A Dataset of Critical Energy for Direct Initiation of Spherical Detonations in Some Hydrocarbon-Oxygen Mixtures

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1 Introduction

Knowledge of explosion hazard of typical hydrocarbon mixtures in enclosures is an important subject in safety assessment for a wide range of operations, connected to production, handling and transportation or use of fuels [1]. Hydrocarbons are easily combustible and can form explosive mixture. Although in many accidents in the chemical process industry involved hydrocarbons, deflagrations are perhaps more likely the probable mode of combustion (when the fuels mix with oxidizer within the flammability limit), the significant explosion hazard caused by the nature of detonation phenomenon still warrants a thorough knowledge of the conditions whereby detonations can be initiated and the magnitude of the resultant consequences.

Among different detonation dynamic parameters, critical energy for direct initiation of detonations provides a direct measure of detonability or sensitive of an explosive mixture [2]. In this paper new measurement results of the critical energy for direct initiation of spherical detonations in four gaseous fuels (C_2H_2 , C_2H_4 , C_3H_8 and H_2) - oxygen mixtures at different initial pressures, amount of argon dilution and equivalent ratios are reported. Results are obtained using a spherical constant volume bomb with a high voltage discharge and the effective energy is estimated adequately from the current output using the procedure given in our previous publications [3-5]. The aim of this paper is to summarize an extended set of reliable experimental data which, on one hand, can provide safety hazard assessment of these fuels and use for theoretical model validation, but also serve as reference base of comparison for the equivalent hazard of explosion of different hazardous chemical substances.

2 Experimental details

Experiment is carried out in a 8" diameter and 2" wall thickness high pressure spherical bomb. A schematic of the apparatus is given in Fig. 1. The ignition system is constructed in previous studies (see [3] for further details). It consists of a high voltage power supply, capacitor bank, a gap-switch and a trigger module (TM-11A). For each direct initiation experiment, the sphere is initially evacuated to at least 80 Pa and then incrementally filled through the ball valve with fuel/oxygen mixtures at various test pressures and equivalent ratios. A PCB piezoelectric pressure transducer is mounted in the

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wall of the chamber to measure the time of arrival of the combustion wave front. It can be determined from the arrival time of pressure signal whether there is a successful detonation or not. At the end of this slender electrode there is a 3.5 mm spark gap through which the energy is delivered inside the chamber through the ignition circuit. The procedure to distinguish detonation initiation and to estimate the actual spark discharge energy from the ignition system is detailed in authors' previous studies [3-5]. In brief, for a given a trace of the current function $i(t) = Ae^{-\alpha t} \sin(\omega t)$ recorded on the oscilloscope, the natural frequency ω_n is determined using ω and ζ where:

$$\omega = \sqrt{1/(LC)_{total} - (R/2L)_{total}^2} = \omega_n \sqrt{1 - \varsigma^2}$$

and attenuation factor equal to $\alpha = R_{\text{total}}/2L_{\text{total}}$. The total circuit inductance and subsequently the total circuit resistance are then calculated from $L_{\text{total}} = 1/\omega_n^2 C_{\text{total}}$ and $R_{\text{total}} = 2L_{\text{total}}\alpha$ accordingly. The spark resistance R_s is determined by subtracting $R_{\text{total}} = R_{\text{circuit}}$ when the spark gap is shorted out $R_s \approx 0$ from $R_{\text{total}} = R_{\text{circuit}} + R_s$ when the spark is not shorted. Finally, the spark discharge energy is found by numerically integrating the square of the current multiplied by spark resistance:

$$E_s = \int_0^\infty i^2 R_s dt$$

According to previous investigation [5, 6], the 1/4 cycle from high voltage capacitor spark discharge is confirmed to adequately estimate the energy responsible for direct initiation by spark ignition analogous to the point blast energy in the ideal case. In the experimental measurement of the critical initiation energy, the amount of initial spark energy is changed via adjusting the capacity of the capacitor or the initial voltage. For each successful and unsuccessful initiation 3 shots are repeated to confirm the critical energy, thus the critical energy should be somewhere inside the interval between the last successful initiation and unsuccessful initiation data points. For the error of measurement of the effective energy from high voltage spark discharge, it is found that at the same voltage and capacitor, the maximum fluctuation of spark energy can be as much as $\pm 8\%$.



