A simple analysis of the blast initiation of detonations

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Abstract—A detonation can be initiated in a fuel-oxidizer cloud by a blast wave of sufficient strength. The Zel'dovich criterion for initiation is that the blast energy must be such that when the pressure ratio across the shock front has decayed to the Chapman-Jouguet value, the distance traveled by the shock must be at least of the order of the reaction zone thickness. A modified version of this criterion has been expressed in quantitative form, and used to determine a dimensionless initiation energy using the stoichiometric value as a reference. Good agreement was found between the theory and experimentally measured initiation energies for MAPP-air, and C_2H_2 - O_2 mixtures. The theory also predicts the variation of initiation-energy with ambient pressure.

Introduction

A DETONATION can be initiated in a fuel oxidizer cloud by a blast wave of sufficient strength. The determination of the minimum or critical blast energy for initiation has been the subject of many experimental and theoretical investigations, and also is the subject of the present paper.

Instantaneous combustion at the blast front would be the simplest model to use as a basis for an initiation theory. However, in this case it can be shown that transition from blast wave to detonation behavior always occurs regardless of the blast energy (Levin, 1967; Korobeinikov, 1969). The observed existence of a critical blast energy below which no detonation occurs must therefore be tied to the ignition delay, characteristic of most combustion. This relation between the ignition delay or induction zone and the critical initiation energy was first recognized by Zel'dovitch et al. (1956), in their qualitative initiation criterion. Thus, direct initiation of spherical detonations requires that when the pressure behind the initiating blast has decayed to the Chapman-Jouguet value, the shock radius must be at least of the order of the reaction zone thickness of the mixture.

Bach et al. (1971) dealt with this problem by retaining the discontinuous combustion front; however, with a reduced heat release Q_e which is only a fraction of the total heat release Q per unit mass of mixture. The ratio Q_e/Q was chosen as an empirical function of both the shock strength and the induction distance, i.e. the distance between the shock front and the start of combustion. This theory, although semi-empirical, appeared to predict the main phenomena which arise during blast initiation. The critical energy, however, can only be determined by the cumbersome computation of a series of shock trajectories for each set of parameters.

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Nicholls et al. (1974a) used an energy balance to develop a direct analytical relation for the critical initiation energy. The energy of the fluid in the induction region behind the blast front decreases as the wave decays. Nicholls et al. (1974a) argue that this decay is opposed by the energy released by combustion, and for initiation to occur the theory requires that the rate of induction zone energy decay equal the rate of combustion heat release before the blast Mach number M_s has dropped below a critical auto-ignition value M_A . M_A is a Mach number below which the Chapman-Jouguet (C-J) detonations fail to propagate because the excessive growth of the induction zone causes uncoupling between the shock and combustion fronts. The choice of the energy in the induction zone essentially ignores the cumulative effect of combustion on the attenuation of the blast wave. During sample computations the theory resulted in induction zone lengths, Δ , which were larger than the blast radius R_s . While there are, thus, some difficulties, the theory contains the main idea that initiation depends on a balance between blast decay and the opposing effect of combustion heat release.

Lee and Ramamurthi (1975) have introduced the concept of a critical detonation kernel to explain initiation. The integrated form of the energy equation is used to show the combined effects of blast energy release and combustion upon the Mach number M_s of the initiating blast wave. Only the heat of combustion released between the blast center and the edge of the induction zone that is to radius $R_s - \Delta$ is taken into account. A critical kernel radius R_s^* is defined by equating the effects of blast energy and combustion upon M_s , the Mach number of propagation. M_s^* , the Mach number corresponding to R_s^* must exceed the auto-ignition limit for initiation to occur, and this condition leads to an expression for the critical initiation energy.

Shock waves are frequently used to detonate liquid and solid explosives. Typically, the shock is applied to the explosive in the form of a pulse of a certain strength and duration, and Walker (1975), among others, has proposed a theory relating the critical energy to the shock pressure and duration. This technique differs considerably from blast ignition so that Walker's theory is not directly applicable.

The theory developed below is based on a modified form of the Zel'dovitch criterion expressed in a quantitative form. The main idea is still that the critical blast energy for initiation depends on a balance between the driving effect of the combustion energy and the induction zone growth due to the decay of the initiating blast.

Formulation

The Zel'dovitch criterion (1956) is that: for initiation the blast energy must be such that when the pressure ratio across the shock front has decayed to the Chapman-Jouguet (C-J) value of the fuel oxidizer mixture, the distance traveled by the shock must be at least of the order of the reaction zone thickness of the mixture. In order to express this criterion in quantitative form the self-similar solution of Taylor (1950), and Sedov (1959) is used to describe the initiating blast. The self-similar point blast theory also was used by Lee *et al.* (1966) in order to compute reaction zone thickness from measured initiation energies via the Zel'dovitch criterion.

