ON THE POWER AND ENERGY FOR INITIATION OF PLANAR DETONATION WAVE

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ABSTRACT

The ignition energy and its rate of deposition (power) required for initiation of planar detonation wave in a reactive gaseous mixture is considered. Their effects on both of the ignition and detonation times are studied, as well. The critical switch-off time of ignition energy required for direct initiation of detonation wave and its relation to the minimum ignition time of the mixture is considered also. Unlike the commonly used model, namely, the constant velocity piston which is set in motion suddenly and results in a constant velocity shock wave required for initiation of detonation wave, that does not correspond to what happens actually, the ignition model presented here mimics, for instance, the spark ignition of the reactive mixture. The model enables us to change the ignition energy, its rate of deposition and its switch-off time. The reactive mixture is assumed to be an ideal gas with constant specific heats and the dissociation at high temperature is neglected. The chemical kinetics are represented by a one-step chemical reaction of Arrhenius type, for simplicity. The results indicate that reduction in the total ignition energy delays the initiation of detonation wave and below certain minimum value of the total ignition energy, detonation is not possible. The results show also that increasing the power of the igniter speeds up the initiation process and there is a minimum value of the power of the igniter below which initiation fails no matter how big the total energy is. It is found also that for successful initiation of detonation, the switch-off time of ignition energy must be greater than the ignition time of the mixture. It is concluded that the ignition source power and the ignition energy released at the ignition zone should be able to generate a shock wave of minimum strength and supports its propagation until chemical reaction starts behind it, for successful initiation.

Keywords: Detonation wave, Ignition energy, Rate of ignition energy, Shack wave, Wave propagation.

NOTATIONS:

A	Power factor
c'_o	Sound speed in the rest state = $\sqrt{(\gamma R' T'_o)}$
C'_p	Specific heat at constant pressure.
C'_v	Specific heats at constant volume.
E'	Activation energy.
E'_i	Total ignition energy per unit area.
L'	Domain length = $c'_o t'_a$
p	Dimensionless pressure.
q	Dimensiionless chemical heat release parameter.
q'_b	Ignition source Power per unit area.
R'	Gas constant.
T	Dimensionless temperature.
t	Dimensionless time.
t_a'	Acoustic time = $1/c'_o$
u	dimensionless velocity.
x	Dimensionless distance.
Y	Dimensionless mass fraction of reactants.

Greek symbols

β	Pre-exponential factor.
γ	Specific heats ratio.
ϵ	Inverse activation energy parameter.
ρ	Density.

Subscripts and superscripts

(')	Dimensional quantity.

('o) Dimensional quantity at rest state.

1- INTRODUCTION

When reactive gaseous mixture is ignited, two modes of combustion waves are available, Lee [7]. A deflagration slow mode, in which the combustion front propagates with velocity of the order of few centimeters per second. The mechanism of propagation of this laminar flame is characterized by the conduction of heat from the reaction zone into the cold unreacted mixture. On the other hand, a detonation fast mode, which is a combustion wave propagating with a velocity of the order of thousands of meters per second. The mechanism of initiation and propagation of such mode is characterized by the auto-ignition of the reactive mixture behind a strong shock wave, propagation ahead in the unreacted mixture.

There are two distinct methods of detonation initiation namely, deflagration to detonation transition (DDT) and direct initiation. In the first method a shock wave is formed by the coalescence of compression waves generated by the accelerating turbulent flame in the reactive mixture. Many shocks may be formed, (Urtiew & Oppenheim [10] and Oppenheim & Kamel [9]) and catch each other to form a strong shock necessary for the initiation of detonation. Turbulence and interaction between waves play the dominant role in the initiation process. On the other hand, in the direct initiation method a shock wave with a certain minimum strength is formed immediately following the deposition of energy from a powerful source in the vicinity of the ignition source. The shock wave heats up the explosive mixture and triggers the chemical reaction behind it which eventually results in a coupled complex of a shock wave followed by a combustion wave (detonation).

Based on the energy-time characteristics of the ignition source, the ignition time and the detonation initiation time vary. The necessary condition for the onset of detonation is the formation of a shock wave of a certain minimum strength and it continues propagation until ignition starts in the heated gas behind it. The chemical heat release supports and strengthens the formed shock and eventually detonation occurs.

