

## DEFLAGRATION PARAMETERS OF PROPANE–AIR MIXTURES IN A CLOSED CYLINDRICAL VESSEL

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*În prezența lucrare a fost realizat un studiu asupra evoluției presiunii în timpul exploziei sub formă de deflagrație produse în amestecuri propan-aer aflate într-o celulă cilindrică ( $\Phi = 10$  cm;  $h = 15$  cm) cu aprindere centrală, la diferite concentrații inițiale de propan (între 2.60 și 5.70%, in vol.), la diferite presiuni inițiale (între 0.3 și 1.3 bar) și la temperatură inițială ambientă. Sunt discutate influența presiunii și concentrației inițiale asupra presiunilor de explozie, a timpilor necesari atingerii presiunilor maxime de explozie și a vitezelor maxime de creștere a presiunii. Presiunile maxime de explozie măsurate au fost comparate cu valorile din literatură și cu presiunile adiabatice de explozie.*

*An experimental study on pressure evolution during the deflagrative explosions of propane–air mixtures in a cylindrical vessel ( $\Phi = 10$  cm;  $h = 15$  cm) with central ignition was performed at various initial propane concentrations (between 2.60 and 5.70%, vol.), initial pressures (between 0.3 and 1.3 bar) and ambient initial temperature. The influence of initial pressure and fuel concentration on explosion pressures, explosion times and maximum rates of pressure rise is discussed. The experimental values of maximum explosion pressures are compared to literature values and to the adiabatic explosion pressures.*

**Keywords:** explosion pressure, explosion time, maximum rate of pressure rise, cylindrical vessel, propane

### 1. Introduction

Knowledge of characteristic parameters of gaseous fuel-air explosions in closed vessels (maximum explosion pressure,  $p_{max}$ , time necessary to reach the explosion pressure,  $\theta_{max}$ , and maximum rate of pressure rise,  $(dp/dt)_{max}$ ) plays a significant role in formulating safe working conditions for various plants. These

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parameters are important not only for safety recommendations, but also for calculating the laminar burning velocities from closed vessel experiments, for vent area design and for characterizing the transmission of explosions between interconnected vessels [1-4].

Results of experiments depend on many different parameters of the investigated process, such as the energy and type of ignition source, size and shape of explosion chamber, initial temperature, pressure and composition of the flammable mixture.

Data on constant-volume combustion of propane-air mixtures, in various conditions (initial pressures within 0.3 – 1.3 bar,  $[C_3H_8] = 2.60 – 5.70$  vol.%) are reported in the present paper. Propane was chosen since it is widely used as fuel for automotive engines and/or as domestic fuel. In addition, propane is one of the major components of LPG (liquefied petroleum gas), recommended as alternative fuel [5].

Experiments were performed in a cylindrical vessel with central ignition, of volume  $V_C = 1.12$  L, with a ratio height/diameter of 1.5. The wide use of cylindrical vessels in laboratory-scale explosion studies enables the comparison of present data with data reported by other authors, for propane-air in various initial conditions [6, 7]. The present data are also compared to those obtained from experiments in a spherical vessel with central ignition [8]. The measured explosion pressures are compared to the corresponding adiabatic values, computed in the assumption that the chemical equilibrium is reached within the flame front.

## 2. Experimental

Experiments were performed in a stainless steel cylindrical vessel with the height  $h = 15$  cm and the diameter  $\Phi = 10$  cm, which can withstand an internal pressure of 40 bar. The vessel was equipped with several ports for the gas feed, an evacuation valve, and two ionization probes (tips mounted 3 mm and 5 mm, respectively, away from the side wall).

A vacuum and gas-feed line, tight at pressures between 0.5 mbar and 1.5 bar, connected the combustion vessel with the gas cylinders containing fuel and air, with a metallic cylinder for mixture storage and a vacuum pump. A scheme of the experimental set-up was previously given [8].

The fuel-air gaseous mixtures were obtained in a metallic cylinder by the partial pressure method and used 24 h after mixing the components, at a total pressure of 4 bar. The initial pressures of propane-air mixtures were measured by a strain gauge manometer (Edwards type EPS-10HM).

