



Deflagration Dynamics of Methane-Air Mixtures in Closed Vessels at Elevated Temperatures

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Abstract: In this paper, we explore the deflagration combustion of methane-air mixtures through both experimental and numerical analyses. The key parameters defining deflagration combustion dynamics include maximum explosion pressure (P_{max}), maximum rate of explosion pressure rise $(dP/dt)_{max}$, deflagration index (K_G) , and laminar burning velocity (S_U) . Understanding these parameters enhances the process of safety design across the energy sector, where light-emissive fuels play a crucial role in energy transformation. However, most knowledge on these parameters comes from experiments under standard conditions (P = 1 bar, T = 293.15 K), with limited data on light hydrocarbon fuels at elevated temperatures. Our study provides new insights into methane-air mixture deflagration dynamics at temperatures ranging from 293 to 348 K, addressing a gap in the current process industry knowledge, especially in gas and chemical engineering. We also conduct a comparative analysis of predictive models for the laminar burning velocity of methane mixtures in air, including the Manton, Lewis, and von Elbe, Bradley and Mitcheson, and Dahoe models, alongside various chemical kinetic mechanisms based on experimental findings. Notably, despite their simplicity, the Bradley and Dahoe models exhibit a satisfactory predictive accuracy when compared with numerical simulations from three chemical kinetic models using Cantera v. 3.0.0 code. The findings of this study enrich the fundamental combustion data for methane mixtures at elevated temperatures, vital for advancing research on natural gas as an efficient "bridge fuel" in energy transition.

Keywords: combustion; laminar burning velocity; methane-air mixtures; explosion safety; Cantera; chemical kinetics

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1. Introduction

Based on energy market needs and future development perspectives, research on the characteristics of gaseous fuel-air mixtures is a key issue for ensuring the process safety of power technologies. While natural resources (including fossil fuels) are constantly shrinking, as well as many efforts being taken to protect the environment, there is an increasing interest in alternative fuels like light hydrocarbons. In order to better understand and estimate the explosion hazards in power technologies, more research (both experimentally and numerically) has to be conducted on the fundamental safety characteristics of such fuels at various and elevated initial conditions, like ignition or fire and explosion characteristics, such as: maximum explosion pressure [1,2], maximum rate of explosion pressure

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rise [3], and heat release rate [4], as well as one of the most important parameters of flame propagation, mainly laminar burning velocity (LBV) [5,6]. LBV is the significant safety property describing the combustible (fuel and oxidizer) mixture in process industries. It is commonly used in the numerical modeling of the combustion phenomenon in power process industries. The LBV yields a measure of the reactivity of combustible mixtures. It is also an important parameter in relation to determining the heat release rate, as well as the testing and validation of many kinetic models. The laminar burning velocity is the velocity of a steady adiabatic one-dimensional free-propagating flame [7]. In other words, it refers to the flame propagation in laminar conditions of unburned gas mixtures. Determination of the LBV is crucial for ensuring power technology safety, especially for the use of gaseous or liquid fuels, including methane, biogas, ethanol, or hydrogen, as well as fuel blends.

Laminar burning velocity can be influenced by many factors, mainly the fuel composition, mixture equivalence ratio and temperature, and initial pressure, as well as the mixture dilution [7]. The general relationship between LBV and the equivalence ratio (ϕ) for different mixtures is non-monotonic. The laminar burning velocity for various fuel blends and different pressure levels reaches its maximum for values of equivalence ratio slightly above 1.0, and it decreases both for more lean and more rich mixtures [8–12]. Measurements of LBV are often conducted for the specified range of equivalence ratio values [8,11]. According to the latter, the relation between the equivalence ratio and laminar burning velocity of mixtures of methane and air at various pressure conditions p (from 1 to 5 atm) is non-monotonic, and the LBV has its maximum at $\phi = 1.1$ for p = 1 atm. The key role of the growth in OH*, O*, and H* radicals' concentrations for the rise in the LBV, due to an increase in reactivity, is highlighted in [10].

