



Temperature and pressure influence on explosion pressures of closed vessel propane–air deflagrations

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ABSTRACT

An experimental study on pressure evolution during closed vessel explosions of propane–air mixtures was performed, for systems with various initial concentrations and pressures ($[C_3H_8] = 2.50\text{--}6.20\text{ vol.}\%$, $p_0 = 0.3\text{--}1.2\text{ bar}$). The explosion pressures and explosion times were measured in a spherical vessel ($\Phi = 10\text{ cm}$), at various initial temperatures ($T_0 = 298\text{--}423\text{ K}$) and in a cylindrical vessel ($\Phi = 10\text{ cm}$; $h = 15\text{ cm}$), at ambient initial temperature. The experimental values of explosion pressures are examined against literature values and compared to adiabatic explosion pressures, computed by assuming chemical equilibrium within the flame front. The influence of initial pressure, initial temperature and fuel concentration on explosion pressures and explosion times are discussed. At constant temperature and fuel/oxygen ratio, the explosion pressures are linear functions of total initial pressure, as reported for other fuel–air mixtures. At constant initial pressure and composition, both the measured and calculated (adiabatic) explosion pressures are linear functions of reciprocal value of initial temperature. Such correlations are extremely useful for predicting the explosion pressures of flammable mixtures at elevated temperatures and/or pressures, when direct measurements are not available.

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1. Introduction

Knowledge of explosion pressures and explosion times characteristic for explosions of fuel–air mixtures in enclosures is required in various applied research fields related to combustion phenomena: design and construction of venting devices, prediction of engines and combustors performance, safety recommendations for the production, transportation or use of fuels [1]. In basic research, the explosion pressures are key values for calculating the laminar burning velocity in various conditions; both the explosion pressures and explosion times are important for validating models of combustion wave propagation, in isolated or inter-connected explosion vessels.

The explosion pressure (defined as the peak pressure developed in a contained deflagration of a flammable mixture) and the explosion time (defined as the time interval from ignition to peak pressure) characteristic for fuel–air gaseous deflagrations in closed vessels, at initial ambient pressure and temperature, were reported in many publications [2–13]. Recent data on explosion pressures characteristic of gaseous closed vessel explosions were obtained from experiments in a spherical 20 L vessel with central ignition, as recommended by European standard EN 13673-1 [14].

The maximum explosion pressure (defined as the maximum pressure developed in a contained deflagration of an optimum mixture) of gaseous hydrocarbons in the presence of air at ambient initial conditions, measured by this method, is given in the German collections of data [15,16]. These sources of data do not include, however, the influence of fuel concentration in fuel–air mixtures or the influence of oxidant/inert concentration in fuel–oxidant–inert mixtures on explosion pressures.

Explosion pressures of fuel–air mixtures at pressures and/or temperatures different from ambient were determined in a wide set of conditions (explosion vessels with various forms and volumes; ignition made by local sources with various energies, from a few mJ up to 20 J; position of the ignition source: central or asymmetric) [5,6,10,11,13,17–27]. The data refer to single fuels, such as hydrogen, methane, propane, propylene or to composite fuels (LPG, gasoline).

Either pure or blended (e.g. in the form of LPG–Liquefied Petroleum Gas), propane is widely used as fuel for automotive engines and domestic heaters, as a refrigerant or as feedstock for the production of base petrochemicals; accordingly, propane is one of the most studied fuels [5–9,12,13,18,27–30]. Measurements of pressure–time history during propane–air deflagrations were performed mostly in symmetrical vessels with central ignition (spheres or cylinders with h/D close to 1) of 20 L, 120 L, 1 m³ or even 25.5 m³ volume [5–8,13,18]; a few data were reported for asymmetrical vessels, as well [12,27]. The authors tried to evaluate

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also the influence of heat losses during explosion development on explosion pressure and maximum rate of pressure rise for various fuel–air mixtures (including propane) and found significant differences between explosion pressures measured in symmetrical and asymmetrical vessels.

In the present paper, data on constant-volume combustion of propane–air mixtures, in various conditions (initial pressures within 0.3–1.2 bar and initial temperatures within 295–435 K) are reported. Experiments performed in two vessels with central ignition: a spherical vessel of volume $V_S = 0.52$ L and a cylindrical vessel of volume $V_C = 1.12$ L, with a ratio height/diameter of 1.5, enable the examination of initial pressure and initial temperature influences on explosion pressures and explosion times. The measured explosion pressures are examined versus the corresponding adiabatic values, calculated in the assumption that the chemical equilibrium is reached within the flame.

2. Experimental

Experiments were performed in two stainless steel combustion vessels: a spherical vessel *S* of diameter $\Phi = 10$ cm and a cylindrical vessel *C* with height $h = 15$ cm and diameter $\Phi = 10$ cm, which can withstand an internal pressure of 40 bar. Each vessel was equipped with several ports for the gas feed and evacuation valve, two ionization probes (tip mounted 3 mm away from the side wall and 5 mm, respectively), ignition electrodes and a pressure transducer. A vacuum and gas-feed line, tight at pressures between 0.5 mbar and 4.5 bar, connected the combustion vessels 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 is given in Fig. 1.