Before each test, the combustion vessels were evacuated down to 0.5 mbar; the explosive mixture was admitted and allowed 15 min. to become

quiescent. Ignition was made with inductive–capacitive sparks produced between stainless steel electrodes (1 mm diameter, round tips). Spark energies were adjusted to a minimum value, between 1 and 5 mJ, in order to avoid the turbulence produced by an excessive energy input at initiation. The pressure variation during explosions was recorded with a piezoelectric pressure transducer (Kistler 601A), connected to a Charge Amplifier (Kistler 5001SN). The signals from the Charge Amplifier and the ionisation probe were recorded with an acquisition data system TestLabTM Tektronix 2505, by means of an acquisition card type AA1, usually at 5000 signals per second.

Propane–air mixtures with fuel concentration between 2.60 and 5.70 vol.% were investigated, at total initial pressures between 0.3 and 1.3 bar. Propane (99.99%) (SIAD – Italy) was used without further purification.

### 3. Data processing and computing programs

The computation of pressure rise rates ( $dp/dt$ ) from pressure-time diagrams was made after smoothing the  $p(t)$  data by Savitzky-Golay method, based on least squares quartic polynomial fitting across a moving window within the data. The method, described in a previous paper [9] has the advantage of producing a smoothed first derivative without filtering the data. This involved the analysis of 500-700 points within ignition and the time necessary to reach the peak explosion pressure. In all cases, we used a 10% smoothing level, since a higher value of this level (e.g. 20%) determined a reduction of the noise accompanied by the signal distortion.

The calculations of adiabatic explosion pressures were made with the program ECHIMAD [10], based on a general algorithm meant to compute the equilibrium composition of products for any fuel–oxidizer gaseous mixture. The algorithm is based on the thermodynamic criterion of chemical equilibrium: the minimum of free Gibbs energy, at constant temperature and pressure or minimum of free Helmholtz energy, at constant temperature and volume. Fifteen compounds, among them one solid compound ( $C_{\text{graphite}}$ ) were considered as products: the fuel ( $C_3H_8$ ),  $CO_2$ ,  $CO$ ,  $H_2O$ ,  $O_2$ ,  $N_2$ ,  $CH_4$ ,  $C_2H_2$ ,  $C_2H_4$ ,  $H_2$ ,  $NO$ ,  $H$ ,  $OH$  and  $O$ ). Their heat capacities (expressed as functions of temperature with the form:  $C_P = a + b \cdot T + c \cdot T^2 + d \cdot T^{-2}$ ), the standard enthalpies of formation at 298 K and the standard entropies at 298 K were taken from references [11, 12]. For each system, the adiabatic flame temperatures were also calculated, both in isobaric and isochoric combustion.

#### 4. Results and discussion

The propagation parameters of gaseous propane-air explosions in the closed cylindrical vessel ( $p_{max}$ ,  $\theta_{max}$ ,  $(dp/dt)_{max}$ ) were determined from pressure-time diagrams, recorded in experiments at variable initial pressure and composition of the flammable mixture.

The influence of initial pressure on peak (maximum) explosion pressures,  $p_{max}$ , is shown in Figure 1, where data referring to several lean propane-air mixtures are plotted. For all examined systems, the maximum explosion pressures are linear function on total initial pressure of the flammable mixture. Linear correlations between the maximum explosion pressures and the initial pressure of fuel-air mixtures were reported for many explosions of quiescent mixtures, in deflagration regime: e.g. propane-air in a 0.5 L spherical vessel [8]; in a 5 L spherical vessel [13]; in a 20 L spherical vessel [14], or propene-air in a 0.5 L spherical vessel and in a 1.12 L cylindrical vessel [15]. The present data, as well as previous data referring to ethylene-air [16], LPG-air [17] or propene-air [15] show a common feature: both the slope and intercept of the linear correlation are dependent on fuel concentration of the flammable mixture. A disagreement is thus observed in respect to results on dimethyl ether-air mixtures reported by Huang and coworkers [18] for initial pressures within 0.8 and 1.5 bar, at ambient initial temperature; in this case, a constant slope was found for all mixtures, regardless on their concentration.