Clarke et al. [3] studied the direct initiation of a planar detonation wave in a slab of reactive mixture confined between two parallel plane walls. In their model, ignition energy is supplied to the mixture at one end of the slab by heat conduction through the wall and transferred to the mixture adjacent to the wall. Their results showed that a strong shock wave is established following energy deposition at the wall, and subsequent ignition of reactive gas occurs. The shock is accelerated as a result of increasingly large chemical heat release. Eventually the reaction zone accelerates, catches up to the lead shock and they move together as an over-driven detonation wave. They concluded that direct initiation of detonation requires sufficient power input to first of all generate a suitably strong shock wave, which then becomes the trigger to switch on vigorous chemical activity behind it.

Knystautas and Lee [6] studied experimentally the effective energy for direct initiation of gaseous detonation. They indicated that the effective energy for direct initiation is the energy deposited up to the time of the peak average power. It is shown also that the peak power of the igniter and the energy release up to the peak power are two parameters that characterize the direct initiation of detonation wave. The peak average power corresponds to a minimum shock strength below which initiation is not feasible.

Abouseif and Toong [1] proposed a model to determine the correlation between the igniter's critical energy and critical power necessary for direct initiation of detonation wave. The model comprises a constant velocity piston which starts motion abruptly into the reactive mixture which results in a formation of constant velocity shock wave. For initiation of planar detonation they demonstrated that the duration of piston motion should not be smaller than the induction time that corresponds to the temperature behind the generated shock. They found also that for cylindrical detonation, there is a minimum average power and minimum critical energy below which initiation fails. These results are qualitatively similar to the experimental results of Knystautas and Lee [6].

Kailasanath and Oran [5] used the same model of Abouseif and Toong [1] to study the power and energy relation for direct initiation of planar, cylindrical and spherical detonation in gaseous mixture. For planar case they noticed that unlike the cylindrical case, each value of power corresponds to a unique value of energy and the shock strength decreases as the power decreases and more energy is needed to initiate a detonation. There is a minimum shock Mach number below which a detonation will not occur. The power corresponding to this minimum Mach number is the minimum power. The shock tube data of Dabora [4] agree well with these results.

From this review it is inferred that the constant velocity piston model which generates constant velocity shock wave does not mimic the commonly used experimental ignition sources, like spark ignition, in which the power and energy are time-dependent and, therefore, the generated shock and flow field behind it are also time-dependent. The present model, however, provides an appropriate mean for studying the power and energy for initiation of detonation wave because it is time-dependent and the energy is distributed in a kernel adjacent to the closed end of the pipe. A schematic diagram of the detonation tube is shown in Figure (1-a).

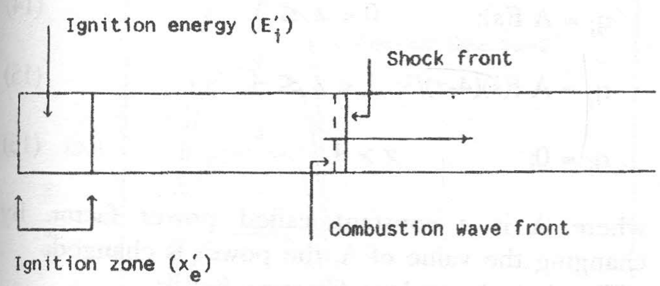

Figure 1-a. Detonation tube model; shock wave followed by combustion wave to form the detonation wave.

The objectives of the present investigation are to find the power and energy relation for initiation of planar detonation wave and their effects on the time to detonation. It is of considerable interest, as well, to obtain the relation between the switch-off time of ignition energy and the time to ignition and whether there is a minimum duration of energy addition below which detonation will not occur or it takes very long time.

2.1 *The governing equations*

The gaseous reactive mixture is assumed to be an ideal gas with constant specific heats. The chemical kinetics are represented by a one-step chemical reaction of Arrhenius type. The governing continuity, momentum, energy, species conservation, and state equations in one-dimensional domain are written below in dimensionless form;

$$\rho_t + (\rho u)_x = 0 \quad (1)$$

$$\rho(u_t + uu_x) = -p_x/\gamma \quad (2)$$

$$\frac{\rho C_v}{(\gamma - 1)}(T_t+uT_x) = -up_x + Q + [\rho\beta\, qY/(\gamma-1)]$$

$$\exp(-1/\epsilon\, T) \quad (3)$$

$$Y_t + uY_x = -\frac{\beta Y}{\gamma}\exp(-1/\epsilon\, T) \quad (4)$$

$$p = \rho T \quad (5)$$

where the subscripts t and x denote partial derivatives with respect to time and space, respectively. The second term in the right-hand side of the energy equation represents the ignition energy and the third is the chemical heat release term.

