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Propagation Velocity of Flames in Inert-Diluted Stoichiometric Propane-Air Mixtures: Pressure and Temperature Dependence

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Abstract: The flammable propane–air mixtures raise specific safety and environmental issues in the industry, storage, handling and transportation; therefore dilution of such mixtures has gained significant importance from the viewpoint of fire safety, but also due to nitrogen oxide's emission control through flameless/mild combustion. In this paper, the propagation of the flame in C_3H_8-air-diluent stoichiometric gaseous mixtures using Ar, N_2 and CO_2 as diluents was investigated. Data were collected from dynamic pressure-time records in spherical propagating explosions, centrally ignited. The experiments were done on stoichiometric C_3H_8-air + 10% diluent mixtures, at initial pressures within 0.5–2.0 bar and initial temperatures within 300–423 K. The flame velocity was determined from laminar burning velocities obtained using the pressure increase in the incipient stage of flame propagation (when the pressure increase is lower than the initial pressure). The experimental propagation velocities were compared with computed ones obtained from laminar burning velocities delivered by kinetic modeling made using the GRI mechanism (version 3.0) with 1D COSILAB package. The thermal and baric coefficients of propagation velocity variation against the initial temperature and pressure are reported and discussed.

Keywords: propagation velocity; propane combustion; diluent addition; temperature and pressure dependence; closed vessel

Highlights

(i)   propagation velocities of stoichiometric C_3H_8-air flames diluted by Ar, N_2 or CO_2 are reported;
(ii)   the propagation velocities are examined as functions on initial pressure and temperature;
(iii) the baric and thermal coefficients of propagation velocities are reported;
(iv)   the propagation velocities from experiments are examined against those obtained by kinetic modeling;
(v)   the comparison of efficiency of the studied inert gases showed that CO_2 has the highest influence, followed by N_2 and Ar.

1. Introduction

The laminar burning velocity (abbreviated further as LBV or S_u) and the propagation velocity of flames (abbreviated further as PV or S_s) are important parameters of flammable mixtures. These parameters are significant for the heat generation rates and rates of fuel conversion to oxidation products.

The LBV was considered as the velocity of a flame with planar one-dimensional geometry relative to the unburnt gas mixture, along the normal to its flame front [1,2]. For engine design, modeling the laminar and the turbulent combustion, and for validation of kinetic models, the LBV is an essential parameter. The PV (propagation velocity or "flame speed"), was defined as the velocity of the flame front in respect to the vessel where

combustion takes place [2,3]. The PV is an important parameter in the design of burners and gas turbines, for predicting the flame flash-back, blow-off, and the dynamic flame instabilities. The PV has a primordial role for assessing risk factors in operating chemical reactors with flammable mixtures, for design of safety devices or explosion vessels [3,4].

The fuel type, fuel-oxidizer ratio, pressure and temperature of the unburned mixture affect both the LBV and PV [1,4–7]. The PV depends also on the flow pattern. It was demonstrated that the presence of turbulence leads to the increase of the propagation speed, resulting in an increase of the maximum rate of pressure rise [8,9].

The LBV and the PV are related [3,4]:

$$S_s = S_u + S_g \tag{1}$$

where S_g, is the gas velocity, determined by the flame front movement due to the expansion of the burnt gas behind the flame front and the compression of the unburnt gas ahead of it.

The study of the influence of diluents (inerts or inhibitors) on gaseous explosions is required by the necessity to mitigate their effects and to characterize and model the combustion processes. Diluent addition changes the thermo-physical properties of the flammable mixture such as heat capacity or thermal conductivity. It also influences the chemistry of the combustion process [3,10]. A better control of the combustion evolution, such as longer induction periods, lower LBVs, lower flame temperatures, lower amounts of pollutants, etc., [5,6] can be due to the additive presence in the explosive mixtures. Furthermore, dilution of flammable mixtures with flue gases (so-called exhaust gas recirculation), could be applied for reduction of NOx emissions [7] of internal combustion engines.

The propagation speed of flammable mixtures is usually determined by the tube method by monitoring the position of the flame front, using various methods: optical sensors and ionization gauges [3,10,11]. In order to obtain reproducible results, the explosion tube is opened at the end, close to the ignition source; this maintains a constant pressure regime during propagation. Using this technique, some problems arise from the unsteady propagation of the flame, especially in the first half of the measuring tube, as a result of flame front increase and progressive change [12]. Therefore, other techniques are used to study the propagation of flames and to determine their propagation speeds: the closed vessel technique, using spherical or cylindrical enclosures (symmetrical or elongated) and central ignition [3,13,14], counterflow-flame technique [15] or flat flame technique [16]. The last two techniques deliver LBV and PV of gaseous mixtures using stationary flames, but only at ambient initial conditions. In comparison, the closed vessel technique can be used at initial temperatures and pressures different from ambient, but requires important corrections to measured data, to account for flame stretch and curvature (in the early stage of the process) and for heat losses (in the late stage of propagation) [11,17,18]. Using this technique, the LBVs and the PVs of fuel-air and fuel-air-inert mixtures were reported: methane-air and natural gas-air [13,19,20], ethane-air [21,22], propane-air and propane-air-nitrogen [23,24], and butane-air [25] at various initial temperatures and/or pressures.