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 and thermally equilibrated. Ignition was made with inductive–capacitive sparks produced between stainless steel electrodes (1 mm diameter, round tips). The spark gap of constant width (3 mm) was located in the geometrical centre of each vessel. 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 piezoelectric pressure transducers (Kistler 601A), connected to Charge Amplifiers (Kistler 5001SN). Each Charge Amplifier was calibrated by means of a Kistler Cali-

brator type 5357. For experiments at elevated temperatures, the spherical vessel *S* was electrically heated; its piezoelectric pressure transducer was mounted in a special adapter, maintained at $(25 \pm 0.1)^\circ\text{C}$ by a water jacket. The temperature of vessel *S* was adjusted by $\pm 1^\circ\text{C}$ using a controller type AEM 1RT96 and monitored by a K-type thermocouple.

The signals from the Charge Amplifier and the ionization probe were recorded with an acquisition data system TestLab™ Tektronix 2505, by means of an acquisition card type AA1, usually at 5000 signals per second.

Propane–air mixtures with fuel concentration between 2.5 and 6.2 vol.% were investigated, at total initial pressures between 0.3 and 1.2 bar and initial temperatures between 298 and 423 K. Propane (99.99%) (SIAD–Italy) was used without further purification. Several tests performed in spherical vessel *S* with a 4.06 vol.% propane–air mixture at ambient initial conditions were used to examine the reproducibility of results. Minimum 3 experiments were performed for each initial condition of explosive mixture. The standard error in measured explosion pressures was $\leq 2\%$.

3. Computing program

The calculations of adiabatic explosion pressures were made with the program ECHIMAD [31], 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_{graphite}) were considered as products: the fuel (C_nH_m), C_{graphite} , 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 [32,33]. Adiabatic flame temperatures were also calculated, for each system, both in isobaric and isochoric combustion.

4. Results and discussion

The pressure–time history of explosions propagating in the spherical vessel, in a near-stoichiometric propane–air mixture at various initial pressures and temperatures is shown in Fig. 2. At any initial pressure, the increase of initial temperature entails the decrease of peak (maximum) explosion pressure p_{max} and the decrease of the explosion time (time from ignition to peak explosion pressure) θ_{max} . A similar variation was found for all examined systems.

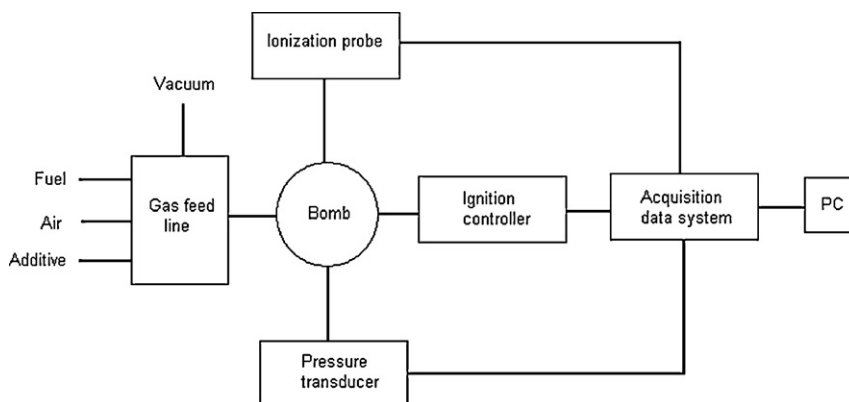


Fig. 1. Schematic diagram of the test equipment.

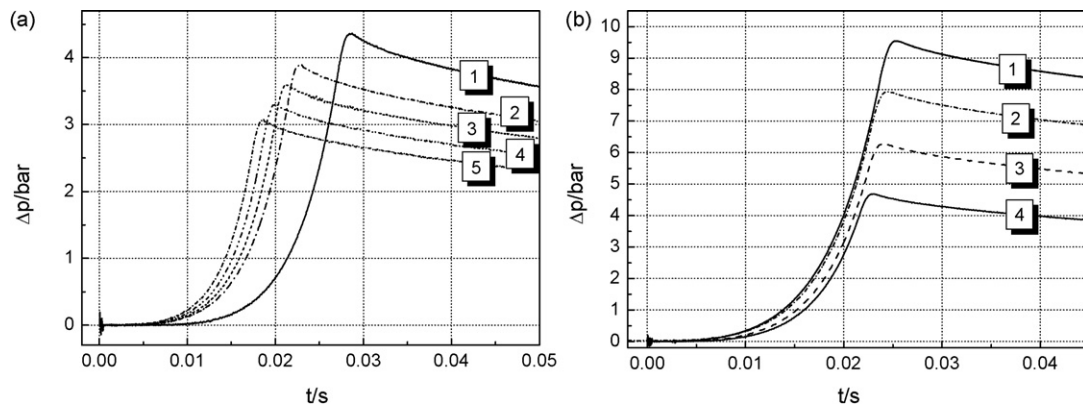


Fig. 2. Pressure–time evolution during explosions of 4.08 vol.% propane–air mixture in spherical vessel S: (a) at $p_0 = 0.5$ bar and various initial temperatures: (1) 298 K; (2) 333 K; (3) 363 K; (4) 393 K; (5) 423 K; (b) at $T_0 = 333$ K and various initial pressures: (1) 1.2 bar; (2) 1.0 bar; (3) 0.8 bar; (4) 0.6 bar.