The variables in eqs.1 through 5 are normalized as the following;

$$\rho = \rho'/\rho'_o,\ p = p'/p_o',\ T = T'/T_o',\ u = u'/c'_o,$$

$$t = t'/t'_a,\ x = x'/L',\ Y = Y'/Y'_o\ \ C_v = C'_v/C'_{vo},$$

$$\beta = \beta'\gamma t'_a,\ q = q'/c'_p T'_o,\ Q = Q'/(p'_o/t'_a) \quad (6)$$

The dimensionless inverse activation energy parameter ϵ is;

$$\epsilon = R'T'_o/E' \quad (7)$$

Since the chemical reaction occurs in times of order 10^{-6} sec., which is much shorter than the acoustic time scale which is of order of 10^{-3} sec., therefore, scaling of time with respect to the acoustic time scale is inappropriate. To solve this problem, the following transformation is used;

$$t = \delta s, \; x = \delta z \qquad (8)$$

where z and s are the new space and time variables and $\delta = O(10^{-3})$. Now, the dimensional time,

$$t' = \delta t'_a s = 10^{-6} s \text{ (sec.)} \qquad (9)$$

where the new dimensionless time s is of order one.

The transformation in eqn.8 is used in eqns.1 through 5 and the governing equations are rewritten in the following semi-conservative form;

$$U_s + F_z + H = 0 \qquad (10)$$

where;

$$U = \begin{bmatrix} \rho \\ \rho u \\ \rho(e+u^2/2) \\ \rho Y \end{bmatrix}, F = \begin{bmatrix} \rho u \\ \rho u^2 + p/\gamma \\ \rho u(e+u^2/2) + pu/\gamma \\ \rho u Y \end{bmatrix}, H = \begin{bmatrix} 0 \\ 0 \\ -q_c - q_i \\ W \end{bmatrix}$$

where $e = C_v T/(\gamma-1)\gamma$ and C_v is assumed to be one. q_c and q_i represent the chemical heat release term and the ignition source term, respectively.

$$q_c = \frac{q}{(\gamma-1)}, q_i = \hat{Q}/\gamma, W = \frac{\hat{\beta}\rho Y}{\gamma}\exp(-1/\varepsilon T) \qquad (11)$$

where now $\hat{\beta} = \delta\beta$ and $\hat{Q} = \delta Q$

2.2 *Initial and Boundary Conditions:*

The initial conditions to be satisfied by the solution of the above set of conservation equations are;

$$s = 0; \; p = \rho = T = Y = 1, \; u = 0; \; z > 0 \qquad (12)$$

The boundary conditions at the closed end are;

$$z = 0; \; u = 0; \; s > 0 \qquad (13)$$

In front of the wave, the conditions are the undisturbed initial state. The physical parameters of the reactive mixture that is used in the present work are shown in Table (1).

Table 1. The physical parameters of the reactive mixture.

Physical parameter	Value and units
Initial pressure (p'_o)	101325 (N/m^2)
Initial temperature (T'_o)	300 (K)
Specific heats ratio (γ)	1.4
Chemical heat release parameter (q')	1808.1 (kj/kg)
Pre-exponential factor (β')	2.86×10^6 (1/s)
The exponential term (E'/R')	3750 (K)
Domain length (L')	1 (m)
Small parameters (δ)	10^{-3}
The gas constant (R')	287 (J/kg K)

According to these parameters, the speed of sound $c'_o = 347$ (m/s) and $t'_a = L'/c'_o$ (sec.)

2.3 *The Power of the Ignition Source:*

The ignition energy is added in a thin layer of thickness z_e (kernel) adjacent to the closed end of the tube. It is represented by the source term Q in the energy equation.

The proposed model for the source power term q_i, Sileem et al. [11] is:

$$q_i = A f(s); \qquad 0 < z \leq 1 \qquad (14)$$

$$q_i = A f(s)(4-z)/3; \quad 1 < z \leq 4 \qquad (15)$$

$$q_i = 0; \qquad z > 4 \qquad (16)$$

where A is a constant called power factor. By changing the value of A, the power is changed.