Propane is one of the most studied fuels due to its utility. Propane, either pure or blended (LPG—Liquefied Petroleum Gas), is widely used instead of gasoline in automotive engines, or in domestic plants. It is also used as feedstock for the production of basic petrochemicals or as a refrigerant (mixtures of C_3H_8 and CO_2) with low global warming potential and low flammability [6,26–43]. Compared to gasoline or diesel, propane is a viable alternative fuel with lower carbon content, used in engine applications. The interest to use C_3H_8 as an alternative transportation fuel rises from its relatively low cost, clean-burning qualities (lower CO and NO_x emissions), domestic availability, and high-energy density. However, the studies were conducted rather to obtain the LBVs of propane-air-inert mixtures, therefore, the data relating to PVs are missing or incomplete and need further explorations. Biopropane could replace the fossil liquified petroleum gas (LPG), because it is being commercialized as a biofuel alternative to liquefied petroleum gas (LPG) [44]. Biopropane can be produced with a one-stage catalytic synthesis of the syngas resulting from biomass gasification [45], and also as a co-product of hydrogenating vegetable or

animal oil/fat [44,46]. The propagation velocities of inert-diluted propane-air mixtures are necessary for delivering specific safety recommendations in all fields of activity where such mixtures are formed. Moreover, the dilution of propane-air mixtures has an increased importance from the viewpoint of fire safety, due to a better control of NOx emissions through flameless/mild combustion.

The present work reports new experimental and computed PVs of propane-air-diluent mixtures (with Ar, N_2 or CO_2 as diluents), under various initial conditions: initial pressures within 0.5 and 2.0 bar and initial temperatures within 300 and 423 K, 10% added diluent. The experimental LBVs and the PVs were obtained from pressure measurements during the incipient stage of closed vessel explosions, when the flame maintains its spherical shape and the heat losses do not influence its development [47].

The PVs of examined systems obtained from experiments are examined against the computed values obtained from adiabatic PVs delivered by kinetic modeling.

The experimental and computed data presented in this paper are important input data for the gaseous explosions database in order to support explosion mitigation in domestic or industrial plants where accidental fires and explosions can occur.

2. Materials and Methods

The experimental set-up, represented in Figure 1, consists of a spherical explosion vessel, the gas-feed line, the ignition controller and the data acquisition system, connected with a computer (PC). The test vessel is a stainless steel sphere (R = 5 cm and V = 0.52 L) designed to withstand a pressure up to 40 bar under static tests. The explosion cell has: (a) gas feed and evacuation valve; (b) ionization gauge (tip at 3 mm away from the side wall); (c) ignition electrodes for ignition by inductive-capacitive sparks; (d) a pressure transducer; (e) an electric heating system which allows experimental measurements at initial temperature higher than ambient.
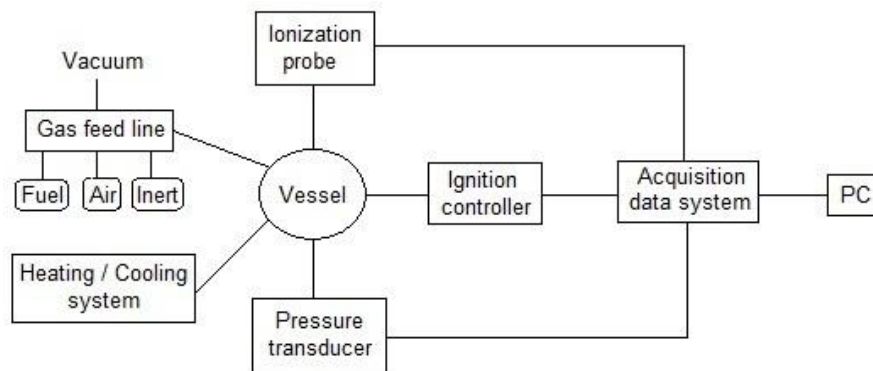

Figure 1. Schematic diagram of the test equipment.

Dynamic pressure-time registrations were made by means of a piezoelectric pressure transducer (Kistler 601A, Kistler, Winterhur, Switzerland) along with a Charge Amplifier (Kistler 5001SN, Kistler, Winterhur, Switzerland). Data were recorded by an oscilloscope (TestLab^{TM} Tektronix 2505, Tektronix, Beaverton, OR, USA). The C_3H_8-air-diluent mixtures were prepared in gas cylinders using the partial pressure method, under the assumption of ideal gas behavior. The gaseous mixtures were prepared at 4 bar total pressure and were used 48 h later.

The cell was electrically heated; its temperature was monitored by a K-type thermocouple and adjusted by ±1 °C using an AEM 1RT96 controller. Other details were previously given [21,38,48–50].

The studied mixtures (C_3H_8-air having ϕ = 1 diluted with 10% gaseous additives: N_2, Ar, CO_2) at variable initial pressures (p_0 = 0.5–2.0 bar) and variable initial temperatures (T_0 = 300–423 K) were allowed 15 min after admission in the combustion vessel to become quiescent and thermally equilibrated before ignition. Each test was repeated 3 times; some

tests were repeated 5–7 times at constant initial conditions of explosive mixtures in order to examine the accuracy and repeatability of the data. The average standard error observed in the measured PV was estimated within 2.5 and 3.5%.

The used gases: C_3H_8 (99.99%), Ar (99.99%), N_2 (99.99%) and CO_2 (99.5%), from SIAD Italy, were used without further purification.