The point blast theory does not account for the effect of combustion; therefore, the present theory can be considered as a zeroth order approximation to the initiation problem. According to the self-similar theory, the blast radius, blast Mach number, and the temperature, induced velocity and pressure immediately behind the blast can be expressed in the form:

$$\frac{R_s}{R_0} = \bar{t}^{2l(\nu+2)} \tag{1}$$

$$M = \frac{2}{(\nu+2)} \sqrt{\left(\frac{k_{\nu}}{\alpha_{\nu}}\right)} \, \bar{t}^{-\nu/(\nu+2)} \tag{2}$$

$$\frac{T_2}{T_0} = \frac{8\gamma(\gamma - 1)}{(\nu + 2)^2(\gamma + 1)^2} \frac{k_{\nu}}{\alpha_{\nu}} \bar{t}^{-[2\nu l(\nu + 2)]}$$
(3)

$$\frac{v_2}{c_0} = \frac{4}{(\nu+2)(\gamma+1)} \sqrt{\left(\frac{k_\nu}{\alpha_\nu}\right)} \, \bar{t}^{-[\nu/(\nu+2)]} \tag{4}$$

$$\frac{p_2}{p_0} = \frac{8\gamma}{(\nu+2)(\gamma+1)} \frac{k_{\nu}}{\alpha_{\nu}} \bar{t}^{-(2\nu/(\nu+2))}.$$
 (5)

Here the subscript zero refers to the undisturbed medium and subscript two refers to conditions immediately downstream of the shock. The dimensionless time \bar{t} is defined by

$$\bar{t} = t/\tau_0; \qquad \tau_0 = R_0/C_0 \sqrt{(k_\nu/\alpha_\nu)} \tag{6}$$

and R_0 , the characteristic explosion radius, is related to the blast energy E by

$$R_0 = (E/k_{\nu}\rho_0 C_0^2)^{1/\nu}. (7)$$

The geometric factors ν and k_{ν} are 1, 2, 3 and 1, 2π , 4π , respectively for plane, cylindrical and spherical waves. The parameter α_{ν} , which is given in Table 1, depends on both ν and the ratio of specific heats γ . ρ_0 and C_0 are the density, and the speed of sound in the undisturbed fuel-oxidizer mixture.

The blast decay is essentially complete by the time $R_s \sim R_0$ or $t \sim 0(\tau_0)$ where τ_0 can be considered a characteristic explosion time. The strong blast theory fails

Table 1. Variation of the blast wave parameter α_{ν} with the ratio of specific heats, γ

γ	$\nu = 1.0$	$\nu = 2.0$	$\nu = 3.0$
1.1	2.9383	2.6449	2.2997
1.2	1.9114	1.7622	1.5383
1.3	1.3620	1.2661	1.1005
1.4	1.0264	0.9666	0.8428
1.5	0.8163	0.7711	0.6743
1.6	0.6695	0.6346	0.5572
1.7	0.5619	0.5356	0.4716

before this point is reached; however, the phenomena relevant to initiation occur at much smaller values of R_s .

The Zel'dovitch criterion is now modified by applying it at the critical blast radius R_s^* , defined by Korobeinkov et al. (1972) as that radius where the blast energy and the energy of combustion inside the blast front are equal. The heat released by combustion will begin to significantly influence propagation at this radius, and the transition from blast wave to C-J behavior, if it occurs, takes place near the critical radius (Bach et al., 1971; Levin, 1967). Using an asterisk to denote blast wave properties at the critical radius, the modified Zel'dovitch criterion becomes

$$\frac{\Delta^*}{R^*} \le \delta. \tag{8}$$

 Δ^* is the reaction length and the parameter δ , which must be less than one, depends on the details of the initiation process. The equality holds in (8) when the blast energy equals the critical value E_c .

By combining eqns (1), (2), (7) and (8), it is now readily shown that

$$E_c = \rho_0 C_0^2 M^{*2} \left(\frac{\Delta^*}{\delta}\right)^{\nu} \alpha_{\nu} \left(\frac{\nu+2}{2}\right)^2 \tag{9}$$

and (9) provides a quantitative statement of the Zel'dovitch criterion. The difficulty is that the parameter δ depends on the coupling between combustion and the blast front for which a detailed analysis is not yet available. The critical initiation energy will vary with the fuel oxidizer mixture ratio. If the critical energy is normalized using the stoichiometric value E_{cs} as reference the normalized critical initiation energy

$$\frac{E_c}{E_{cs}} = \left(\frac{M^*}{M^*_s}\right)^2 \left(\frac{\Delta^*}{\Delta^*_s}\right)^{\nu} \left(\frac{\rho_0 C_0^2 \alpha_{\nu}}{\rho_{os} C_{os}^2 \alpha_{\nu s}}\right) \tag{10}$$

will be independent of δ provided that this parameter does not vary appreciably with the mixture ratio. Stoichiometric quantities are denoted by the subscript s.