The time-dependent function f(s) is;

$$f(s) = 0.5[\tanh 5(s-0.5) - \tanh 5(s-s_o)] \qquad (17)$$

The function f(s) increases very rapidly with time s to the value of one and then remains constant until the switch-off value s_o, when it decreases very rapidly again to the value of zero.

The rate of energy deposition per unit time per unit area in an element of volume with a differential length dx' is given by;

$$dq_b' = Q' \, dx' \qquad (18)$$

If the previous equation is put in dimensionless form, then;

$$dq'_b = p'_o c'_o \hat{Q} dz \qquad (19)$$

The total power deposition per unit cross-sectional area q'_b is found by integrating dq'_b from z = 0 to $z = z_e$; z_e is the thickness of the layer (kernel) in which ignition energy is deposited, Therefore;

$$q'_b = \gamma p'_o c'_o \int_0^{z_e} q_i (s,z)\, dz = \gamma p'_o c'_o q_b \qquad (20)$$

The integration in eqn. 20 is found by using the model of q_i given in eqns. 14 through 16. The result is;

$$q_b = 2.5 A f(s) \qquad (21)$$

The variation of dimensionless power q_b, in eqn. 21, with time s is shown in Figure (1-b) for different values of the power constant A when the switch-off time s_o = 2. When A = 6, f(s) ≃ 1, the source power is 0.0738 Mw/cm^2.

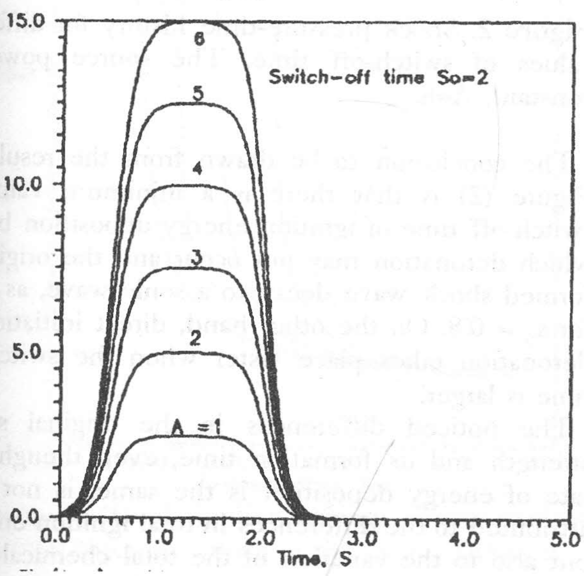

Figure 1-b. Ignition source power variation with time at different values of the power factor, A.

2.4 *The Ignition Energy* (E'_i)

The total ignition energy is found by integrating the power, eqn.20, with respect to time from s = 0 to the time at which the power goes to zero (s_m). The calculations showed that $s_m \approx s_o + 0.8$. Therefore;

$$dE'_i = q'_b \, dt' \qquad (22)$$

by integration, we obtain the total ignition energy as;

$$E' = \gamma p_o' c'_o \delta t'_a (2.5 A) \int_0^{sm} f(s)\, ds \qquad (23)$$

or

$$E'_i = \gamma p'_o c'_o \delta t'_a (2.5 A) I$$

$$= \gamma p'_o c'_o \delta t'_a E \qquad (24)$$

Where;

$$I = 0.1 [\ln \frac{\cosh 5 (s_m - 0.5)}{\cosh 5 (s_m - s_o)} - \ln \frac{\cosh 5 (0 - 0.5)}{\cosh 5 (0 - s_o)}] \qquad (25)$$

The total ignition energy E varies almost linearly with the switch-off time s_o, as shown in Figure (1-c), for different values of the power factor A. For the parameters shown in Table 1, and A = 1, $E'_i = 4.92 \times 10^{-3}$ E (j/cm^2).

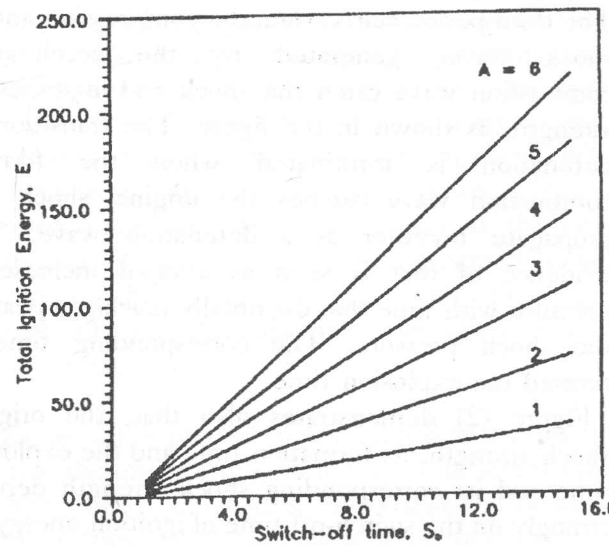

Figure 1-c. Variation of the total ignition energy E with the switch-off S_o, at different values of A.