3. Data Evaluation

The PVs of propane-air-diluent flames were calculated from the LBVs and the expansion coefficients of unburnt mixtures in the combustion at constant pressure p_0, as [3,4]:

$$S_s = S_u \cdot E_0 \tag{2}$$

The expansion coefficient of the unburnt gas mixtures, E_0, is available from thermodynamic data as the ratio of burnt and unburnt gas volumes:

$$E_0 = \frac{V_e}{V_0} \tag{3}$$

where V_0 is the volume of reactants and V_e is the volume of burned ("end") gas obtained from combustion of V_0.

The LBVs of gaseous flammable mixtures at initial pressure p_0 used in Equation (2) were calculated in the early stage of the flame propagation as [21,47]:

$$S_u = R \cdot \left(\frac{k}{\Delta p_{max}} \right)^{1/3} \cdot \left(\frac{p_0}{p_{max}} \right)^{2/3} \tag{4}$$

where R is the radius of the explosion cell, k is the cubic law coefficient of pressure increase, Δp_{max} is the maximum (peak) value of the pressure increase during the explosion and $p_{max} = p_0 + \Delta p_{max}$. Equation (4) was derived under the assumption of the compression of the unburned gas ahead of the flame front, at constant temperature. The experimental values of Δp_{max} and p_{max} were used as input values in Equation (4). The coefficient of the cubic law was obtained for each experiment using a nonlinear regression of the form [21,47,50]:

$$\Delta p = a + k \cdot (t - b)^3 \tag{5}$$

where a is the pressure correction and b is the time correction, made to avoid any possible delays in the signal recording or in the signal shift of pressure transducer. For all experiments, the computation was limited to a pressure variation $p_0 \leq p \leq 2p_0$, to minimize the disturbing effects of the flame curvature and stretch on the LBV.

The cubic law method [47], approached in the present work for determining the LBV and further on, the PVs, is based on the examination of the incipient stage of flame propagation (for $\Delta p \leq p_0$). During this stage, the flame is still far from the vessel's wall, as shown by flame radius measurements reported in our earlier publications, so that thermal losses towards the vessel's wall can be neglected.

4. Computing Programs

The burned gas volume, V_e, and the expansion ratio, E_0, in the isobaric combustion of flammable mixtures were delivered by equilibrium calculations made by means of COSILAB 0-D package (Bad Zwischenhahn, Germany) [51]. The algorithm used by this program affords the computation of the flame temperature and the equilibrium composition of burned gas under adiabatic conditions for any flammable gaseous mixtures. The program uses the thermodynamic criteria of chemical equilibrium considering 53 compounds as combustion products.

The LBVs were calculated with COSILAB-1D package [51] by the kinetic modeling of the laminar adiabatic premixed flames in various conditions. In the present case, the GRI mechanism (version 3.0), involving 53 chemical species and 325 elementary reactions

was used. The thermodynamic and molecular databases (format for CHEMKIN) of Sandia National Laboratories, USA, provided the input data for the runs. More details were given in [21,50,52,53]. Premixed 1D laminar adiabatic-free flames have been considered.

COSILAB package [51] is a tool for simulating a variety of laminar flames including unstrained (such as premixed freely propagating flames, premixed burner-stabilized flames) or strained premixed flames (such as diffusion flames, partially premixed cylindrically or spherically). This software allows solving complex chemical kinetics problems which involve thousands of reactions. The runs can be made by varying some physical parameters such as equivalence ratio, temperature, pressure, and strain rate. The COSILAB capabilities allow a detailed study on a complex chemical reaction considering intermediate compounds, trace compounds and pollutants.

5. Results and Discussion

The expansion coefficients of flammable mixtures were found to depend strongly on the initial temperature. Their variation against the initial temperature of stoichiometric C_3H_8-air–10% diluent mixtures (diluent: Ar, N_2 or CO_2) at constant initial pressure (p_0 = 1.5 bar) is given in Figure 2, while the variation of the expansion coefficients at various initial pressures and constant initial temperature (T_0 = 333 K) is given in Table 1. Such values were computed for all propane-air-diluent examined systems at variable initial pressures and temperatures, and were further used for calculating the PVs, both experimental and computed.
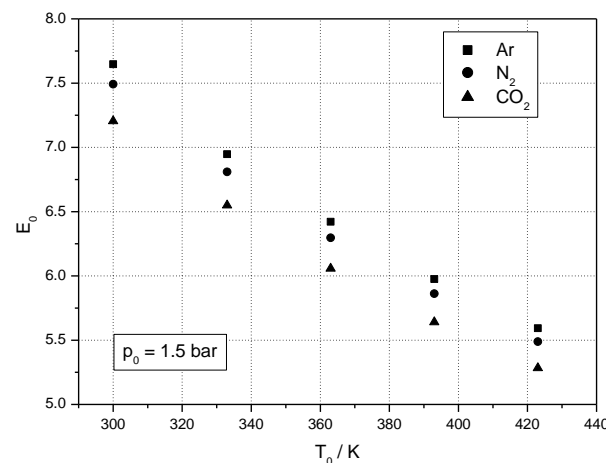

Figure 2. Expansion coefficients, E_0, at p_0 = 1.5 bar and T_0 from 300 to 423 K for propane-air–10% diluent mixtures (Ar, N_2 or CO_2).