The normalized initiation criterion (10) has the advantage that it does not depend on δ , and hence on a detailed consideration of combustion-blast front coupling. If the critical energy of initiation is known for any one mixture ratio, (10) can be used to determine E_c for any other fuel-oxidizer mixture. First, however, (10) must be expressed in terms of parameters related to the propagation properties of C-J detonations and to the kinetics of the combustion reaction. For this purpose it is convenient to express M^* in terms of the dimensionless time \bar{t}^* using (2). At the critical blast radius the blast energy E equals the combustion energy contained inside the radius R^* . From this condition and (1) it follows that

$$\tilde{t}^* = (\nu C_0^2/Q)^{(\nu+2)/2\nu} \tag{11}$$

where Q is the heat of combustion per unit mass of fuel oxidizer mixture. \bar{t}^* can be related to the properties of a C-J detonation propagating through the mixture under consideration if it is assumed that Q is constant and equal to the C-J value. For most C-J detonations $M_c^2 \gg 1$, where M_c is the Mach number of propagation, and then it can be shown (Nicholls *et al.*, 1974b) that Q is related to M_c by

$$Q \cong \frac{C_0^2 M_c^2}{2(\gamma_2^2 - 1)} \tag{12}$$

where γ_2 is the ratio of specific heats of the products of combustion. Equation (12) is derived by assuming that the fluid behaves as a perfect gas both upstream and downstream of the detonation. Then, combining (11) and (12) results in

$$\bar{t}^* = \left[\frac{2\nu(\gamma_2^2 - 1)}{M_c^2}\right]^{(\nu + 2)/2\nu} \tag{13}$$

the desired relation between \bar{t}^* and C-J properties.

Immediately behind the leading shock the fluid moves with velocity $(R_s - v_2)$ relative to the shock front. If τ_1 is an induction or characteristic reaction time, the induction distance Δ can be approximated by

$$\Delta = \tau_1(\dot{R}_s - v_2) = \tau_1 C_0 M(\gamma - 1)/(\gamma + 1). \tag{14}$$

The relative velocity, and τ_1 , will change as the fluid moves away from the shock; however, in the early stages of blast initiation, while the temperature T_2 behind the shock is high, τ_1 and hence Δ/R_s will be small so that (14) should be a reasonable approximation. Now combining (2) and (14) with (10) results in

$$\frac{E_c}{E_{cs}} = \eta \left(\frac{\bar{t}_s^*}{\bar{t}^*} \frac{\tau_s^*}{\tau_s^{\dagger}}\right)^{\nu} \tag{15}$$

with

$$\eta = \left[\frac{C_0}{C_{0s}} \left(\frac{\gamma-1}{\gamma+1}\right) \left(\frac{\gamma_s+1}{\gamma_s-1}\right)\right]^{\nu} \left(\frac{\alpha_{\nu s}}{\alpha_{\nu}}\right)^{(1/2)(\nu+2)}.$$

Equation (15) provides a relation for the normalized initiation energy in terms of \bar{t}^* , which is related to C-J properties by (13), and τ_1^* , which is governed by the kinetics of the combustion reaction.

A kinetic model for the induction chemistry or an empirical formula is needed to evaluate the induction time τ_1 . The simplest kinetic scheme which takes the influence of ambient density ρ_0 into account is the second order irreversible reaction

$$A + B \xrightarrow{k_f} C \tag{16}$$

where A is the fuel, B the oxidizer, C the combustion products, and k_f the forward rate constant. This model has been adopted here. With (A_0) and $(B)_0$ the initial concentrations of fuel and oxidizer, a characteristic reaction time τ_1 can be defined by

$$\tau_1 = |(A)_0/[d(A)/dt]_0| = 1/k_f(B)_0. \tag{17}$$

Now, assuming that k_f follows an Arrhenius law so that

$$k_{\rm f} = (1/\kappa) \exp\left(-E_1/\Re T\right) \tag{18}$$

 τ_i will be given by

$$\tau_1 = [\kappa/(B)_0] \exp(E_1/\Re T). \tag{19}$$

Since many of the induction reactions in combustion are second order, the model (16), though extremely simple, is not unreasonable. A number of empirical formulas for the induction time have the form (Schott and Kinsey, 1958; White, 1967)

$$\ln \left[(A)^m (B)^{1-m} \tau_1 \right] = A + B/T \tag{20}$$

which agrees with (19).