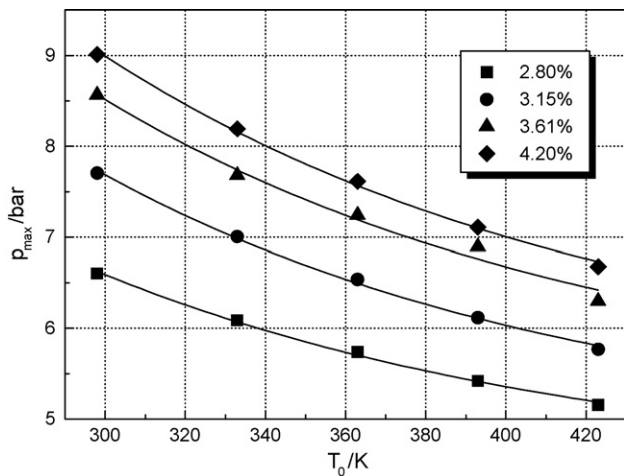


Fig. 3. Peak explosion pressures of propane–air mixtures in spherical vessel S, at various initial temperatures and $p_0 = 1.0$ bar.

Diagrams of peak explosion pressures reached at ambient initial pressure in preheated propane–air mixtures are given in Fig. 3 for several lean (2.80–3.61 vol.%) and one near-stoichiometric mixture (4.20 vol.%). The same data, plotted as dimensionless explosion pressures $\pi_{max} = p_{max}/p_0$ against the reciprocal values of initial temperature are linear, as seen in Fig. 4. Similar plots were obtained for rich mixtures ($[C_3H_8] = 5.5\text{--}6.22$ vol.%) as well.

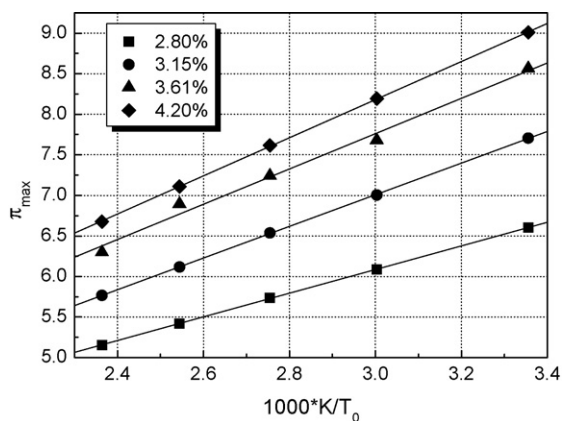


Fig. 4. Variation of dimensionless explosion pressures reached in spherical vessel S at $p_0 = 1.0$ bar, in correlation to the reciprocal temperature of lean- and near-stoichiometric propane–air mixtures.

The data in Fig. 4 are well fitted by equation:

$$\pi_{max} = a + \frac{b}{T_0} \quad (1)$$

The slopes and intercepts of the correlations found for data measured in the spherical vessel at ambient initial pressure are given in Table 1. Data measured at other initial pressures fit well (Eq. (1)), for all examined propane–air mixtures.

Such a variation was reported for both experimental and calculated (adiabatic) explosion pressures of various gaseous mixtures: methane–air, by Pekalski et al. [21] (measurements made in a standardized 20 L sphere); synthetic biogas ($CH_4\text{--}CO_2$ mixture)–air, by Dupont and Accorsi [25] (20 L sphere); propane–air, by Desoky et al. (14 L sphere) [5]; LPG–air, by Huzayyin et al. [13] (2.56 L cylinder). In contrast to them, measured explosion pressures on $CH_4\text{--}air$ (experiments made in a 40 L sphere) were fitted versus temperature by a linear equation [23]. In all cases, the observed decrease of peak pressures in preheated flammable mixtures was explained by the decrease of density for the burning charge, which releases thus a lower heat amount.

The influence of initial pressure on peak explosion pressures is shown in Fig. 5, where data referring to a lean propane–air mixture ($[C_3H_8] = 3.15$ vol.%) are plotted. At constant initial temperature, the measured explosion pressures are correlated to initial pressure by the linear equation:

$$p_{max} = \alpha + \beta \cdot p_0 \quad (2)$$

The slope and intercept of such equations are listed in Table 2 and in Table 3, together with the determination coefficients.