Table 1. Expansion coefficients, E_0, at T_0 = 333 K and various initial pressures for propane-air–10% diluent mixtures (Ar, N_2 or CO_2).

p_0/bar	E_0		
	Ar	**N_2**	**CO_2**
0.50	6.883	6.755	6.501
0.75	6.908	6.776	6.520
1.00	6.923	6.791	6.533
1.25	6.937	6.801	6.543
1.50	6.947	6.810	6.550
1.75	6.955	6.816	6.556
2.00	6.962	6.822	6.561

The experimental PVs of the stoichiometric C_3H_8-air mixture diluted with 10% N_2 at various initial temperatures and various initial pressures are given in Figure 3. The pressure and temperature influence on present PV (obtained from the experimental LBV)

follow the same trend as the LBV founded by Tang et al. (2010) [24] for propane-air diluted with nitrogen. Maintaining constant initial pressure and composition, the increase of the initial temperature leads to increase of PVs. Maintaining constant the initial temperature and composition, the increase of the initial pressure causes the decrease of PVs. A similar behavior was found for the stoichiometric propane-air mixture diluted with 10% Ar or CO_2 and it was already observed for other fuel-air and fuel-air-diluent mixtures [13,21,54–56].
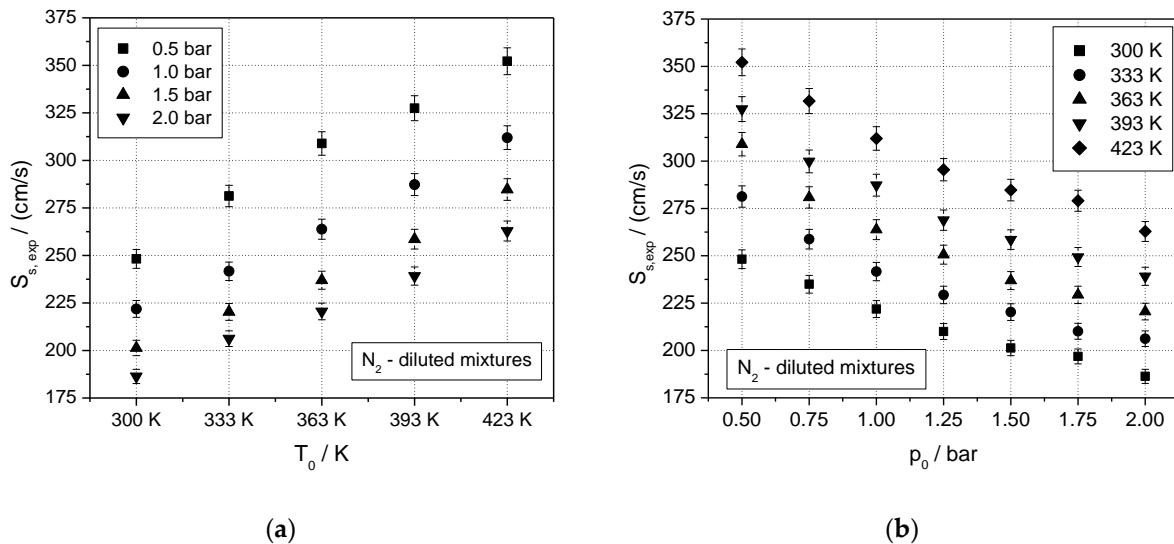

Figure 3. Experimental PVs of stoichiometric C_3H_8-air diluted with 10% N_2: (**a**) S_s versus the initial temperature at various initial pressures; (**b**) S_s versus the initial pressure at various initial temperatures.

Among the studied diluents, carbon dioxide has the most important influence on propane-air PVs, followed by N_2 and Ar. This behavior corresponds to the ranking of specific heats of the inert gases: 37.12 J/mol K for CO_2; 29.12 J/mol K for N_2; 20.79 J/mol K for Ar. A higher specific heat capacity means better inerting effect. Through its high specific heat, CO_2 reduces both the adiabatic flame temperature and the reaction rates. This leads to a decrease of LBV and hence of PV. Additionally, under the flame condition, CO_2 can dissociate leading to an increase of its inerting effect. Moreover, due to its high specific heat, CO_2 absorbs energy from reactions and emits radiation to the surroundings due to its high emissivity. This leads to a decrease in PV.

The PVs of propane-air–10% CO_2 are lowest at all pressures, as shown by data from Figure 4. By adding CO_2 to a fuel-air mixture, the burning velocity (and as a consequence the PV of the mixture) may be affected through several mechanisms [3,14]: the variation of the transport and thermal properties of the mixture, the possible direct chemical effect of CO_2, and the enhanced radiation transfer. The average standard errors observed in the measured propagation velocities were estimated within 2.5 and 3.5%, and are represented in Figures 3 and 4 as error bars.