When the oxidizer is a mixture of nitrogen and oxygen, $(B)_0$, the initial concentration of oxygen behind the shock is given by

$$(B)_0 = \left(\frac{\gamma + 1}{\gamma - 1}\right) \rho_0 [32(1 + r_N)(\nu_s \phi + 1)]^{-1}$$
 (21)

with r_N the nitrogen oxygen ratio by mass, ν_s the stoichiometric fuel-oxidizer mass ratio and ϕ the equivalence ratio. $\nu_s \phi$ is the actual fuel-oxidizer mass ratio of the mixture.

Taking T in (19) as T_2 , the temperature immediately downstream of the shock, and combining (3), (15), (19) and (21) yields the following expression for the normalized initiation energy:

$$E_c/E_{cs} = \eta \{ (\bar{t}_s^*/\bar{t}^*) [(1+\nu_s\phi)/(1+\nu_s)] \}^{\nu} \exp \nu B_{\nu} (E_1/\Re T_0) (\bar{t}_s^{*2\nu/(\nu+2)} - \bar{t}_s^{*2\nu/(\nu+2)})$$
 (22)

where

$$B_{\nu} = [(\nu + 2)^{2}(\gamma + 1)^{2}/8\gamma(\gamma - 1)](\alpha_{\nu}/k_{\nu}).$$

The direct expression (9) for the critical initiation energy E_c also can be related to the kinetic and C-J parameters using (2), (14) and (19) so that

$$E_{c} = \rho_{0}^{1-\nu} C_{0}^{\nu+2} \bar{t}^{*-\nu} \delta^{-\nu} D_{\nu} \exp\left(\frac{\nu B_{0} E_{1}}{\Re T_{0}} \bar{t}^{*2\nu/(\nu+2)}\right)$$
 (23)

with

$$D_{\nu} = \left[32\kappa (1 + r_{\rm N})(\nu_s \phi + 1) \left(\frac{2}{\nu + 2} \right) \right]^{\nu} \left(\frac{\gamma - 1}{\nu + 1} \right)^{2\nu} \alpha_{\nu} \left(\frac{k_{\nu}}{\alpha_{\nu}} \right)^{(1/2)(\nu + 2)}$$

Equation (23) shows how the critical initiation energy E_c varies with the ambient density ρ_0 . Thus, assuming that the C-J Mach number M_c , and the parameter δ are independent of ρ_0 , it follows that $E_c \propto \rho_0^{1-\nu}$.

Comparison with experiment

Critical initiation energies for MAPP gas-air mixtures have been measured by Collins and Parsons (1973) and by Fry and Nicholls (1974). Lee and Matsui (1976) have measured initiation energies in acetylene oxygen mixtures.

The Collins and Parsons (1973) experiments were made by placing an explosive charge at one end of a plastic bag $4 \times 4 \times 20$ ft long. Detonation was observed before any appreciable interaction with the walls of the bag could occur; hence, these tests corresponding closely to initiation by a point charge with $\nu = 3$. The Fry-Nicholls (1974) experiments were made in a pie-shaped shock tube designed to simulate cylindrical clouds. This shock tube has an included angle of 20° and is 2.05 in. high. The initiating charge was placed at the vertex of the pie-shaped tube, and these tests thus corresponded closely to cylindrical symmetry with $\nu = 2$. The Collins-Parsons (1973) data, which has been taken from the plot of critical threshold energy vs % MAPP in air by volume, is reproduced in Table 2 below. The Fry-Nicholls (1974) data, reproduced from Nicholls et al. (1973) is shown in Table 3. In each case, E_c/E_{cs} was computed from the data and tabulated as a function of the % MAPP by volume of the fuel-air mixture.

Lee and Matsui (1976) used an electric spark discharge to initiate cylindrical detonations in a chamber 13 cm in dia. and 3.7 cm wide. Only the spark energy released during the first quarter cycle of the discharge is effective in producing initiation, and this energy is reported as the critical initiation energy in Table 4. Here E_c/E_{cs} is also tabulated as a function of the % C_2H_2 by volume of the C_2H_2 — O_2 mixture.

