EXPANSION COEFFICIENTS AND NORMAL BURNING VELOCITIES OF PROPANE-AIR MIXTURES BY THE CLOSED VESSEL TECHNIQUE

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abstract: The normal burning velocities of propane-air mixtures were calculated from the expansion coefficients and the cubic law constants of flame propagation in the early stage of closed vessel explosions, using the adiabatic compression model. The experiments were made in a spherical vessel with central ignition in various initial conditions: pressure within 0.3÷1.3 bar, temperature within 298÷423 K, propane concentration within 2.80÷6.22 vol.%. The expansion coefficients were computed for the adiabatic isobaric combustion, assuming equilibrium is reached in the flame front. The normal burning velocities are compared with literature data and with normal burning velocities calculated from the same cubic law constants, using the isothermal compression model.

key words: closed vessel; expansion coefficients; burning velocities; propane.

1. Introduction

The determination of flammability characteristics of gaseous combustible mixtures in various conditions is the key for achieving the performance and safety of combustion systems. A special attention is paid to flammability limits, peak explosion pressure, explosion index and normal burning velocity.

The normal burning velocity is a fundamental property of any combustible mixture, influenced mainly by the overall combustion rate in the flame front. The normal burning velocity is useful for design of venting devices and of combustors, such as internal combustion or rocket engines, power plant burners, etc. or for modeling turbulent flame propagation and pollutant formation in internal combustion engines. Determination of the normal burning velocity is made by various methods, making use of stationary flames (e.g. the burner method or the counter-flow twin flames method) or non-stationary flames (the tube method or the constant volume method). The constant volume method, where the normal burning velocity is evaluated from pressure-time records obtained during centrally-

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ignited explosions in various initial conditions, is frequently used [1-4]. The method has several advantages (a small amount of fuel is necessary; a good control of initial conditions (mixture composition, pressure and temperature) is possible), but it requires an advanced mathematical treatment. A simple way to determine the normal burning velocity by this method is to restrict the examination of flame propagation just to the early stage, when the temperature gradients in both unburned and burned gas are small and can be neglected. Such a simple procedure, recently developed [5], was based on the relationship between the pressure increase in the early stage Δp and the time from ignition, t [6]:

$$\Delta p = kt^3 = Kp_0 \frac{S_u^3 t^3}{V_0} \tag{1}$$

where S_u is the normal burning velocity, k – the constant of cubic law, V_0 – the volume of explosion vessel, K – a constant dependent on the flammable mixture composition. Assuming the compression of unburned gas ahead of the flame front is adiabatic, the normal burning velocity S_u was correlated with the constant of cubic law k as:

$$S_u = R \left[\frac{k}{E^2 (E-1)\gamma_u} \right]^{1/3} \tag{2}$$

where: R – the radius of the explosion vessel, E – the expansion factor of the flammable mixture in the early (near-constant pressure) stage of explosion and γ_u – the adiabatic compression coefficient. The expansion coefficient is defined as the ratio of unburnt to burnt gas densities across the flame front:

$$E = \frac{\rho_u}{\overline{\rho_b}} = \left(\frac{T_{f,p}}{T_0} \right) \left(\frac{n_e}{n_0} \right) \tag{3}$$

where: ρ_u – the unburnt gas density; $\overline{\rho_b}$ – the average burnt gas density, $T_{f,p}$ – the adiabatic flame temperature of isobaric combustion; T_0 – the initial temperature; n_e – the end (final) number of moles; n_0 – the initial number of moles. The expansion coefficients can be easily computed for any flammable mixture, using results obtained in equilibrium computations: the adiabatic flame temperature of the isobaric combustion and the end mole number.

In the present paper, the normal burning velocities of propane-air mixtures at various initial pressures, temperatures and mixture compositions, calculated by means of the adiabatic compression model, are reported. The expansion coefficients were computed for the adiabatic isobaric combustion, assuming equilibrium is reached in the flame front.

The comparison of normal burning velocities obtained by this model with literature data and with normal burning velocities calculated from the same cubic law constants, by means of the isothermal compression model [7] affords the choice of the best procedure for calculating normal burning velocities from the early stage of constant-volume explosions.

2. Experimental procedure

Experiments were made in a spherical vessel of 5 cm radius, at various initial pressures (0.3÷1.2 bar), various initial temperatures (298÷423 K) and various initial propane-air

concentrations (2.80÷6.22 vol.%). The ignition of the gaseous mixtures was made with high voltage inductive-capacitive sparks produced between stainless steel electrodes. The spark gap of constant width 3.5 mm was located in the geometrical centre of the vessel. The pressure variation during explosions was recorded with a piezoelectric pressure transducer (Kistler 601A), connected to a Charge Amplifier (Kistler 5001SN) and an Acquisition Data System Tektronix TestLab 2505. The detection of flame front position was made using two ionization probes mounted in equatorial position, with tips at various distances from the wall.