The experimental PVs were compared by those obtained from computed LBVs using the 1D COSILAB package. Such a comparison for the stoichiometric propane-air diluted with 10% Ar is given in Figure 5. One can observe that the PVs obtained from computed LBVs are systematically higher than the PVs obtained from experimental LBVs. Increasing the initial temperature and/or initial pressure, the GRI mechanism (version 3.0) simulates the evolution of the LBV, but the runs globally overestimate the measured ones. Therefore, at all examined mixtures and initial conditions, the computed values of PVs are higher than experimental ones.
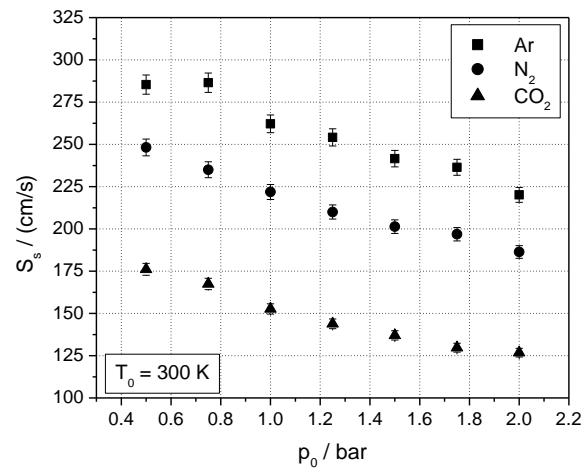
Figure 4. PVs of propane-air–10% diluent mixtures (Ar, N_2 or CO_2) at initial ambient temperature and various initial pressures.
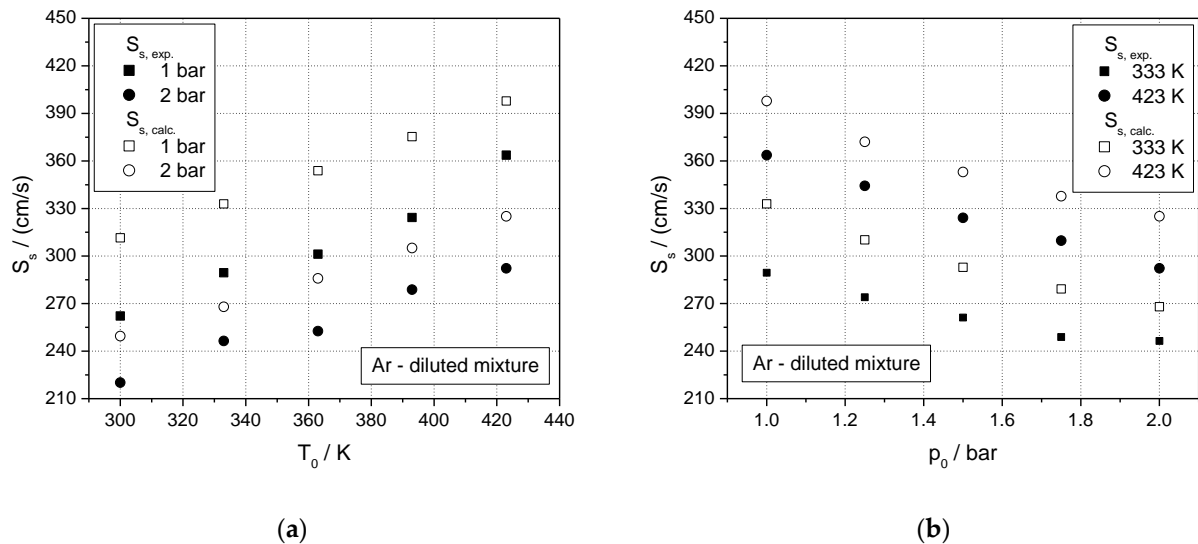

(**a**)

(**b**)

Figure 5. Comparison of experimental and calculated PVs of stoichiometric C_3H_8-air diluted with 10% Ar at: (**a**) various initial temperatures; (**b**) various initial pressures.

Even if GRI mechanism (version 3.0) was constructed to match the evolution of flames in the constituents of natural gas, i.e., CH_4, C_2H_6 and C_3H_8 mixed with air, this mechanism overestimates measurements. For example, discrepancies between measured and modeling data using GRI mechanism (version 3.0) were reported by Cardona et al. [57] for LBV of propane-air, biogas with oxygen-enriched air, biogas-propane-hydrogen oxygen-enriched air mixtures, at 295 K and 0.83 atm. This behavior was already reported in [41] for propane-air-inert mixtures at different temperature and pressure. Kishore et al. [58] also observed large discrepancies between experimental and computed with GRI mechanism (version 3.0). They reported data regarding the laminar burning velocity of methane-air and ethane-air mixtures at 307 K, 1 bar and various equivalence ratios. Moreover, high values of computed LBV were reported when other mechanisms are employed as reported by Akram et al. [59] on C_3H_8-air mixtures diluted with N_2 and CO_2. This prompts a further examination of GRI mechanism (version 3.0) through sensitivity analyses, in order to improve some of the reaction rate constants.

PVs are obtained from LBVs. Thus, high-computed LBVs conducted to high-computed PVs. Additionally, in the present paper, LBVs were obtained under adiabatic conditions, without heat loss, while the measurements are done under non-adiabatic conditions. Therefore, this could also be a reason for these discrepancies.

If the initial pressure is kept constant, both experimental and computed data exhibit the same slope. The same behavior of experimental and computed PVs was also observed for constant initial temperature. The same behavior was also observed when N_2 or CO_2 were used as diluents, and other fuel-air-diluent mixtures compared to experimental ones [19,55].