Table 2. (energy Parsons (1973)		mixtures
%MAPP by vol.	%MAPP by wt.	Equivalence ratio (φ)	E _c (J)	$\frac{E_c}{Ec_s}$

%MAPP by vol.	%MAPP by wt.	Equivalence ratio (ϕ)	E_c (J)	$\frac{E_c}{Ec_s}$
3.48	5.12	0.777	2.25 × 10 ⁶	25.40
3.65	5.36	0.816	3.44×10^{5}	3.89
4.25	6.23	0.957	8.38×10^4	0.95
5.00	7.30	1.134	1.01×10^{5}	1.14
6.93	10.03	1.605	1.80×10^{5}	2.04
8.25	11.86	1.938	4.40×10^{5}	4.98
9.45	13.51	2.249	9.39×10^{5}	10.62
9.85	14.06	2.355	2.25 × 10 ⁶	25.40

Table 3. Critical initiation energy MAPP-air mixtures (Fry-Nicholls (1974) shock tube tests)

% MAPP by vol.	% MAPP by wt.	Equivalence ratio (ϕ)	E _c (J/cm)	$\frac{E_c}{E_{cs}}$
2.9	4.28	0.643	19,490	6.086
3.3	4.86	0.736	9,552	2.980
3.8	5.58	0.851	5,359	1.672
4.3	6.30	0.968	3,035	0.947
6.0	8.72	1.376	3,716	1.159
6.8	9.85	1.572	4,740	1.479
8.5	12.21	2.002	10,506	3.278
9.7	13.85	2.315	18,178	5.663

Table 4. Critical initiation energy acetylene-oxygen mixtures, p_0 = ambient pressure = 100 torr (from Lee-Matsui (1976) spark discharge tests)

% C₂H₂ by vol.	% C₂H₂ by wt.	Equivalence ratio (ϕ)	E_c (J/cm)	$\frac{E_c}{E_{cs}}$
20.0	16.88	0.625	3.6 × 10 ⁻¹	3.08
28.6	24.55	1.000	1.17×10^{-1}	1.00
40.0	35.14	1.667	8.4×10^{-2}	0.718
50.0	44.83	2.500	8.4×10^{-2}	0.718
60.0	54.93	3.750	2.5	21.4

Table 5. Critical initiation energy, theoretical results for MAPP-air mixtures

				Cylindrical $\nu = 2$		-	cal wave‡ = 3
Equivalence ratio (φ)	% MAPP† by vol.	M_c	γ_2	\bar{t}^*	E_c/E_c	<u></u>	E./E.s
0.400	1.831	4.13	1.2661	1.41 × 10 ⁻¹	73.9	0.275	133.1
0.600	2.722	4.71	1.2218	8.89×10^{-2}	4.61	0.186	14.53
0.660	2.984	4.84	1.2068	7.78×10^{-2}	2.76	0.167	6.14
0.888	3.974	5.20	1.7668	5.34×10^{-2}	1.070	0.122	1.164
1.000	4.456	5.30	1.1651	5.09×10^{-2}	1.000	0.117	1.000
1.122	4.974	5.41	1.1632	4.83×10^{-2}	0.950	0.112	0.896
1.361	5.969	5.51	1.1868	5.38×10^{-2}	1.152	0.123	1.305
1.605	6.964	5.53	1.2196	6.37×10^{-2}	1.713	0.141	2.64
1.854	7.951	5.50	1.2434	7.21×10^{-2}	2.50	0.157	5.02
2.109	8.955	5.46	1.2603	7.91×10^{-2}	3.52	0.169	8.95

[†]MAPP composition: methyl acetylene (C_3H_4), 35.91%; propadiene (C_3H_4), 24.48%; propane (C_3H_6), 18.58%; (C_4H_{10}), 13.74%; propylene (C_3H_6), 7.29%. Molecular wt. = 43.37. Stoichiometric mixture: 4.434% by vol.; ν_1 = stoich. fuel-air mass ratio = 0.06946.

[‡]Other parameters used in the theory: $\gamma = 1.4$; $\alpha_2 = 0.9666$; $B_2 = 3.165$; $T_0 = 298.16$ °K; $\alpha_3 = 0.8428$; $B_3 = 2.156$.

Equation (22) was used to compute E_c/E_{cs} from the theory developed above. The results of the theoretical calculations are shown in Table 5 for MAPP-air, and in Table 6 for C_2H_2 -oxygen. M_c and γ_2 which are needed to compute \bar{t}^* from (13) were obtained using the Gordon-McBride Program (1971) for detonation properties.