Linear correlations between the peak explosion pressures and the initial pressure of fuel–air gaseous mixtures were reported for many explosions of quiescent mixtures, in deflagration regime, e.g. methane–air in a 20 L spherical vessel [21] or in a 40 L vessel [23]; propane–air in a 2.56 L cylindrical vessel [13] and in a 5 L spherical

Table 1

Parameters of linear correlations between the dimensionless explosion pressure and the reciprocal temperature, for propane–air mixtures at $p_0 = 1.0$ bar.

$[C_3H_8]$ (vol.%)	a	$b \times 10^3$ (K)
2.80	1.710	1.458
3.15	1.151	1.952
3.61	1.230	2.177
4.08	1.042	2.287
4.20	1.125	2.352
4.51	0.907	2.432
5.06	1.167	2.349
5.50	1.674	2.061
6.22	2.106	1.674

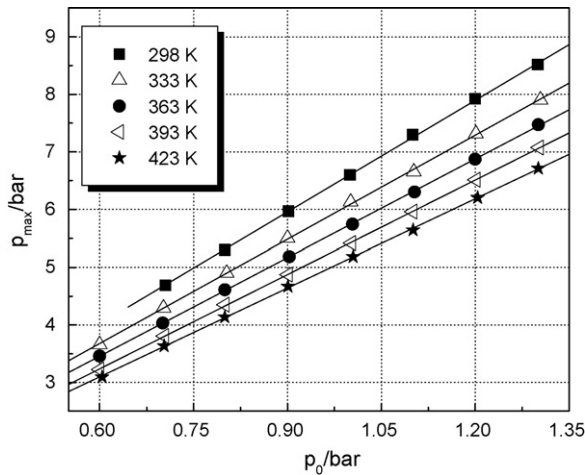


Fig. 5. Peak explosion pressures of 3.15 vol.% propane–air mixture reached in spherical vessel S, at various initial pressures and temperatures.

Table 2

The fit parameters of linear correlations between the peak explosion pressure and the initial pressure (Eq. (2)) for two sets of data obtained in vessel S, at various initial temperatures.

T_0 (°C)	α (bar)	β	r_n
$[\text{C}_3\text{H}_8] = 3.15\% (\varphi = 0.774)^a$			
25	-0.049 ± 0.025	7.755 ± 0.026	0.9996
60	-0.087 ± 0.034	7.093 ± 0.036	0.9991
90	-0.093 ± 0.010	6.630 ± 0.011	0.9999
120	-0.078 ± 0.032	6.195 ± 0.041	0.9991
150	-0.092 ± 0.013	5.858 ± 0.018	0.9998
$[\text{C}_3\text{H}_8] = 4.20\% (\varphi = 1.044)$			
25	-0.091 ± 0.023	9.104 ± 0.031	0.9998
60	-0.110 ± 0.015	8.303 ± 0.018	0.9998
90	-0.103 ± 0.010	7.718 ± 0.012	0.9999
120	-0.109 ± 0.024	7.217 ± 0.032	0.9993
150	-0.101 ± 0.011	6.777 ± 0.016	0.9998

^a φ is the equivalence ratio of fuel–air mixture, defined as $\varphi = ([\text{fuel}]/[\text{O}_2])/([\text{fuel}]/[\text{O}_2])_{\text{stoich}}$.

vessel [6]; propylene–air in a 0.5 L spherical vessel [11]; LPG–air in a 2.56 L cylindrical vessel [13] and in a 1.12 L cylindrical vessel [34]; dimethyl ether–air in a 1.57 L cuboid vessel [26]. The present data, as well as previous data we obtained in the same enclosures [10,11,34] 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 et al. [26] 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.

From the examination of the heat balance during the constant volume combustion of a gaseous fuel–air mixture [35] a correlation

Table 3

The fit parameters of linear correlations between the peak explosion pressure and the initial pressure (Eq. (2)) for data obtained in vessel C, at various initial concentrations and ambient initial temperature.

$[\text{C}_3\text{H}_8]$ (vol%)	φ	α (bar)	β	r_n
2.60	0.636	-0.390 ± 0.382	6.368 ± 0.345	0.9956
3.22	0.792	-0.173 ± 0.010	7.309 ± 0.010	0.9999
3.67	0.907	-0.185 ± 0.023	7.937 ± 0.028	0.9999
4.14	1.036	-0.229 ± 0.013	8.414 ± 0.015	0.9999
4.70	1.174	-0.188 ± 0.031	8.489 ± 0.036	0.9999
5.38	1.354	-0.165 ± 0.007	8.362 ± 0.009	0.9999
5.70	1.439	-0.336 ± 0.047	8.404 ± 0.055	0.9998