3- THE NUMERICAL SOLUTION

The solution of the system of equations in eqs.10 with the initial and boundary conditions in eqs.12 and 13 is obtained numerically by using the finite-difference scheme of MacCormack [8] and the Flux-Corrected Transport scheme of Book et al. [2].

4- RESULTS AND DISCUSSIONS:

4.1 Shock Pressure -Time History:

Figure (2) presents the shock pressure-time history at different values of the ignition energy switch-off time (s_o),while keeping the ignition source power constant; A = 6. At constant value of s_o =1.5; for instance; one can distinguish three periods of time. At the first period, an original shock wave is formed due to the deposition of ignition energy with rapid rate in the ignition zone. The shock pressure is almost 9 units and its formation time is almost 2.5 time units. The second period is characterized by a noticeable decrease in the shock pressure because of the switch-off of the ignition energy. This period takes almost 5 time units. During this period an auto-ignition of the shocked gas occurs and forms hot spot that eventually becomes a combustion wave accelerating behind the shock (Sileem et al. [11]). The third period starts when the compression and/or shock waves generated by the accelerating combustion wave catch the shock and increases its strength, as shown in the figure. The transition to detonation is terminated when the formed combustion wave catches the original shock and propagate together as a detonation wave. The evidence of that is seen as a rapid increase of pressure with time that eventually reaches a peak in the shock pressure. The corresponding time is termed the explosion time.

Figure (2) demonstrates also that, the original shock strength, its formation time and the explosion time and its corresponding shock strength depend strongly on the switch-off time of ignition energy. In other words, it is seen that the original shock strength decreases and its formation time increases with a decrease in s_o , while the corresponding explosion time increases. When the switch-off time becomes as small as 0.8 units, the transition to detonation does not occur in the present time and length scales. On the other hand, the transition occurs very rapidly as s_o increases as shown for s_o = 3 units. It is worth to remember that the ignition energy increases with the increase in switch-off time.

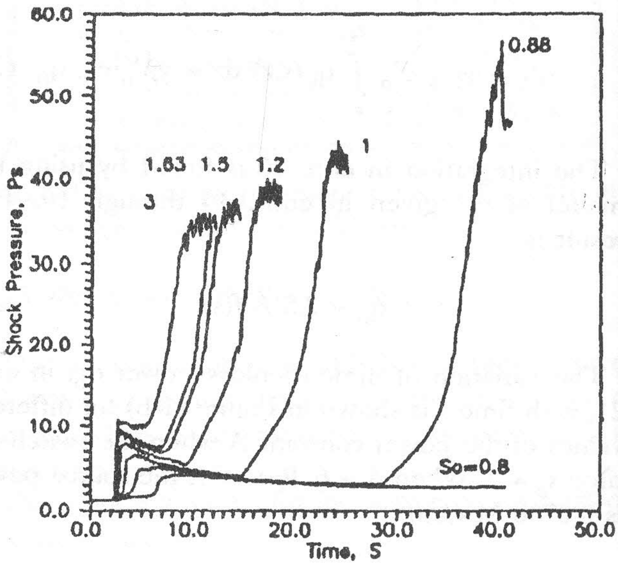

Figure 2. Shock pressure-time history for different values of switch-off time. The source power is constant, A=6.

The conclusion to be drawn from the results in Figure (2) is that there is a minimum value of switch-off time of ignition energy deposition below which detonation may not occur and the originally formed shock wave decay to a sonic wave, as seen for s_o = 0.8. On the other hand, direct initiation of detonation takes place faster when the switch-off time is larger.

The noticed differences in the original shock strength and its formation time, even though, the rate of energy deposition is the same, is not only attributed to the differences in total ignition energy, but also to the variation of the total chemical heat release in the ignition zone. One notice the sensitivity of the explosion time to any small change in the switch-off time. For example, a decrease in s_o from 0.88 to 0.8 causes no explosion. It is also noticed the delay in shock formation when s_o < 1.2, because the ignition of the mixture in the kernel is delayed and therefore, the contribution of the chemical heat release in the formation of the shock is smaller. These results agree qualitatively with that of Abousief and Toong [1].