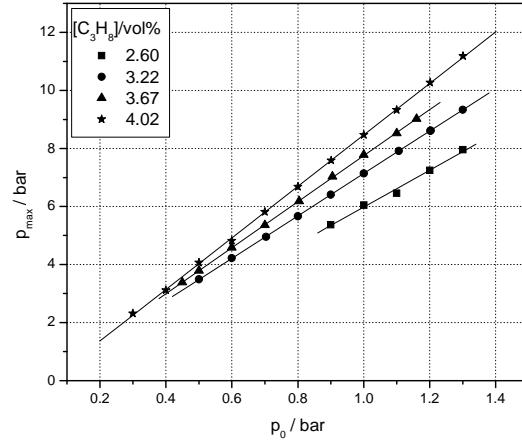


Fig. 1. Maximum explosion pressures of propane-air mixtures, at ambient initial temperature and various initial pressures

The maximum explosion pressures of propane-air mixtures in experiments at various initial pressures and concentrations are given in Figure 2, where data were fitted by 2-nd order polynomials. In Figure 3, a comparison of data referring to explosions at ambient initial conditions (experimental and computed peak explosion pressures) with literature data is given. As expected, for every concentration and/or initial pressure, the adiabatic explosion pressures are higher as compared to experimental values measured in systems with heat losses.

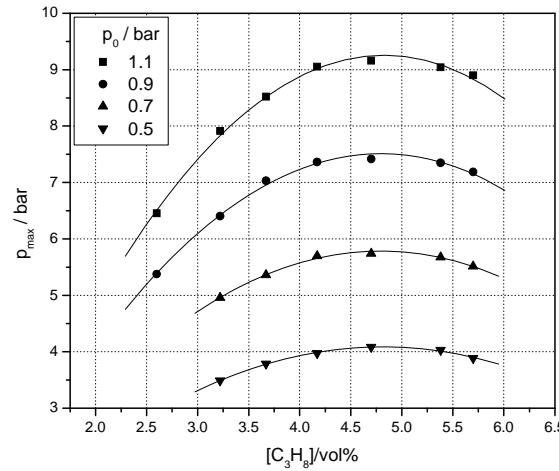


Fig. 2. Maximum explosion pressures of propane-air mixtures, at various initial pressures and concentrations

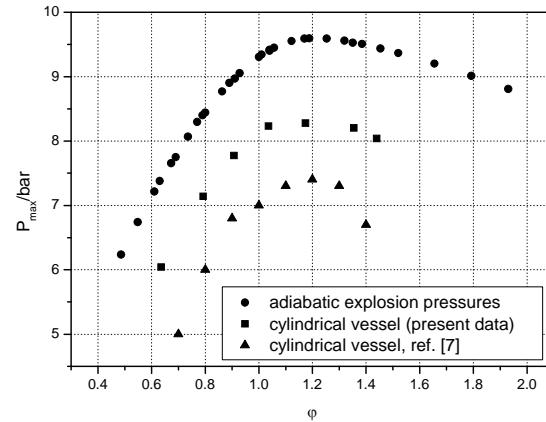


Fig. 3. Maximum explosion pressures of propane-air mixtures, at ambient initial conditions

In the present study, the maximum explosion pressure of the stoichiometric propane-air mixture ( $[C_3H_8] = 4.02\%, \text{ vol.}$ ) at ambient initial conditions is 8.2 bar. In the same initial conditions, the highest explosion pressure is 8.3 bar, reached in a 4.70%, vol. propane-air mixture. For this mixture, considered “the most reactive”, the maximum explosion pressure measured in a spherical vessel is 9.1 bar [8] and the adiabatic explosion pressure is 9.6 bar. For this most reactive mixture, other authors reported maximum explosion pressures between 8.0 bar and 8.2 bar in cylindrical vessels [6, 7] and between 8.8 bar and 9.4 bar in spherical vessels [13, 19, 20]. The asymmetry of the vessel determines important heat losses during flame propagation and accounts for the systematic lower explosion pressures in cylindrical vessels in comparison with spherical vessels. A comparison of data referring to explosions at ambient initial conditions (experimental and computed peak explosion pressures) with literature data is given in Figure 3, where the maximum explosion pressures are plotted against the equivalence ratio  $\varphi$  of propane-air mixtures<sup>6</sup>. As expected, for every concentration and/or initial pressure, the adiabatic explosion pressures are higher as compared to experimental values measured in systems with heat losses.