Other relevant data obtained from experiments and kinetic modeling of flames referring to the initial pressure and temperature influence on PVs are plotted in Figure 6a,b. At initial ambient temperature and pressure, the experimental PVs vary between 153 cm/s for mixtures diluted with 10% CO_2 and 262 cm/s for mixtures diluted with 10% Ar. The reference PV of the stoichiometric propane-air mixture, under present conditions, is 328 cm/s [55], close to 305 cm/s, from experimental measurements in a cylindrical explosion vessel [23]. The decrease of the PVs of the propane-air-diluent mixtures can be attributed mainly to the decrease of the initial fuel concentration, after diluent addition. This leads to a decrease of the available amount of the heat released and the reaction rate, followed by the reduction of the flame temperature and the PV [56]. The decrease of the flame temperature can be observed as well from Figure 7a,b where significant values of flame temperatures ($T_{f,p}$) under adiabatic conditions for C_3H_8-air-diluent mixtures are given.

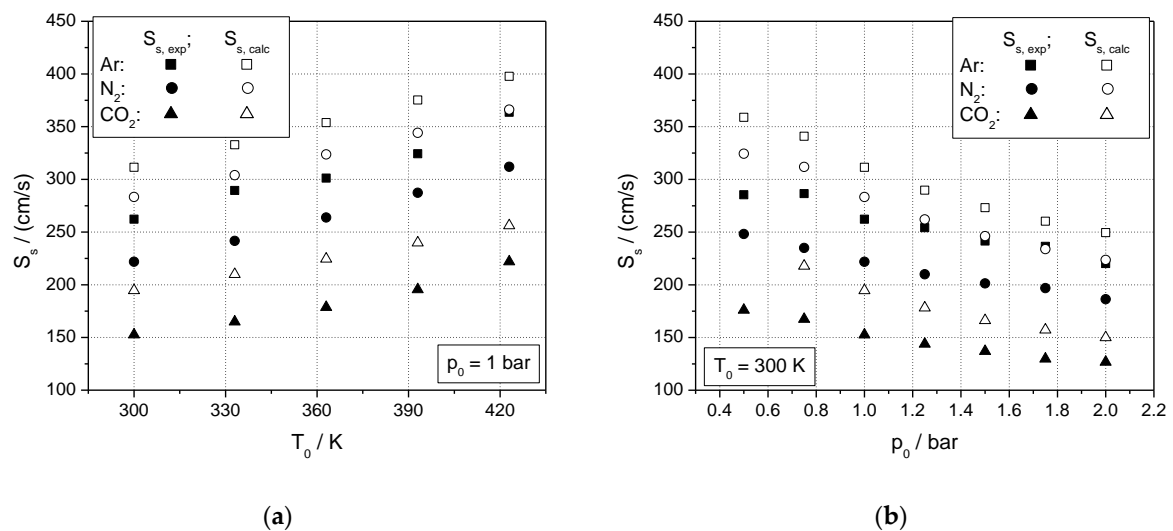(a)

(b)

Figure 6. Comparison of experimental and calculated PVs of stoichiometric (C_3H_8-air) + diluent: (**a**) at various initial temperatures; (**b**) at various initial pressures.
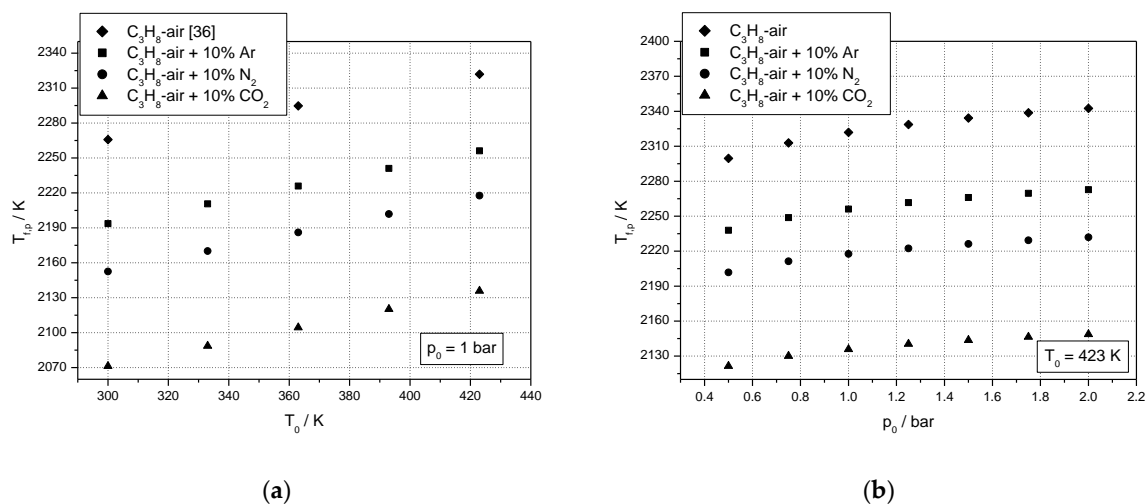

(a)

(b)

Figure 7. Adiabatic flame temperatures of isobaric combustion of stoichiometric C_3H_8-air+diluent mixture: (**a**) at various initial temperatures; (**b**) at various initial pressures.

The new results obtained from this study may present additional insights about the mitigation phenomena when inerts are added to propane-air mixtures, and could help to develop safety measures for these mixtures in industrial installations.

