Normal burning velocity and propagation speed of ethane–air: Pressure and temperature dependence

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HIGHLIGHTS

- Normal burning velocities S_u and propagation velocities S_s of ethane–air are reported.
- $p(t)$ records in a spherical bomb with central ignition were used.
- S_u – determined from the coefficients of the cubic law of pressure rise.
- S_s – calculated from S_u using the expansion coefficient of the unburnt gas.
- Both S_u and S_s are examined against the initial composition, p_0 and T_0.

ARTICLE INFO

ABSTRACT

Experiments in a spherical bomb with central ignition using ethane–air mixtures of variable composition ([C_2H_6] = 3.4–7.6 vol%), at various initial pressures (p_0 = 30–130 kPa) and initial temperatures (T_0 = 298–423 K) afforded the calculation of the normal burning velocities S_u and propagation velocities S_s. The normal burning velocities (NBV) were determined from the coefficients of the cubic law of pressure rise during the early stage of explosion, using a previously proposed procedure. The propagation velocities (PV) were calculated from the normal burning velocities using the expansion coefficient of the unburnt gas during isobaric combustion. The experimental NBVs are examined against computed values, obtained with the package INSFLA for free laminar premixed flames, using the mechanism CH_4–C_4 based on 53 chemical species, which participate to 592 elementary reactions. The baric and thermal coefficients of NBVs and of PVs are determined and discussed in comparison with literature data.

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1. Introduction

The normal burning velocity of a laminar premixed flame S_u characterizes the propagation of a quiescent flame front through a homogeneous gaseous mixture of a flammable substance and oxidizer at rest. NBV is considered to be a fundamental property of a fuel–air mixture, depending on the fuel type, equivalence ratio, pressure, temperature and mass fraction of any gases, with a significant impact on many aspects of combustion [1,2]. NBV is influenced mainly by the overall rate of fuel oxidation in the flame front. Therefore, it is often used as a target parameter for development and validation of kinetic mechanisms [3–5]. Using the values of experimental NBVs, the apparent activation energies and the overall reaction orders of fuel oxidation can be calculated; they are input parameters in Computational Fluid Dynamics (CFD) mod-

eling of explosion propagation in closed vessels. The NBVs are used also for predicting the emissions and performance of internal and external combustion systems [6,7]. Another useful property of flammable mixtures is the propagation velocity (or "flame speed") S_s, defined as the velocity of the flame front in respect to the vessel where combustion takes place, i.e. a fixed reference system. Similar to NBVs, PVs depend on the same operational parameters [7,8] and, additionally, on the flow pattern. The propagation velocity of a flame is an interesting property in many areas of combustion science such as the design of burners and of gas turbines, for predicting the flame flash-back, blow-off, and the dynamic instabilities. It plays an essential role for assessing risk factors in operating chemical reactors where flammable mixtures are formed, for design of active safety devices (vents) and explosion proof vessels.

In the present paper we report NBVs and PVs of ethane–air mixtures with various initial compositions ([C_2H_6] = 3.4–7.6 vol%), temperatures (298–423 K) and pressures (30–130 kPa), obtained from pressure–time records in a closed spherical vessel with

central ignition. These transient $p(t)$ data have been recently analyzed and NBVs have been calculated over an extended period of flame propagation [9,10] using a recently developed model based on burned mass fraction [11,12]. An alternative, simpler method to determine NBV from $p(t)$ records uses the coefficients of the cubic law of pressure rise, valid in the early stage of spherical flame propagation [13]. The method can be extended to experiments in cylindrical vessels but it does not account for stretch and curvature effects, present in the early stage of flame propagation and extracts a limited amount of information from pressure–time history of each experiment. However, its use for $p(t)$ data referring to propane–air [14], propylene–air [13,15] and LPG (liquefied petroleum gas)–air mixtures [16] delivered NBVs in a very good agreement with those obtained by other experimental methods. In the present case, the accuracy of results obtained from the same $p(t)$ records using this simple method and the alternative method, based on use of burned mass fraction, is examined over the mentioned ranges of initial concentrations, pressures and temperatures of ethane–air mixtures. Additional information on ethane–air flames is provided by their PVs corresponding to the initial state of unburnt mixtures, S_s^0, analyzed in correlation with the initial concentration, pressure and temperature of ethane–air mixtures.