The explosion time  $\theta_{max}$  (the time necessary to reach the maximum explosion pressure) is dependent on mixture composition, as shown in Figure 4. The initial pressure variation, within the investigated range, has little influence on explosion times.

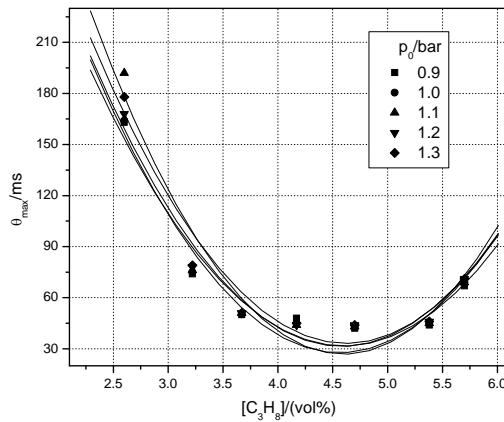


Fig. 4. The time necessary to reach the maximum explosion pressure, at various initial concentrations of propane-air mixtures and initial pressures

<sup>6</sup> The equivalence ratio  $\varphi$  of any flammable mixture is defined as:  $\varphi = \frac{[\text{fuel}]/[\text{oxygen}]}{([\text{fuel}]/[\text{oxygen}])_{st}}$ , where the index “st” refers to a stoichiometric fuel-air mixture.

Linear correlations were found also between the maximum rate of pressure rise and the initial pressure, at constant initial concentration of propane-air mixtures. Data referring to the examined systems are given in Figure 5.

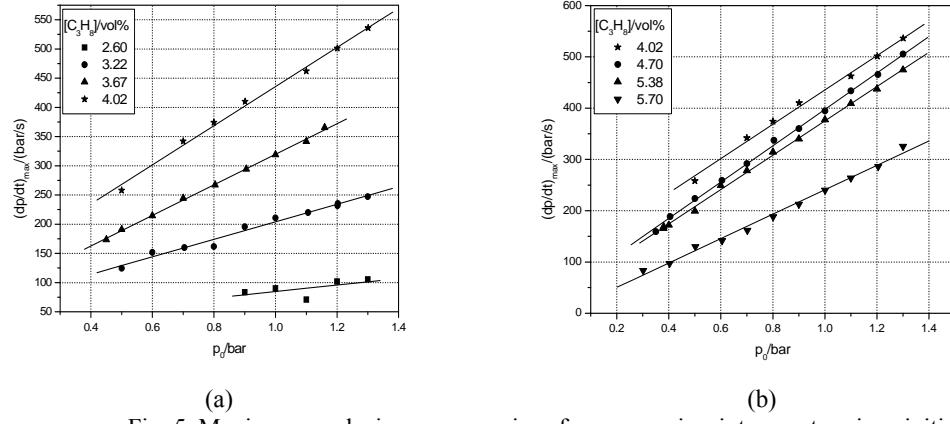


Fig. 5. Maximum explosion pressure rise of propane-air mixtures, at various initial pressures and concentrations:

(a) – lean ( $[C_3H_8] = 2.60\text{--}3.67\%$ , vol.) and stoichiometric ( $[C_3H_8] = 4.02\%$ , vol.) mixtures;  
 (b) – rich ( $[C_3H_8] = 4.70\text{--}5.70\%$ , vol.) and stoichiometric mixtures

In Figure 6 the maximum rate of pressure rise of propane-air mixture at ambient temperature and pressure are plotted versus the equivalence ratio  $\phi$ , in comparison with literature data [7].

