. *Comb. Science and Technology*, in press.

Gordon, S., and McBride, B. J. (1971). Computer program for calculation of complex chemical equilibrium compositions, rocket performance, incident and reflected shocks and Chapman-Jouguet detonation. NASA SP-273.

Lce, J. H. (1977). Initiation of gaseous detonation. Ann. Rev. Phys. Chem. 28, 75.

Lee, J. H., and Matsui, H. (1977). A comparison of the critical energies for direct initiation of spherical detonations in acetylene-oxygen mixtures. *Comb. and Flame* 26, 61.

Matsui, H., and Lee, J. H. (1979). On the measure of the relative detonation hazards of gaseous fuel-oxygen and air mixtures. *Seventeenth Symposium (International) on Combustion*, p. 1269, Combustion Institute.

Mitrofanov, V. V., Pinaev, A. V., and Zhdan, S. A. (1979). Calculations of detonation waves in gas-droplet systems. Acta Astronautica 6, 281.

Schelkin, R. I., and Troshin, Y. K. (1964). Gas Dynamics of Combustion. NASA T F231.

Sichel, M. (1977). A simple analysis of the blast initiation of detonations. Acta Astronautica 4, 409.

Zel'dovich, Ya. B., and Kompancets, A. S. (1960). *Theory of Detonation*. New York: Academic Press.