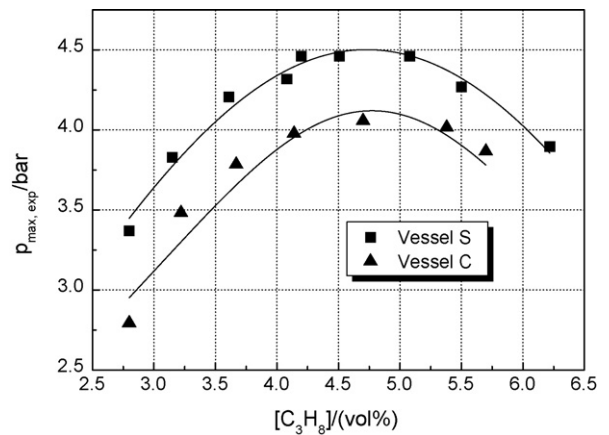


Fig. 6. Peak explosion pressures of propane–air mixtures, at ambient initial temperature and ambient initial pressure, obtained in spherical vessel S and cylindrical vessel C.

between p_e , the pressure reached at the end of combustion and the initial pressure and temperature, p_0 and T_0 was found:

$$p_e = p_0 \left(\xi + \frac{r_1}{\nu_l} \cdot \frac{\Delta^c U'}{T_0 \cdot \bar{C}_{e,V}} \right) - q_{tr} \frac{\gamma_e - 1}{V_0} = \pi_{ad} \cdot p_0 - q_{tr} \frac{\gamma_e - 1}{V_0} \quad (3)$$

where π_{ad} is the adiabatic coefficient of the pressure increase during explosion, defined as $(p_{ad,max}/p_0)$; q_{tr} is the total amount of heat losses, transferred by the gas to the vessel before the end of combustion. The signification of ξ , r_1 , ν_l , γ_e , $\Delta^c U'$ and $\bar{C}_{e,V}$ is given in Appendix A.

Eq. (3) can be rewritten as:

$$p_{max} = \left(\xi + \frac{r_1}{\nu_l} \cdot \frac{\Delta^c U'}{T_0 \cdot \bar{C}_{e,V}} \right) \cdot p_0 - q_{tr} \frac{\gamma_e - 1}{V_0} = \pi_{ad} \cdot p_0 - q_{tr} \cdot \frac{\gamma_e - 1}{V_0} \quad (4)$$

by assuming that p_e , the pressure reached at the end of combustion, is equal or very close to the peak (maximum) explosion pressure p_{max} . Indeed, data measured in vessel S for various fuel–air mixtures support this approximation [11,35].

From Eq. (4), the variation of the peak (maximum) explosion pressure with initial temperature T_0 (according to Eq. (1)) and initial pressure p_0 (according to Eq. (2)) of the flammable mixture is confirmed. Such dependencies are valid, however, for restricted variation ranges of initial temperature and pressure.

In comparison to explosion pressures measured in vessel S, those reached in vessel C (at identical p_0) are smaller, for all examined compositions.

Two sets of data obtained in experiments at $T_0 = 298$ K and $p_0 = 1$ bar are plotted in Fig. 6 versus propane concentration. They were fitted against propane concentration by 2nd degree polynomials:

$$\text{vessel S: } p_{max}/\text{bar} = -3.918 + 5.505[\text{C}_3\text{H}_8]/(\text{vol.}\%)$$

$$- 0.586([\text{C}_3\text{H}_8]/\text{vol.}\%)^2;$$

$$\text{determination coefficient} = 0.979 \text{ (17 points)} \quad (5)$$

$$\text{vessel C: } p_{max}/\text{bar} = -4.892 + 5.542[\text{C}_3\text{H}_8]/(\text{vol.}\%)$$

$$- 0.576([\text{C}_3\text{H}_8]/\text{vol.}\%)^2;$$

$$\text{determination coefficient} = 0.983 \text{ (7 points)} \quad (6)$$

The left (ascendent) branch of each plot corresponds to $r_1 < 1$ when propane is the limiting component of the mixture; the right

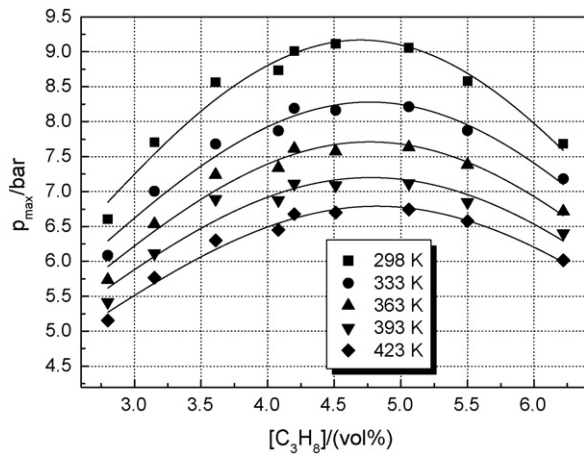


Fig. 7. Peak explosion pressures of propane-air mixtures at $p_0 = 1$ bar and various initial temperatures, measured in vessel S.

(descendent) branch of each plot corresponds to $r_1 < 1$ when oxygen is the limiting component of the mixture.