Figure 1. A schematic of the experimental setup

3 Measurement results

The critical initiation energies of C_2H_2 mixtures measured from the present experiments are first given in Fig. 2 for different initial pressures and mixture compositions. Also shown are available data published in literature [7]. The present results follow well with previous data and are extended to higher initial pressures. It is well known that acetylene has the lowest critical energy for direct initiation measured to-date of most of the common hydrocarbon and represents the most detonation sensitive hydrocarbon mixtures. Even at high inert gas dilution, the mixtures can support detonation and may detonate with relatively small initiation energy comparable to other undiluted hydrocarbon mixtures.



Figure 2. Critical energy as a function of initial pressure for a) C_2H_2 -2.5 O_2 ; b) C_2H_2 - O_2 ; c) C_2H_2 -4 O_2 ; d) C_2H_2 -2.5 O_2 -50% Ar and e) C_2H_2 -2.5 O_2 -70% Ar mixtures.

It can be seen from Fig. 2a) that, although electrical spark was used as energy source in both cases, there appears some deviation between the present results and that of [7], particularly at low initial pressure. This discrepancy may be due to the dependence of the electrode geometry. In [7], the critical energy was reported on a per unit length basis and represented the limiting value for large spark gap

lengths corresponding to the cylindrical geometry. While in this study, an ideal point energy source is assumed, which is justified with the use of a relatively small electrode spacing compared to the diameter of the electrode and the formation distance of the detonation wave.



Figure 3. Critical energy for C_2H_4 -3 O_2 mixtures as a function of a) initial pressure and b) equivalence ratio at $p_0 = 100$ kPa.

Critical energy plots are shown in Fig. 3 for $C_2H_4-O_2$ mixtures at different initial pressures and equivalent ratios. It is worth noting that ethylene is often an important reference fuel in transportation research. Fig. 3b) also includes some experimental data from previous study [1] and it appears that there is also a discrepancy with the present results. It should be pointed out that the method of obtaining initiation energy in [1] is not explicitly measured. The energy is estimated by first obtaining the critical tube diameter which is then put into a theoretical model using the work-done formula of Lee and Matsui [1].



Figure 4. Critical energy as a function of initial pressure for C₃H₈-5O₂ mixtures.

Propane is the last hydrocarbon fuel considered in this study. By comparing the critical energy of direct initiation among the three hydrocarbon fuels considered here, the detonation hazard posed by propane is the lowest and the critical energy is an order magnitude larger compared to that of acetylene mixtures at the same initial condition.

For completeness, Fig. 5 summarizes some new experimental data for hydrogen-oxygen mixtures at higher initial pressure than those previously archived in Caltech Detonation database [8]. Some higher initial pressure data was previously obtained and reported in [3].



Figure 5. Critical energy as a function of equivalence ratio for 2H₂-O₂ mixtures.

4 Concluding remarks

In this study, a new dataset of critical energy for direct initiation of detonations in some common gaseous fuel-oxygen mixtures is reported. The experimental setup and procedure used in this study provide accurate results through direct measurement of the energy from the current discharge output than those estimated by Matsui and Lee using the critical tube diameter approach with a work-done model [1]. These results should found applications in safety hazard assessment of these fuels and in developing and validating new thorough theoretical model for direct initiation of gaseous detonations.

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References

[1] Matsui H, Lee JHS. (1978) On the measure of the relative detonation hazards of gaseous fueloxygen and air mixture. Proc. Combust. Inst. 17: 1269.

[2] Lee JHS. (1984) Dynamic parameters of gaseous detonations. Ann. Rev. Fluids Mech. 16: 311–36.

[3] Kamenskihs V, Ng HD, Lee JHS. (2010) Measurement of critical energy for direct initiation of spherical detonations in high-pressure H_2 -O₂ mixtures. Combust. Flame 157(9): 1795-1799.

[4] Zhang B, Kamenskihs V, Ng HD, Lee JHS. (2010) Direct blast initiation of spherical gaseous detonation in highly argon diluted mixtures. Proc Combust. Inst. 33(2): 2265-2271.

[5] Zhang B, Ng HD, Lee JHS. (2010) Measurement of effective blast energy for direct initiation of spherical gaseous detonations from high-voltage spark discharge. Revision submitted to Shock Waves Journal (SHOC381).

[6] Knystautas R, Lee JHS. (1976) On the effective energy for direct initiation of detonations. Combust. Flame 27: 221-228.

[7] Lee JH, Matsui H. (1977) A comparison of the critical energies for direct initiation of spherical detonation in acetylene-oxygen mixtures. Combust. Flame, 28(1): 61-66.

[8] Kaneshige M, Shepherd JE. Detonation database, GALCIT Technical Report FM97-8, _http://www.galcit.caltech.edu/detn_db/html/_, 1997.