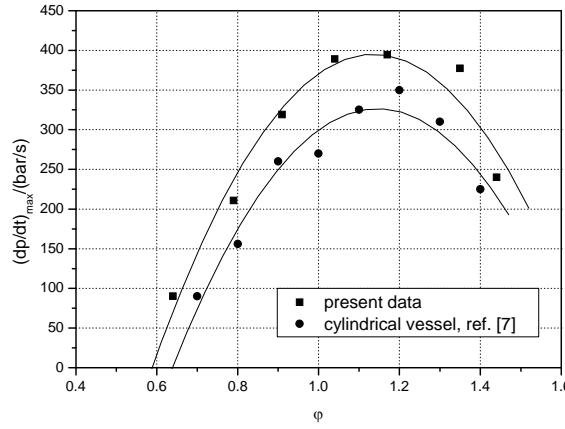


Fig. 6. Maximum explosion pressure rise of propane-air mixture; present data and data measured in a 2.56 L cylinder with central ignition [7]

The maximum rate of pressure rise for the stoichiometric propane-air mixture at ambient pressure and temperature is  $(dp/dt)_{max} = 391$  bar/s in the present measurements. For comparison, Senecal [6] obtained  $(dp/dt)_{max} = 270$  bar/s in a cylindrical vessel with volume  $V = 22$  L, Huzayyin reported  $(dp/dt)_{max} = 350$  bar/s [7] from experiments made in a cylindrical vessel of volume  $V = 2.56$  L and Cashdollar [20] reported  $(dp/dt)_{max} = 304$  bar/s from experiments made in a spherical vessel of volume  $V = 120$  L. The differences of dimensions of these explosion vessels account for the wide range of rates of pressure rise. A better comparison of data can be made by means of the severity index  $K_G$ , defined as:

$$K_G = \sqrt[3]{V} \cdot \left( \frac{dp}{dt} \right)_{max}$$

which is used for scale-up of gaseous explosions in enclosures with variable volume.

Table 1 gives a set of representative  $K_G$  values referring to explosions of a stoichiometric propane-air mixture at ambient initial conditions, in various closed vessels.

Table 1

Severity indices  $K_G$  of propane-air mixtures in various conditions

Explosion vessel	$K_G$ (bar.m/s)	Reference
Cylinder, $h = 15$ cm; $\Phi_C = 10$ cm	53	Present data
Cylinder, $h = 35$ cm; $\Phi_C = 30.4$ cm	76	[6]
Cylinder, $h = 15$ cm; $\Phi_C = 14.5$ cm	92	[7]
Sphere, $\Phi_S = 10$ cm	85	[8]
Sphere, $\Phi_S = 21.2$ cm;	100	[13]
Sphere, $\Phi_S = 61.2$ cm;	150	[20]

One could expect that  $K_G$  should be independent of vessel's volume; however, the severity factor is still influenced by the dimension and asymmetry of the enclosure.

A summary of information concerning the explosive combustion of propane with air in vessel C and in a spherical vessel S (10 cm diameter;  $V = 0.52$  L)[8] with central ignition is given in Table 2.

Table 2

Extreme values of deflagration parameters for explosions of propane-air mixtures in two closed vessels at  $p_0 = 1$  bar and  $T_0 = 298$ K

	Vessel S	Vessel C	Concentration range where extreme values of flammability parameters are observed
$p_{max}$ / bar	9.10	8.70	
$(dp/dt)_{max}$ / (bar.s <sup>-1</sup> )	1200	400	4.60 – 4.80 vol.%
$\theta_{max}$ /ms	20	35	

## 5. Conclusions

At constant initial temperature and fuel concentration, in explosions of quiescent propane-air mixtures in a cylindrical vessel with central ignition, both peak pressures and maximum rates of pressure rise are linear functions on total initial pressure. The slope and intercept of found correlations are influenced by the amount of heat losses from the burned gas to the vessel. The obtained correlations enable the calculation of peak pressure or of maximum rate of pressure rise at any value of initial pressure - important aspect from safety reasons point of view, for explosions occurring in conditions different from ambient, when direct measurements are not available.

The maximum rates of pressure rise and deflagration index of propane-air explosions have maxima at concentrations higher than stoichiometric, usually at equivalence ratios 1.2–1.4.

The reported measurements made with a cylindrical vessel different from the EU standard (recommending a 20 L sphere), provide useful results concerning explosion evolution of propane-air systems. They are useful data for scaling explosions in chemical reactors and for the design of safety (venting) devices.

## Acknowledgement

The present study was partly financed by the Romanian Ministry of Education, by the contract PN II - IDEI No. 546/2009, code ID 458 in the frame of the National Program for Research and Innovation.

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