The influence of initial composition on peak explosion pressures measured in vessels S and C was examined at various initial pressures (both vessels) and various initial temperatures (in vessel S). A set of representative results obtained in vessel S at ambient initial pressure and various initial temperatures is plotted in Fig. 7. A comparison of data referring to explosions at ambient initial conditions, from the present measurements and from literature, is given in Fig. 8. In the present study, the highest peak pressure of propane-air at ambient initial conditions is 9.1 bar, measured in spherical vessel S for $[C_3H_8] = 4.51$ vol.%. In the same initial conditions, the peak explosion pressure of the stoichiometric mixture is 8.7 bar. For comparison, literature data are listed in Table 4. In symmetrical vessels (sphere or cylinder with h/Φ close to 1) the measured maximum explosion pressure vary between 8.2 [7] and 9.4 [16]. Any factor, determining the flame asymmetry (such as a slight deviation of the spark gap position from vessel's geometrical centre) and/or appearance of cellular flames account for such scatter, observed already for many other systems [11].

In comparison to measured values, the highest adiabatic explosion pressure is 9.6 bar, reached at propane concentrations in the range $4.50 < [C_3H_8] < 4.80$ vol.%. Data calculated at various initial temperatures and ambient initial pressures are plotted in Fig. 9; the plots are similar to those obtained for experimental explosion pressures (Fig. 7). As expected, for every concentration and/or ini-

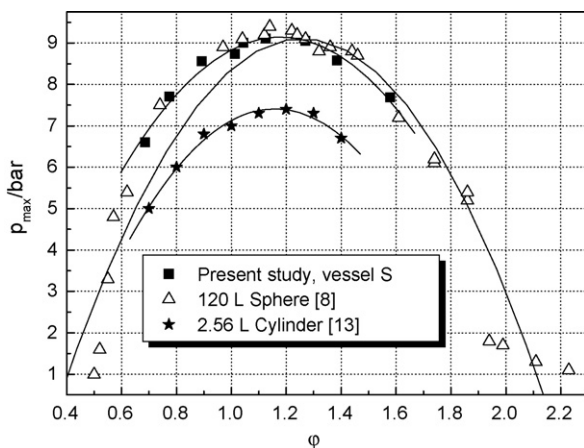


Fig. 8. Peak explosion pressures of propane-air mixtures at ambient initial conditions, measured in vessel S (present study), compared to literature data.

Table 4

Measured explosion pressure of propane-air mixtures, at ambient initial pressure and temperature; literature data.

Nr.	p_{exp} (bar abs)	$[C_3H_8]$ (vol%)	Explosion vessel	Reference
1	9.2	4.5–5.0	Sphere, $V = 1.7$ L	[5]
2	8.9	4.5	Sphere, $V = 5$ L	[6]
3	8.2	4.5–5.0	Cylinder, $h/D = 1.15$, $V = 22$ L	[7]
4	9.2	4.8–5.2	Sphere, $V = 120$ L	[8]
5	8.8	4.5–5.0	Sphere, $V = 25$ m ³	[8]
6	3.3	4.5–5.0	Cylinder, $h/D = 143$	[12]
7	8.4	4.8–5.2	Sphere, $V = 2.56$ L	[13]
8	9.4	4.5–5.0	Sphere, $V = 20$ L, conditions as in EN 13673-1	[16]

tial temperature, the adiabatic explosion pressures are higher as compared to experimental values measured in systems with heat losses. At constant initial pressure, the adiabatic explosion pressure depends on the reciprocal value of initial temperature according to Eq. (1); at constant initial temperature and composition, Eq. (2) holds for adiabatic explosion pressures as well. The correlations are easily derived from Eq. (4), after neglecting the term associated to heat losses.

The explosion times are dependent on mixture composition and on temperature. The initial pressure variation, within the investigated range, has little influence on explosion times. Illustrative data obtained in vessels S and C are plotted in Fig. 10. Larger explosion times are recorded in vessel C as compared to vessel S, as a consequence of the larger amount (volume) of flammable mixture burning in vessel C ($V_S = 0.52$ L; $V_C = 1.12$ L). The influence of initial temperature and concentration of propane-air mixtures on explosion times measured in vessel S is plotted in Figs. 11 and 12. The increase of preheat temperature determines the decrease of the time necessary to reach the peak explosion pressure, as already reported for various fuel-air mixtures [6,13,23]. The variation of explosion times plotted in Fig. 11 is highest for lean mixtures (e.g. $[C_3H_8] = 2.80$ and 3.15 vol.%); for a near-stoichiometric propane-air mixture, the increase of initial temperature has a much smaller influence. The increase of the initial temperature causes the increase of both reaction rate and normal burning velocity. At constant propane concentration and constant initial pressure, this increase of burning velocity accounts for the decrease of explosion times. The influence of the initial temperature on explosion times is seen also in Fig. 12, where data measured at ambient initial pressure are plotted. For all examined initial temperatures, the