The author is not aware of measurements of activation energies for the induction reaction in MAPP-air mixtures. Hence E_1/\Re for MAPP-air was determined, here, by requiring the computed curve of E_c/E_{cs} vs % MAPP and the curve drawn using the Fry-Nicholls (1974) data to match at one point. In this case, the point where $E_c/E_{cs}=2.5$ and the mixture contains 7.95% MAPP by volume was arbitrarily chosen. Then E_1/\Re was found to have the value of 3350°K. This value does not appear unreasonable although considerably lower than the values of 8700 and 9130°K reported for acetylene oxygen (White, 1967) and diluted hydrogen oxygen mixtures (Schott and Kinsey, 1958), respectively. In the case of MAPP-air the variation of γ , the ratio of specific heats of the unburned mixture is very small; hence, it was possible to take $\eta \cong 1$ and to use constant values for B_{ν} and α_{ν} in the calculations.

There are small disparities between the MAPP compositions quoted by Collins and Parsons (1973), Fry and Nicholls (1974) and used here. The quoted compositions and the mixture properties are summarized in Table 7, and it can be seen that the differences in molecular weight and stoichiometric mixture composition are small. The composition and MAPP C-J properties used here were taken from Sichel and Hu (1973). The measured and theoretical values of $(E_c|E_{cs})$ are all plotted vs the % MAPP in air by volume without adjustment for the slight differences in composition for, as Table 7 indicates, these differences should not have large effects on the results.

The experimental and theoretical values of E_c/E_{cs} for MAPP-air are compared in Fig. 1. The theory and experiment are in remarkable agreement. The theory appears to confirm that the difference between the Collins-Parsons (1973) and Fry-Nicholls (1974) results are mainly due to the different geometries of the test apparatus used, i.e. $\nu = 2$ for the Fry-Nicholls (1974) tests and $\nu = 3$ for the Collins-Parsons (1973) tests. The theory also appears to predict detonation limits reasonably well and reproduces the skewness of the E_c/E_{cs} curves relative to the stoichiometric mixture composition. Agreement appears to be best for rich mixtures; for lean mixtures the theory underestimates E_c/E_{cs} .

From Table 6 it is evident that the variation of γ is appreciable in the case of C_2H_2 – O_2 so that variations in η , α_{ν} and B_{ν} must be taken into account in the computations. Soot formation becomes appreciable when the proportion of C_2H_2 exceeds 50% by volume, and then eqn (13) for \bar{t}^* will no longer be valid. Hence, theoretical calculations were only made for mixtures up to 50% C_2H_2 . Computations were made for $E_1/\Re = 8700$ and 13,880°K. The first value corresponds to that reported by White (1967) for very lean C_2H_2 – O_2 mixtures; the second value was determined by equating theoretical and experimental values of E_c/E_{cs} for the $20\% C_2H_2$ – O_2 mixture.

Theory and experiment for C_2H_2 — O_2 are compared in Fig. 2, and are in good agreement. The theory reproduces the skewness of the E_c/E_{cs} curve with respect

Table 6. Critical initiation energy, theoretical results for C₂H_z-O₂ mixtures

Equivalence ratio (ϕ)	% C ₂ H ₂ by vol.	M _c	γ,	# ± 12	~	α_2	B_2	۴	E_c/E_{cs} $(E_1/\mathscr{R}=13,880^{\circ}\mathrm{K})$	E_c/E_{cs} $(E_1/\Re = 8700^{\circ}\text{K})$
0.625	20.0	6.33	1.130	2.76	1.346	1.128	4.243	1.186	3.08	1.807
0.769	23.53	6.648	1.1317	2.541×10^{-2}	1.339	1.149	4.408	1.106	1.551	1.256
1.000	28.60	7.013	1.1382	2.403×10^{-2}	1.329	1.179	4.656	1.000	1.000	1.000
1.319	34.53	7.441	1.1458	2.260×10^{-2}	1.319	1.213	4.953	0.899	0.611	0.781
2.051	45.07	8.150	1.1687	2.203×10^{-2}	1.306	1.267	5.472	0.746	0.507	0.742
2.514	50.17	8.421	1.1894	2.339×10^{-2}	1.292	1.305	5.784	0.674	0.947	1.077
3.077	55.17	7.838	1.1686	2.381×10^{-2}	1.284	1.343	6.095	0.609	1.246	1.306

 $T_0 = 298.16$ °K; $p_0 = 100$ torr.

Table 7. Quoted MAPP gas compositions (% by vol.)

Constituents	Source	Source Collins-Parsons Fry-Nicholls Sichel-Hu (1973) (1974) (1973)	Fry-Nicholls (1974)	Sichel-Hu (1973)
Methyl acetylene (C3H4)	(C,H,)	37%	51%	35.91%
Propadiene (C3H4)		25	23	24.48
Propane (C3H8)		20	26	18.58
C ₄ compounds		6	1	13.74
Propylene (C,H,)		6	i	7.29
Molecular wt.		42.24	41.04	43.37
Stoichiometric				
% MAPP in air		4.614	4.738	4.434
(by vol.)				