Ethane was chosen for this investigation because it naturally occurs as a dissolved component in petroleum oil and it is a chief by-product during the operations involving the refinery of oil and coal-carbonization. At the same time, the natural gas, widely used nowadays as a clean fuel, contains methane and ethane as main constituents. The composition of natural gas can vary appreciably from region to region, a fact which has a great impact on its burning velocity and propagation speed. Among components of natural gas, only methane has been extensively studied in various initial conditions and flame configurations. NBVs of ethane–air mixtures have been reported for wide ranges of initial conditions, using experimental techniques based on stagnation flames, on spherically expanding flames or the heat flux method [4,9,17–34]. In this article, we examine the experimental NBVs of ethane–air against computed values, obtained with the package INSFLA for free laminar premixed flames. In a previous study the kinetic modeling of ethane–air flames has been made with the GRI Mech 3.0 mechanism by means of COSILAB package [9,35] and delivered higher NBVs in comparison with most literature data. As an alternative, in the present study we use the mechanism CH_4–C_4, described by Warnatz [2] and recommended for flames of C_1–C_4 hydrocarbons with air. For both experimental and computed NBVs, their baric and thermal coefficients were determined and discussed in comparison with available literature data.

2. Experimental

The important parts of the experimental set-up are the combustion vessel, the vacuum and gas-feed line, the ignition controller and the data acquisition system, connected with a PC.

Measurements on spherical expanding flames of ethane–air mixtures were performed in a stainless steel spherical vessel of diameter Φ = 10 cm (V = 0.524 L) which can withstand an internal pressure of 4 MPa under static conditions. The vessel was equipped with several ports for the gas feed and evacuation valve, the ionization probe (tip mounted 3 mm away from the side wall), the ignition electrodes and the pressure transducer. A vacuum and gas-feed line, tight at pressures between 50 Pa and 450 kPa, connected the combustion vessel with the gas cylinders containing fuel and air, with a metallic cylinder for mixture storage and with the vacuum pump. These components have been described in ear-

lier papers [12–16] together with the components of the ignition system and the acquisition data system.

The ethane–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 400 kPa. The initial pressures of ethane–air mixtures were measured by a strain gauge manometer (Edwards type EPS-10HM). Before each test, the combustion vessel was evacuated down to 50 Pa; the explosive mixture was admitted and allowed 15 min to become quiescent and thermally equilibrated. GC analyses of several test ethane–air mixtures revealed no change of the initial composition as a result of preheating, in the range 333–450 K, at heating duration within 15–30 min. The data accuracy and repeatability was examined by repeating 3–5 times some tests in chosen experimental conditions. The average standard error observed in explosion pressures was 2%; the average standard error in the cubic law coefficients was 2.5% and in the corresponding burning velocities was under 3.5%.

Ethane–air mixtures with fuel concentration between 3.4 and 7.6 vol% were investigated, at total initial pressures between 30 and 130 kPa and initial temperatures between 298 and 423 K. Ethane (99.99%) (SIAD—Italy) was used without further purification.

3. Data evaluation

3.1. Normal burning velocity determination

The NBV of a gaseous flammable mixture at initial pressure p_0 is related to the coefficient k of the cubic law of pressure rise by Eq. (1), derived by assuming an isothermal compression of the unburned gas in the early stage of flame propagation [35]:

$$S_u = R \left(\frac{k}{\Delta p_{max}} \right)^{1/3} \left(\frac{p_0}{p_{max}} \right)^{2/3} \tag{1}$$

where R is vessel's radius, k is the coefficient of the cubic law of pressure rise, Δp_{max} is the maximum (peak) pressure rise of the explosion and $p_{max} = p_0 + \Delta p_{max}$ [13]. As input values for Eq. (1) we used the experimental values of Δp_{max} and p_{max}. The coefficient k is given by Eq. (2) [37,38], where K is a dimensionless constant dependent on the nature and state of the explosive mixture and V_0 is the volume of the explosion vessel:

$$\Delta p = K \cdot p_0 \frac{S_u^3 t^3}{V_0} = k \cdot t^3 \tag{2}$$

The coefficient k was determined for each experiment by a nonlinear regression method of $p(t)$ data, assuming the validity of the relationship:

$$\Delta p = \alpha + k \cdot (t - \beta)^3 \tag{3}$$

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

3.2. Propagation velocity determination

The propagation velocity of ethane–air flames at the initial moment of flame propagation, S_s^0, was calculated from S_u, the normal burning velocity and E_0, the expansion coefficient of the unburnt fuel–air mixture in the isobaric combustion at pressure p_0, as:

$$S_s^0 = S_u \cdot E_0 \tag{4}$$

$$E_0 = \left(\frac{T_{f,p}}{T_0} \right) \cdot \left(\frac{n_e}{n_0} \right) \tag{5}$$