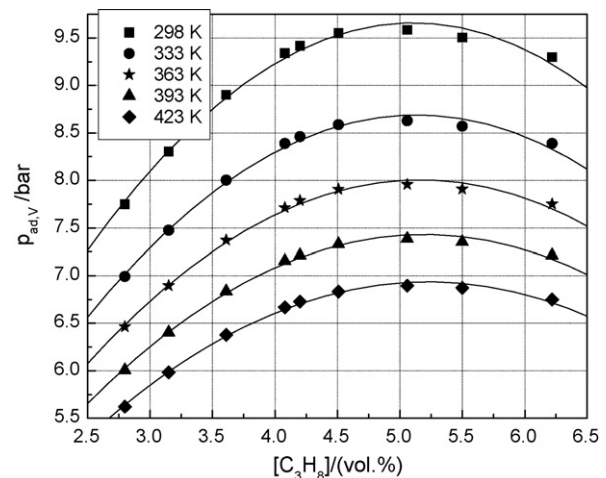


Fig. 9. Calculated adiabatic explosion pressures of propane-air mixtures at $p_0 = 1$ bar and various initial temperatures.

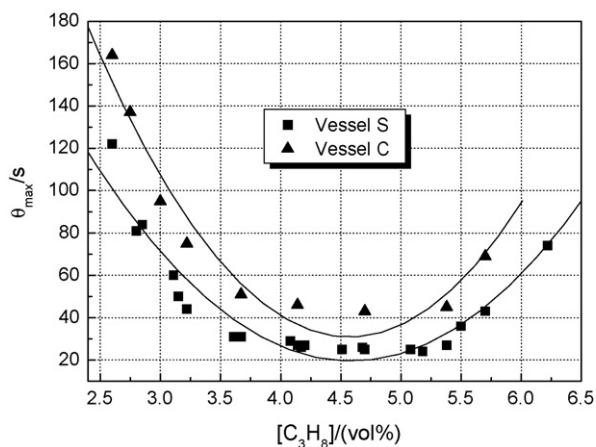


Fig. 10. The time to peak pressure, measured at ambient initial pressure and temperature in vessels S and C.

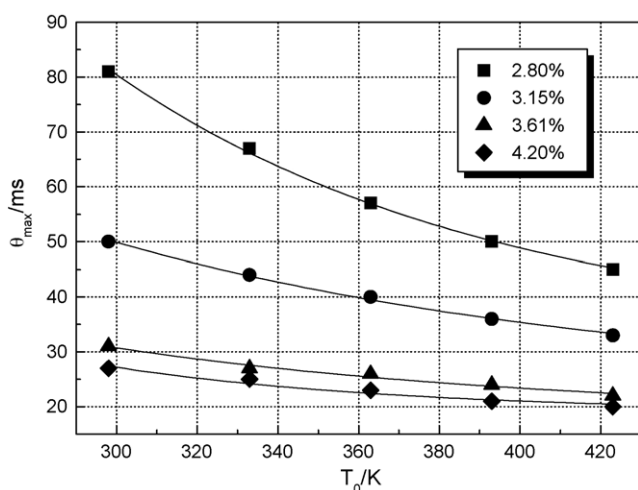


Fig. 11. The time to peak pressure, measured at ambient initial pressure and various initial temperatures in vessel S.

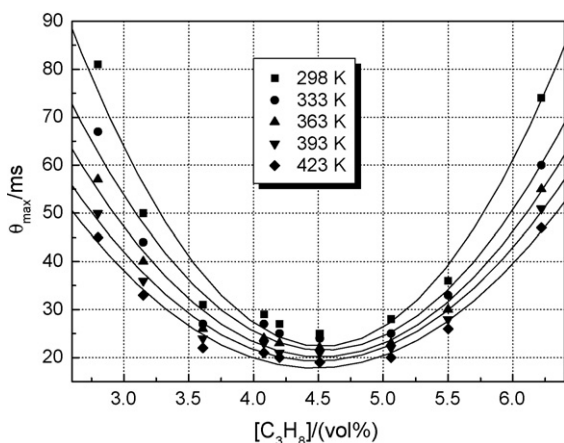


Fig. 12. The time to peak pressure, measured at ambient initial pressure and various initial temperatures in vessel S.

minimum values of explosion times are observed in the concentration range 4.4–4.7 vol.% (rich mixtures). In this concentration range of propane–air mixtures, maximum burning velocities and maximum flame temperatures were obtained [23,36]. In the near-limit mixtures, higher explosion times are measured, determined

by the combined effect of lower burning velocities and enhanced heat losses at vessel's wall.

5. Conclusions

For all propane–air mixtures, the peak explosion pressures, measured or calculated at constant initial pressure and temperature are obtained at fuel concentrations higher than stoichiometric, usually at equivalence ratios 1.2–1.4.