4-2 *Effect of Ignition Energy and Power on the Explosion Time*:

Figure (3) demonstrates the dependence of the explosion time on both of the ignition source power (represented by the power factor A) and the total ignition energy, E. It shows clearly that at constant power, the explosion time increases as the energy decreases and below certain minimum value of energy the explosion time increases significantly and the detonation may not occur in the present time and length scales. As the power decreases the explosion is delayed at the same amount of ignition energy. That is because the formed shock is weaker and the formation of hot spot behind the shock (necessary for the initiation) is delayed.

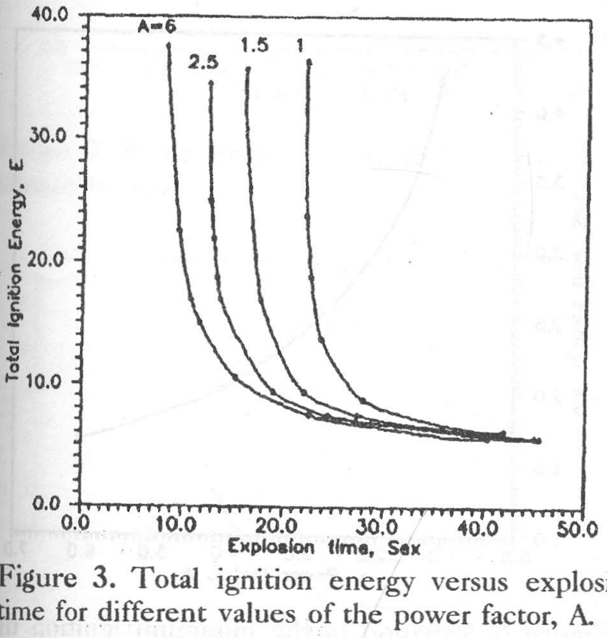

Figure 3. Total ignition energy versus explosion time for different values of the power factor, A.

It is also seen that at constant ignition source power, the explosion time reaches an asymptotic minimum value, no matter how big the total ignition energy is. This means that, for each value of the ignition source power there exists a minimum explosion time. This minimum value occurs when the ignition energy is greater than certain value. This may be explained by the fact that the ignition delay time becomes very small when the temperature behind the lead shock is much greater than the auto-ignition temperature of the mixture. Therefore, the particles burns immediately as it is processed by the shock and the explosion occurs suddenly.

It is interesting to note also, in Figure (3) that, the explosion time is almost independent of the igniter power, represented by A, as the energy decreases below certain value. This is noticed when the energy takes values below $\approx$ 7 units, where it is clearly seen that the explosion time becomes almost the same irrespective of the source power.

These findings emphasis that when the ignition energy is below certain minimum value, the initiation of detonation occurs through deflagration to detonation transition, irrespective of the source power. On the other hand, direct initiation of detonation does depend on the source power.

4-3 *Effect of Switch-Off Time* (s_o) *on the Ignition Time* (s_i)

The dependence of the ingition time of the reactive mixture in the kernel, on the switch-off time of energy deposition at different values of the source power is depicted in Figure (4). It is noticed that, for constant value of the source power, s_i does not change if s_o greater than certain minimum value s_{oc}. One the hand s_i increases significantly if s_o is lower than s_{oc}. It is believed that the critical switch-off time of energy deposition is related to the induction time of the reactive mixture, which essentially depends on the source power. Figure (4) demonstrates also that s_i decreases as the power increases. Based on the aforementioned relation between the induction time and the critical switch-off time, the induction time decreases as the power increases.

Figure (5). is plotted for the critical switch-off time versus the minimum ignition time at different values of the power factor A. It shows that the minimum ignition time is almost equal to the critical switch-off time.