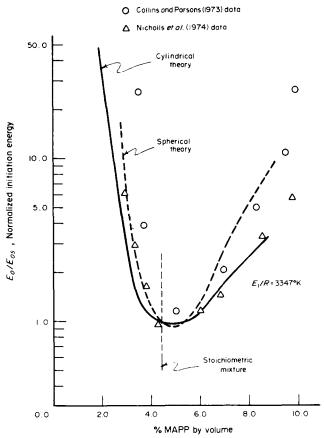


Fig. 1. Experimental and theoretical variations of normalized initiation energy for MAPP-air mixtures.

to the stoichiometric mixture and essentially appears to reproduce the detonation limits. The theory also reproduces the initial drop in initiation energy as the mixture ratio exceeds the stoichiometric value. With $E_1/\Re=8700^\circ \mathrm{K}$ the theoretical value of E_c/E_{cs} is below experiment for lean mixtures and is somewhat above the measured value for rich mixtures. With $E_1/\Re=13,880^\circ \mathrm{K}$, the theory produces the correct rich detonation limit but yields low values of E_c/E_{cs} between 30 and 50% C_2H_2 by volume. Optimum agreement between theory and experiment would probably be obtained for an activation temperature E_1/\Re lying between the two values above. What is significant is the essential agreement between the value E_1/\Re suggested by the initiation theory presented here and the value reported by White (1967).

Equation (23) suggests that $E_c \propto \rho_0^{1-\nu}$, or for fixed ambient temperature, that $E_c \propto \rho_0^{1-\nu}$. Measured initiation energies for C_2H_2 at reduced pressures have been reported by Bach *et al.* (1971), Matsui (1973), Lee and Ramamurthi (1975) and Lee and Matsui (1976). Some of this data which is discussed in detail by Lee

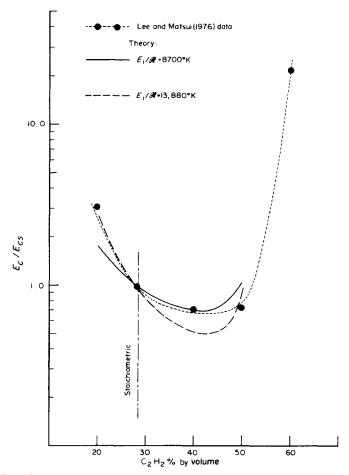


Fig. 2. Experimental and theoretical variation of normalized initiation energy for acetylene-oxygen mixtures.

and Matsui (1976), is plotted in Fig. 3 along with curves corresponding to cylindrical and spherical symmetry with $E_c \propto p_0^{-1}$, p_0^{-2} .

The electric spark initiation experiments reported by Lee and Matsui (1976) were designed to produce waves with cylindrical symmetry and, it can be seen from Fig. 3, that the variation of E_c with p_0 closely follows $E_c \propto p_0^{-1}$ as predicted by the present theory. The earlier laser spark measurements by Bach et al. (1971) also appear to vary inversely with p_0 , again suggesting cylindrical symmetry. The actual value of E_c is very sensitive to the energy source used for initiation, as discussed in detail by Lee and Matsui (1976). The different properties of laser and electric sparks thus result in the difference in the absolute values of E_c shown in Fig. 3.

Matsui (1973) used a planar detonation wave traveling in a tube as the initiation source and determined the minimum tube diameter needed to initiate a detonation in a larger surrounding volume. This method of initiation closely simulates the initiation of a spherical detonation with a point source of energy.

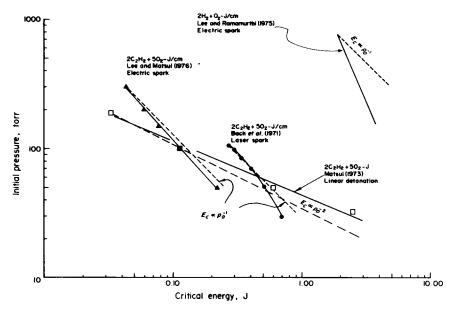


Fig. 3. The variation of critical initiation energy with pressure.

Lee and Matsui (1976) used the critical tube diameter data to estimate the critical initiation energies plotted in Fig. 3. There is close agreement between the Matsui (1973) data and the variation $E_c \propto p_0^{-2}$ predicted for spherical symmetry by the present theory.

Lee and Ramamurthi (1975) also measured the variation of E_c with p_0 for a stoichiometric hydrogen oxygen mixture. Figure 3 shows that while the $2H_2$ - O_2 initiation energy increases with decreasing p_0 , the rate of increase appears to be much less than indicated by (20), possible because (16) is not a good approximation for H_2 - O_2 kinetics. An interesting consequence of (23) is that E_c should be independent of ρ_0 for plane waves.