At constant fuel/air ratio and initial temperature, the maximum explosion pressure is a linear function on total initial pressure, for both explosion vessels and for all examined propane–air mixtures. The adiabatic maximum explosion pressures are higher than experimental values.

At constant initial pressure and composition, both the measured and the calculated (adiabatic) explosion pressures are linear functions of the reciprocal value of initial temperature.

Such correlations are extremely useful for predicting the explosion pressures of propane–air flammable mixtures at elevated temperatures and/or pressures, when direct measurements are not available.

For all propane–air mixtures, the explosion times measured at constant initial pressure decrease at increase of the preheating temperature. Minimum explosion times are obtained at fuel concentrations higher than stoichiometric, usually at equivalence ratios 1.2–1.4.

Nomenclature

a, b	parameters of linear correlations between π_{max} and T_0 , b (K)
C	heat capacity, $\text{J mol}^{-1} \text{K}^{-1}$
h	height, cm
n	mole number
p	pressure bar
q	heat amount, J
r	ratio of mole numbers
R	universal gas constant, $\text{J mol}^{-1} \text{K}^{-1}$
S	referring to spherical vessel
t	time, s
T	temperature, K
U	internal energy, J
V	volume, L

Subscripts and superscripts

ad	referring to adiabatic combustion
c	referring to combustion
e	referring to the end state of mixture
f	referring to flame
G	referring to gas
l	referring to the limiting component
max	maximum value
$sens$	referring to sensible heat
tr	referring to transferred heat
u	unburned gas
V	referring to a constant-volume process
0	referring to the initial state of mixture

Greek letters

α, β	parameters of linear correlations between p_{exp} and p_0 α (bar)
γ	adiabatic coefficient (C_p/C_v)
θ	time to peak explosion pressure, s
ν	stoichiometric coefficient

π	dimensionless pressure
ξ	ratio of final to initial mole numbers
φ	equivalence ratio
Φ	diameter

Acknowledgements

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Appendix A.

The state equations applied to the initial and end conditions of the fuel–air gaseous mixture burning in a constant volume vessel (volume V_0) are:

$$p_0 V_0 = n_0 R T_0 \quad (\text{A.1})$$

$$p_e V_0 = n_e \overline{R T_{e,V}} \quad (\text{A.2})$$

where index “0” refers to the initial conditions and “e” refers to the end conditions.

The heat balance during the adiabatic combustion of the gaseous mixture can be written as [35]:

$$(q_c)_V = (q_{sens})_V \quad (\text{A.3})$$

where $(q_c)_V$ is the combustion heat, evolved during combustion of n_0 moles of mixture and $(q_{sens})_V$ is the sensible heat necessary to the end products to raise their temperature from T_0 to $\overline{T_{e,V}}$, the average flame temperature.

The terms in Eq. (A.3) can be calculated as:

$$(q_c)_V = \frac{n_0 \cdot r_l}{\nu_l} \cdot \Delta^c U' \quad (\text{A.4})$$

$$(q_{sens})_V = n_e \cdot \overline{C_{e,V}} \cdot \Delta T = n_e \cdot \overline{C_{e,V}} (\overline{T_{e,V}} - T_0) \quad (\text{A.5})$$

where $r_l = (n_l/n_0)$ is the ratio of the number of moles corresponding to the limiting component of the mixture and the total initial number of moles; ν_l is the stoichiometric coefficient of the limiting component in the mixture and $\Delta^c U'$ is the combustion heat (at constant volume and T_0) corrected by taking into account the endothermic processes; $\overline{C_{e,V}}$ is the molar heat capacity of the end gaseous mixture, averaged for the end components and for the temperature range T_0 to $\overline{T_{e,V}}$.

In adiabatic conditions, the heat balance is equivalent to [35]:

$$p_e = p_0 \left(\xi + \frac{r_l}{\nu_l} \cdot \frac{\Delta^c U'}{T_0 \cdot \overline{C_{e,V}}} \right) = \pi_{ad} \cdot p_0 \quad (\text{A.6})$$

where $\xi = (n_e/n_0)$ is the ratio of final to initial mole numbers and $\pi_{ad} = (p_{ad,max}/p_0)$ is the adiabatic coefficient of the pressure increase during explosion, defined as the ratio of the adiabatic explosion pressure, $p_{ad,max}$, and the initial pressure, p_0 . Within a restricted pressure range, one can assume that ξ , $\Delta^c U'$ and $\overline{C_{e,V}}$ are independent of p_0 (or their variations compensate each other).

Under non-adiabatic conditions, a heat amount q_{tr} is transferred by the gas to the vessel before the end of combustion and the heat balance is:

$$(q_c)_V = (q_{sens})_V + q_{tr} \quad (\text{A.7})$$

Eq. (A.7) can be rewritten as:

$$p_{exp} = \pi_{ad} \cdot p_0 - q_{tr} \frac{\gamma_e - 1}{V_0} \quad (\text{A.8})$$

where γ_e is the adiabatic coefficient of the burned gas, at the end of combustion.

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