Lower PVs for fuel-air-diluent mixtures compared with fuel-air mixtures were already observed for other fuels. For example, for the stoichiometric CH_4-air mixture at ambient initial conditions, the reported PVs determined by experiments in spherical vessels range between 210 cm/s [13] and 280 cm/s [56], with an intermediate value of 270 cm/s [19]. The PVs for stoichiometric CH_4-air-diluent mixtures, measured in the same conditions are: 129 cm/s for CH_4–air–10% CO_2 mixture, 235 cm/s for CH_4–air–10% N_2 mixture and 257 cm/s for CH_4–air–10% Ar mixture [56].

Similar to the LBVs, the PVs also depend on the initial pressure. This dependence of PVs for propane-air-diluent mixtures was examined by a power law, used for other flammable mixtures as well [21,50–55]:

$$S_s = S_{s,ref} \cdot \left(\frac{p}{p_{ref}} \right)^{\beta} \tag{6}$$

where $S_{s,ref}$ is the PV at reference conditions (p_{ref} = 1 bar) and β is the baric coefficient. The baric coefficients of experimental PVs, determined by a non-linear regression analysis of S_s versus P data, are given in Tables 2 and 3.

Table 2. Reference PVs (experimental data) and their baric coefficients, β, for stoichiometric C_3H_8–air–10% diluent mixtures (*Ss,ref* at p_0 = 1 bar).

C_3H_8–Air–Diluent	T_0/K	$S_{s,ref}$/(cm/s)	$-\beta$	$r_n{}^2$
Ar	300	262.2	0.182 ± 0.026	0.904
	333	289.5	0.191 ± 0.016	0.966
	363	301.2	0.214 ± 0.015	0.975
	396	324.3	0.190 ± 0.010	0.987
	423	363.7	0.199 ± 0.024	0.933
N_2	300	221.9	0.201 ± 0.012	0.983
	333	241.7	0.228 ± 0.004	0.998
	363	263.8	0.240 ± 0.240	0.998
	396	287.3	0.221 ± 0.008	0.994
	423	311.9	0.203 ± 0.010	0.987
CO_2	300	152.7	0.267 ± 0.016	0.979
	333	164.9	0.232 ± 0.008	0.993
	363	178.7	0.196 ± 0.014	0.974
	396	195.5	0.201 ± 0.011	0.987
	423	221.9	0.187 ± 0.023	0.939

Table 3. Baric coefficients, -β, of calculated PVs, S_s, for stoichiometric C_3H_8–air–diluent mixtures at p_0 = 1 bar.

Diluen T_0/K	Ar	N_2	CO_2
300	0.319 ± 0.001	0.340 ± 0.001	0.383 ± 0.004
333	0.312 ± 0.001	0.331 ± 0.002	0.375 ± 0.004
363	0.305 ± 0.001	0.323 ± 0.002	0.366 ± 0.003
396	0.296 ± 0.001	0.314 ± 0.002	0.357 ± 0.003
423	0.288 ± 0.002	0.308 ± 0.002	0.349 ± 0.003

At initial ambient temperature, the baric coefficients of experimental PVs vary from −0.267, when carbon dioxide is used as diluent, to −0.182 when argon is used as diluent. One can observe that the baric coefficients of the PVs do not depend significantly on the initial temperature. The baric coefficients of calculated PVs exceed the values characteristic

for experimental PVs, for all examined systems. The baric coefficients of the PVs for C_3H_8-air-diluent mixtures are smaller when compared to the baric coefficients of LBVs previously reported [39], as it results from Table 4 where data at initial ambient temperature are given. It is an expected variation, since the expansion coefficients themselves depend on pressure, as seen from Table 1.

Table 4. Baric coefficients from LBVs and from PVs, at initial ambient temperature.

Inert	β from S_u [40]	β from S_s (Present Data)
Ar	−0.253	−0.319
N_2	−0.276	−0.340
CO_2	−0.237	−0.383

The PVs depend also on the initial temperature. This dependence was examined using an empirical power law, as in previous cases [21,53–55]:

$$S_s = S_{s,ref} \cdot \left(\frac{T}{T_{ref}} \right)^\alpha \tag{7}$$

where $S_{s,ref}$ is the PV at reference temperature (T_{ref} = 300 K) and α is the thermal coefficient.

The PVs of stoichiometric C_3H_8–air + 10% diluent mixtures at reference conditions ($S_{s,ref}$ at p_0 = 1 bar and T_{ref} = 300 K) used in Equation (7) are given in Table 5 together with reference PVs ($S_{s,ref}$) of stoichiometric CH_4–air + 10% diluent mixtures; both sets of experimental and calculated data are given. Data from Table 5 confirm the influence of diluent gases on PVs, which vary in the order of $CO_2 > N_2 > Ar$.

Table 5. Reference PVs for stoichiometric CH_4–air + 10% diluent and for C_3H_8–air + 10% diluent mixtures.

Inert	$S_{s,ref}$/(cm/s)			
	CH_4–Air + 10% Diluent [56]		C_3H_8–Air + 10% Diluent (Present Data)	
	Experimental	Calculated	Experimental	Calculated
Ar	256.6	225.0	262.2	311.5
N_2	234.8	200.9	221.9	283.3
CO_2	128.7	130.2	152.7	194.6

The thermal coefficients, α, of experimental PVs, from the non-linear regression of S_s versus T data, are shown in Table 6. The thermal coefficients of calculated PVs are slightly lower in comparison with these values.