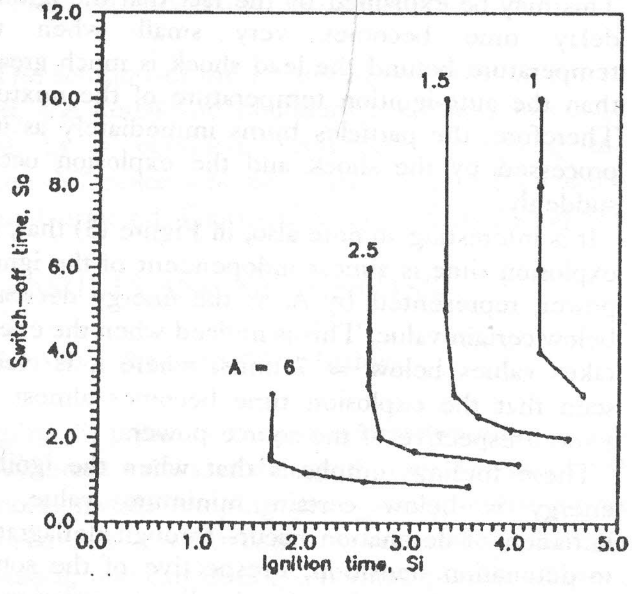

Figure 4. Ignition time against switch-off time for different values of the power factor, A.

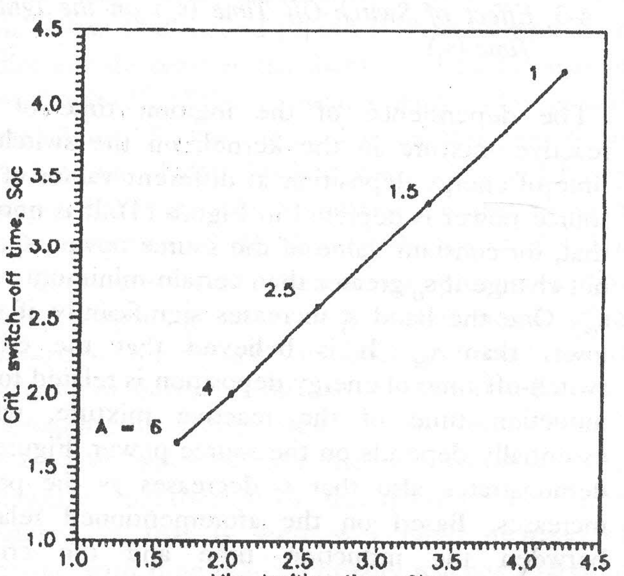

Figure 5. The minimum ignition time versus critical switch-off time at different values of the power factor, A.

By consulting the results in Figure (2), one interestingly note that if the switch-off time of energy deposition is equal or greater than the critical value, the initiation of detonation is likely to occur after small period of time. In other words, direct initiation of detonation is achieved if the switch-off time of energy deposition is greater than s_{oc}. This can be seen clearly in Figure (2), where one notices that the explosion occurs faster when the switch-off time is equal or greater than s_{oc}. However, the time to detonation increases sharply or detonation may not occur at all, if $s_o < s_{oc}$. For example, in the case of Figure (2) where A =6, s_i = 1.668, s_{oc} = 1.668 and the corresponding explosion time s_{ex} = 10.7 time units. When $s_o = 1 < s_{oc}$, the explosion time become as large as 22.56 time units. When $s_o = 3 > s_{oc}$, the explosion time s_{ex} = 8.1. It is worth to mention here that, by using the piston model, Abousief et al. [1] concluded that the period of piston motion must be greater than the induction time of the mixture for direct initiation of detonation, which coincides with our conclusion.

Figure (6) demonstrates the variation of the minimum ignition time with the variation of the ignition source power (represented by the power factor A). It shows clearly that the minimum ignition time diminishes with the increase of the source power.

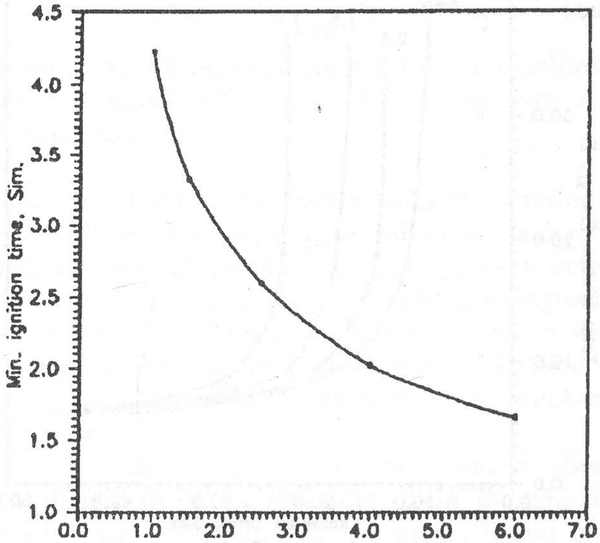

Figure 6. Variation of the minimum ignition time with the ignition source power.