Bach et al. (1971) expressed their critical initiation energy in terms of the ratio of Δ_c , the induction distance of the C-J detonation to the explosion radius R_0 . The modified Zel'dovich criterion presented here can be expressed in the same form by combining eqn (8) with the expressions (14) and (19) for the induction distance Δ and the ignition delay time τ_1 with the result

$$\frac{\Delta_c}{R_0} \leq \delta M_c \bar{t}^* \left(\frac{\nu+2}{2}\right) \sqrt{\left(\frac{\alpha_{\nu}}{k_{\nu}}\right)} \exp \frac{E_1}{\Re T_0} \left(\frac{T_0}{T_{2c}} - B_{\nu} \bar{t}^* \frac{2\nu}{\nu+2}\right). \tag{24}$$

Here T_{2c} is the temperature downstream of the shock but upstream of the reaction zone for the C-J detonation. Bach *et al.* (1971) computed a critical value of $(\Delta_c/R_0) = 0.091$ for the initiation of a spherical detonation in a stoichiometric C_2H_2 - O_2 mixture with $p_0 = 100$ torr. By using (24), this value of (Δ_c/R_0) and the detonation parameters of C_2H_2 - O_2 , it now is possible to determine the corresponding value of the parameter δ . With $M_c = 7.013$, $E_1/\Re = 8700^{\circ}$ K,

 $\alpha_3 = 1.0$, $B_3 = 3.085$, $\bar{t}^* = 6.272 \times 10^{-2}$, $T_{2c}/T_0 = 8.887$, the result is $\delta = 0.282$. This certainly is not an unreasonable value.

Discussion

The theory developed here verifies that the minimum initiation energy is determined by a balance between the combustion heat release and the growth of the induction zone. The simple relation (22) for the variation of the initiation energy with the fuel-oxidizer mixture ratio, which is developed on the basis of the Zel'dovich criterion, is in excellent agreement with experimental measurements for two quite different, fuel-oxidizer combinations. The theory can be used to compute the initiation energy E_c at any fuel-oxidizer ratio, given a measured value of E_c for one particular mixture and an estimate of the activation energy of the induction reaction. The experimentation required to establish the initiation characteristics of a given fuel can thereby be reduced appreciably. With sufficient information about the chemistry of the induction zone, the theory will also predict the effect of ambient density upon the initiation energy.

The simplicity of the theory comes from the use of self-similar strong blast theory to describe the initiating blast. Thus, the theory really is the zeroth order solution of an expansion scheme in which the first order solution would account for the influence of combustion on the initiating blast. The success of this simple theory in the case of explosively and spark initiated detonation waves suggests that non-ideal blast behavior during the initial phases of blast formation will not have a large effect on initiation. At the same time, the critical phenomena which determine whether or not the initiating blast wave quenches appear to occur near $R_s = R_s^*$ where the influence of combustion on wave propagation is still relatively small.

The present theory by no means represents a complete solution of the initiation problem. No explicit means of determining the parameter δ is provided. A key feature of the present development is that the parameter δ is not required for the computation of E_c/E_{cs} . However, an absolute theory for computing E_c depends crucially upon δ , and here many problems remain. Determination of δ will require a detailed consideration of the processes in the induction zone leading to uncoupling of combustion from the blast front. Liñan (1975) has attempted to relate this coupling to the rate of increase of the induction distance in reacting blast waves. In the Bach *et al.* (1971) and Lee and Ramamurthi (1975) theories, uncoupling occurs whenever the wave Mach number drops below the auto-ignition limit. The work of Strehlow (1968), among others, indicates that transverse waves in the reaction zone of detonation waves may also play an important role in the coupling process. A greater understanding of combustion-shock coupling is needed to determine such parameters as δ and the auto-ignition Mach number a priori.

Another shortcoming of the present theory is that conditions immediately behind the blast wave are used to compute the induction length Δ . In a more complete theory the variation of the temperature and velocity of a fluid particle as it traverses the induction zone should be taken into account.

The rate of energy release at the blast source can have a large influence on the initiation energy if the rate falls below a certain minimum value. This problem has been studied extensively by Bach et al. (1971), Knystautas and Lee (1975) and Matsui and Lee (1975) using spark initiators. The effect of energy release rate has been ignored in the present theory; hence, this theory will only be valid for initiation sources with high rates of energy deposition.

The theory developed here appears to take the important physical parameters involved in initiation into account, and provides a simple means of estimating minimum initiation energies.

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