Propane (99.99%) (SIAD Italy) was used without further purification.

Other details were previously given [8-9].

3. Computing programs

The adiabatic flame temperature and the end mole number of isobaric combustion for propane-air mixtures were calculated using the program ECHIMAD [10], assuming that the thermodynamic equilibrium is reached within the flame. The program is based on a general algorithm for computing the equilibrium composition of products for fuel-oxidizer gaseous mixtures by determining the minimum of the free enthalpy. Fifteen compounds ($C_{graphite}$, O_2, N_2, H_2O, CO, CO_2, H_2, NO, CH_4, C_2H_2, C_3H_8, C_4H_{10}, H, OH and O) were taken into account. The heat capacities (expressed as $C_p = f(T)$ polynomials), the standard enthalpies of formation at 298 K and the standard entropies at 298 K were taken from literature [11,12].

The coefficient k, from equation (1), characteristic for the early stage of combustion, was determined for each experiment using a nonlinear regression, applied to an equation of the form:

$$\Delta p = a + k\left(t - b\right)^3 \tag{4}$$

where a and b are pressure and time corrections respectively, meant to eliminate the signal shift of pressure transducer and any possible delay in signal recording [5]. The computation was restricted to a pressure range $p_0 \leq p \leq 2p_0$, for all experiments.

4. Results and discussions

The adiabatic flame temperature and hence the expansion factor depend on flammable mixture concentration, having maximum values at a fuel concentration slightly higher than the stoichiometric one ($[C_3H_8]$ = 4.03 vol.%). In Fig. 1 the variation of expansion factors against propane concentration is given, for systems at constant ambient initial pressure and variable initial temperatures. Such values were computed for all propane-air systems at variable initial pressures and variable initial temperatures and were further used for normal burning velocity calculation by means of the adiabatic compression model.
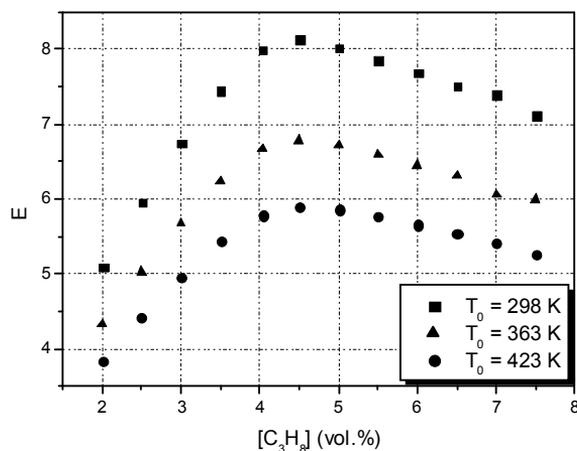
Fig. 1 *Expansion factors of C_3H_8-air mixtures at ambient pressure and various initial temperatures*

Typical values of cubic law coefficients k of propane-air systems at variable initial pressures, temperatures and concentrations are given in Tables 1 and 2.

Table 1 *Cubic law constants ($k*10^{-3}$) of C_3H_8-air mixtures, at ambient initial pressure and various initial temperatures*

[C₃H₈] (vol%)	T_0 (K)				
	298	333	363	393	423
2.80	14.50	21.87	29.86	41.01	53.64
3.15	53.75	74.17	92.81	120.3	148.7
3.61	223.0	301.5	340.3	425.5	513.7
4.08	280.9	355.6	417.8	486.8	613.2
4.20	411.1	450.2	550.1	660.5	737.5
4.51	399.0	514.4	574.2	696.3	819.0
5.08	284.1	363.1	426.3	490.9	610.0
5.50	129.4	148.0	195.7	243.7	272.8
6.22	19.81	28.64	31.98	34.29	40.61

At constant pressure and composition the coefficients of cubic law k increase with increase of the initial temperature. At constant initial pressure and temperature, the coefficients k depends on the concentration having a maximum at near-stoichiometric mixture, similar to the expansion factor E.

A set of representative results referring to a near-stoichiometric propane-air mixture at various initial temperatures and ambient pressure are given in Table 3: the expansion factors E, the adiabatic compression coefficients γ_u and the normal burning velocities S_u obtained by means of equation (2). Table 3 includes also the normal burning velocities $(S_u)^*$, computed by means of the isothermal compression model, as reported in [15]. Very

close values of the normal burning velocities were obtained, at all examined conditions. Their dependency on initial temperature was examined using a power law equation:

$$S_u = S_{u,ref} \left(\frac{T}{T_{ref}} \right)^{\mu} \tag{5}$$

The thermal exponents of normal burning velocities, determined for the two sets of data by means of equation (5) are quite close: $\mu = 1.71$ from the present set of data, $\mu = 1.63$ from data obtained by means of isothermal compression model. They are also in good agreement with values reported by other authors: 2.13 [2]; 1.66 [18]; 1.81 [19]. This behavior was observed for all examined systems.