4-4 *Power and Energy Relation for Direct Initiation of Detonation*:

Figure (7) shows a plot of power versus energy for direct initiation of planar detonation. It shows clearly that the energy increases as the power decreases for the successful initiation. The trend of the curve indicates that more and more energy is needed as the source power decreases. It shows also that there is a minimum value of power for initiation and the necessary amount of energy at this minimum value is huge.

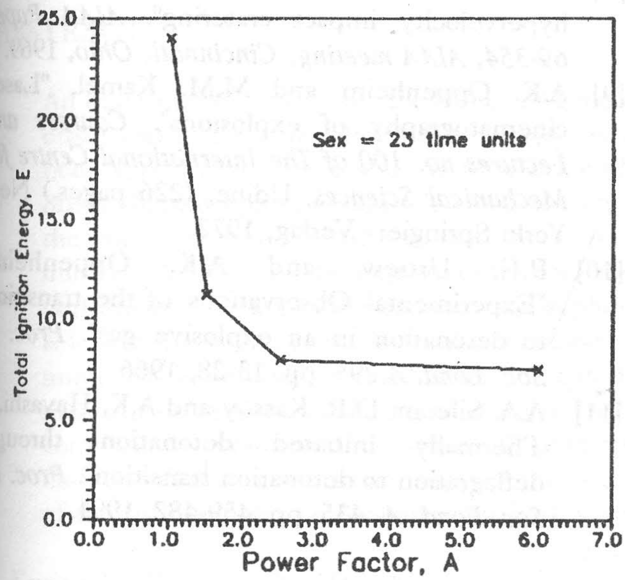

Figure 7. Power-energy variation for initiation of detonation wave.

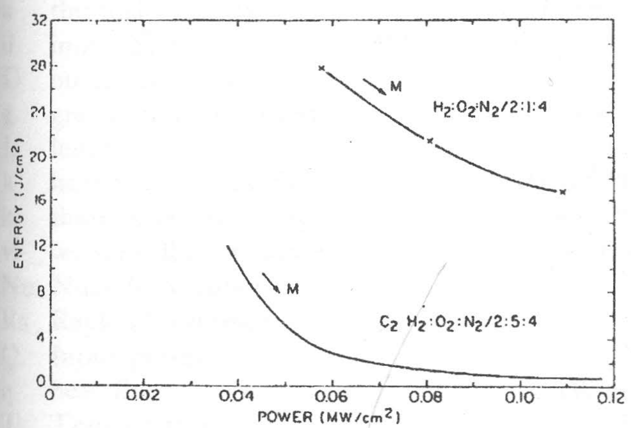

Figure 8. Power energy relation for the initiation of planar detonation by Kailasanath & Oran. The x's are data from shock tube experiments of Dabora (4).

The present results agree qualitatively with the shock tube experimental results of Dabora [4] and with the piston model results of Kailasanath et al. [5] for planar initiation of detonation shown here in Figure (8), for comparison. Quantitative comparison is impossible because the used reactive mixture is different.

5- CONCLUSIONS

This paper presents a theoretical model to study the power and energy required for initiation of planar detonation wave. The following conclusions could be inferred from the present investigation:

1- The results show clearly that the used ignition model is a good simulation to the actual ignition systems.
2- The results confirmed the dependence of direct initiation of detonation on the ignition source characteristics and there is almost no effect of the ignition source power on the deflagration to detonation transition when the ignition energy is below certain minimum value.
3- The most important conclusion is that for direct initiation of planar detonation, the switch-off time of ignition energy addition must be equal or greater than the ignition time of the mixture which depends on the source power.
4- The time to detonation depends on both of the ignition source power and energy as noticed experimentally by Lee et al. [6].
5- If the switch-off time of ignition energy is much less than the ignition time, the initiation of detonation takes very long time to occur or it may not occur at all.
6- It is shown also that for direct initiation, the ignition energy increases as the power of the igniter decreases and there is a minimum value of the power below which direct initiation of detonation is impossible.

Acknowledgement

The author appreciates the valuable comments and suggestions of Prof. M. M. Kamel, the Dean of the Higher Technological Institute at Ramadan 10th. city.

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