Table 6. The thermal coefficients, α, of experimental PVs for stoichiometric C_3H_8–air + 10% diluent mixtures.

Diluent p_0/bar	Ar	N_2	CO_2
0.50	0.918 ± 0.025	0.989 ± 0.049	0.890 ± 0.034
0.75	0.746 ± 0.051	0.990 ± 0.052	0.871 ± 0.096
1.00	0.918 ± 0.105	1.010 ± 0.035	1.107 ± 0.113
1.25	0.872 ± 0.093	0.996 ± 0.044	1.094 ± 0.055
1.50	0.877 ± 0.086	1.014 ± 0.059	1.037 ± 0.068
1.75	0.809 ± 0.094	1.042 ± 0.096	1.131 ± 0.059
2.00	0.809 ± 0.073	0.990 ± 0.050	1.084 ± 0.062

At p_0 = 1 bar, the thermal coefficients of the PVs range between 0.92 for C_3H_8–air + 10% Ar mixture and 1.11 for C_3H_8–air + 10% CO_2 mixture. It can be observed that the thermal coefficients of the PVs do not vary significantly with the initial pressure.

The thermal coefficient of the experimental PV for C_3H_8-air-N_2 mixture at p_0 = 1 bar (α = 1.010) is lower compared to any thermal coefficient of the LBV reported in literature

for propane-air-N_2 mixtures ($\alpha = 1.77$ [40], $\alpha = 1.83$ [59], $\alpha = 2.13$ [60]). Once more, the explanation is based upon the influence of temperature on expansion coefficients, as seen from data in Figure 2.

The expansion coefficients do not depend significantly on the initial pressure. That determines close baric coefficients of propagation velocities and of laminar burning velocities as previously reported [21]. Due to the simultaneous temperature influence on flame temperature and LBV, the thermal coefficients of propagation velocity are lower than the corresponding thermal coefficients of normal burning velocities. The baric and thermal coefficients of propagation velocities can be used to illustrate the dependence of PV on initial pressure and temperature as do the baric and thermal coefficients of laminar burning velocity.

The new results of experimental and computed propagation velocities of propane-air in the presence of various diluent gases (CO_2, N_2, Ar) at initial pressures within 0.5 and 2.0 bar and initial temperatures within 300 and 423 K, are useful data for fire safety equipment, flame flashback, explosion protection, fuel tank venting systems and other combustion systems.

6. Conclusions

In this work, the flame propagation in inert-diluted propane-air gaseous mixtures was experimentally investigated, using pressure records from a small spherical vessel with central ignition. The propagation velocities were determined by means of laminar burning velocities, evaluated in the early stage of outwardly propagating flames. Simultaneously, the kinetic modeling of flame propagation was performed and delivered adiabatic laminar burning velocities and flame propagation velocities.

It is observed that for the studied ranges of initial pressure p_0: 0.5–2 bar and initial temperature T_0: 300–423 K, the propagation velocities of propane-air-inert flames strongly depend on initial pressure and temperature of flammable mixtures. The experimental values of PVs range between 220–393 cm/s for stoichiometric mixture C_3H_8–air + 10% Ar, 186–354 cm/s for stoichiometric mixture C_3H_8–air + 10% N_2, 127–237 cm/s for stoichiometric mixture C_3H_8–air + 10% CO_2. The computed values of PVs range between 250–424 cm/s for stoichiometric mixture C_3H_8–air + 10% Ar, 224–398 cm/s for stoichiometric mixture C_3H_8–air + 10% N_2, and 150–282 cm/s for stoichiometric mixture C_3H_8–air + 10% CO_2.

The PVs of studied systems obtained from experiments are examined against the computed values obtained from adiabatic PVs delivered by kinetic modeling. As expected, the propagation velocities obtained from computed laminar burning velocities are higher than propagation velocities obtained from experimental data.

A particular interest was paid to the impact of the initial pressure and temperature of flammable mixtures on propagation velocities. From the dependencies of propagation velocities on initial pressure and temperature, expressed as simple power laws, the corresponding thermal and baric coefficients were obtained.

The comparison of efficiency of the studied inert gases showed that CO_2 is the most influent additive, followed by N_2 and Ar.

At constant composition, the propagation velocity depends on the pressure and temperature being correlated by a power law. In the present work, the thermal coefficients range between 0.74 and 1.31 while the baric coefficients range between -0.383 and -0.288.

The present results could predict the propagation velocities of propane-air at initial pressures and/or temperatures different from ambient, in the presence of various diluent gases, having thus a high practical interest. The data can be directly used to deliver safety recommendations for reactors or plants where flammable propane-air mixtures are formed.

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Nomenclature

a [bar]	pressure correction
b [s]	time correction
E [–]	expansion coefficient
k [bar/s^3]	coefficient of the cubic law of pressure rise
LBV [m/s]	laminar burning velocity (Su)
p [bar]	pressure
PV [m/s]	propagation velocity of flames (Ss)
R [m]	vessel radius
S [m/s]	speed, velocity
t [s]	time
T [K]	temperature
V [m^3]	volume
Greek	
α [–]	thermal coefficient of the normal burning velocity
β [–]	baric coefficient of the normal burning velocity
Δ [–]	variation
Subscripts	
f	referring to the flame
g	gas
max	maximum value
u	unburned gas
s	spatial
ref	reference value
p	referring to an isobaric value
0	initial condition

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