Table 2 *Cubic law constants ($k \times 10^{-3}$) of C_3H_8-air mixtures, at various initial pressures and ambient initial temperature.*

[C$_3$H$_8$] (vol%)	p_0 (bar)				
	0.4	0.6	0.8	1.0	1.2
3.15	–	39.14	52.94	53.75	56.52
3.61	129.8	177.2	203.6	223.0	248.5
4.08	158.1	227.6	256.7	280.9	295.7
4.51	222.1	302.1	387.0	399.0	415.2
5.08	196.5	238.9	274.7	284.1	316.0
5.50	96.78	109.4	120.2	129.4	136.3
6.22	17.37	16.79	16.61	19.82	21.11

Table 3 *Normal burning velocities of near-stoichiometric mixture (4.08 vol.% C_3H_8-air), at various initial temperatures and ambient pressure.*

T_0 (K)	E	γ_u	S_u (cm/s)	$(S_u)^*$ (cm/s)
298	8.035	1.3673	38.4	38.9
333	7.244	1.3592	46.4	47.9
363	6.688	1.3530	53.3	53.7
393	6.212	1.3472	60.8	61.2
423	5.808	1.3420	70.6	69.5

The normal burning velocities at ambient initial pressure and temperature, obtained using the equation (2), are given in Fig. 2, together with data obtained by other authors (measurements by the closed vessel technique [16] and by the heat-flux method [17]). A good agreement is observed between our results and the literature data, especially for lean propane-air mixtures. The normal burning velocities have a peak value of 42.1 cm/s, reached at 4.5 vol.% propane in air (the most reactive concentration). At the stoichiometric composition, the normal burning velocity was 38.4 cm/s – a value close to literature data obtained by means of the closed vessel method as well: $S_u = 38.3$ cm/s [2]; $S_u = 38.1$ cm/s [13]; $S_u = 38.7$ cm/s [14].
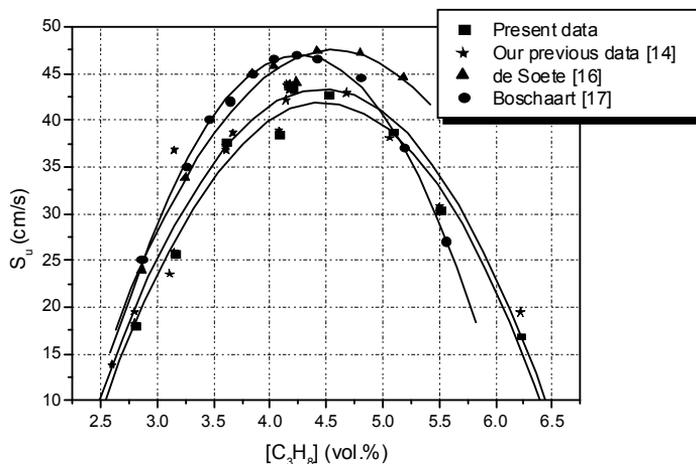
Fig. 2 *Burning velocities of C₃H₈-air mixtures at ambient pressure and temperature.*

It is worth mentioning that both calculation methods based on cubic law constants of flame propagation in the early stage of closed vessel explosions require the measurement of pressure-time history, limited to the early stage defined by the restriction $p_0 \leq p \leq 2p_0$. Whereas the method based on the isothermal compression model requires also other measurable quantities (the initial pressure and the peak explosion pressure for each experiment), the method based on the adiabatic compression model requires only calculable quantities: the expansion factor, E and the adiabatic compression coefficient, γ_u. This feature recommends the present method for evaluation of early-stage variation of pressure in cylindrical vessels, so frequently used in laboratory-scale explosion studies.

5. Conclusions

The normal burning velocities of propane air-mixtures with variable concentration, pressure and temperature were calculated by means of expansion factors obtained from adiabatic flame temperature, computed for the isobaric combustion and from the cubic law constants of flame propagation in the early stage of closed vessel explosions. A good agreement was observed between the present data and the normal burning velocity obtained by other techniques, over the whole range of studied concentrations. As the present method of normal burning velocity calculation requires only calculable quantities (the expansion factor, E and the adiabatic compression coefficient, γ_u) besides the cubic law coefficients (evaluated from experimental p(t) records, limited to the early stage of flame propagation), the method is suitable for evaluation of data recorded in cylindrical vessels with central ignition.

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