In the scientific literature, the laminar burning velocity of fuel blends (or mixtures) containing methane is frequently examined, as is the influence of the presence of another substances in methane-air flames, especially hydrogen [10,13,14]. For example, in the literature [15], it was found that the addition of halons causes a reduction in the burning velocity of stoichiometric methane-air mixtures. In another paper [16], the authors experimentally and numerically investigated (with the use of kinetic models) the LBV of mixtures of methane, ammonia, and air. Some other authors [8] discussed the laminar burning velocity and burned gas Markstein length of methane-air mixtures diluted with N₂, H₂O, and CO₂. The influence of hydrogen and carbon dioxide on the LBV values for mixtures of CH₄ and air was analyzed experimentally and numerically in [17]. Some of the experimental results revealed that there was a strong impact of hydrogen addition and carbon dioxide dilution on laminar burning velocity in the investigated cases [9–15]. The LBV decreased with an increase in the CO₂ mole fraction and increased with the addition of H₂. Moreover, the results obtained both from the experiments and numerical models were in agreement. The authors of [18] performed experimental and numerical studies on methane-air flames suppressing abilities of dimethyl methylphosphonate (DMMP). They measured the laminar burning velocities with the use of the Bunsen flame method at 373 K. A kinetic model ensured a good prediction of the LBV for the methane-air premixed flames with the addition of DMMP. Experimental and numerical studies of the LBV of methane-air and natural gas-air mixtures under the influence of the addition of hydrogen were carried out in [9]. A 14-litre closed spherical vessel with central ignition was utilized in these experiments. It was found that the increasing amounts of hydrogen added to the methane–air mixture resulted in a rise in the laminar burning velocity. In boiling, the removal of vapor becomes more challenging at higher superheats due to increased vapor production, which can act as a barrier [19,20]. Analogously, in combustion, elevated initial temperatures can significantly alter the flame structure and propagation speed, impacting the efficiency and stability of the combustion process. The intricate interplay between heat release, flame stretch, and diffusive processes at varying temperatures necessitates comprehensive experimental and numerical analyses. In the literature [21], some authors also investigated the dilution effect of carbon dioxide and water on the laminar burning velocity of methane-air flames, as well as the coupling effect between CO₂ and H₂O. It

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was concluded that the strongest chemical effects were observed with the simultaneous supplementation of CO_2 and H_2O . The laminar burning velocity and burned gas Markstein length of methane–air mixture correlations can be found in the literature [8]. The obtained results showed that the LBV increased by 23–29% with a rise in temperature from 373 K to 423 K and by 22–34% with a temperature increase from 423 K to 473 K. In a well-known review paper [12], some authors also showed the application of polynomial regression curves fitting to LBV measurement data from various publications, including those related to methane–air mixtures [22,23].

Akram et.al. [24] demonstrated that, for slightly richer mixtures, a minimal temperature exponent and an increase in adiabatic flame temperature were observed. This phenomenon was due to the fact that the normalized sensitivity to methane of the dominant reactions increases with temperature for mixtures close to the lean flammability limit and slightly decreases for stoichiometric mixtures. A linear change in the temperature exponent as a function of the equivalence ratio should be avoided. The maximum flame speed has been observed for slightly richer methane—air mixtures, which is consistent with computational results and contrasts with available experimental results that show peak values for lean or very rich mixtures at high temperatures. This discrepancy is attributed to the inaccuracy and variability of the temperature exponent with equivalence ratios.

Ghosh and co-authors [25] demonstrated that the laminar burning velocity of hydrogen–air mixtures was measured under stoichiometric conditions for temperatures ranging from 160 to 295 K. The laminar burning velocity decreased by 50% when the unburned mixture temperature was reduced by 100 K. This decrease followed a power law relationship between the unburned mixture temperature and the ambient temperature, with an exponent of 1.571. This exponent, as reported in the literature, was determined for temperatures above ambient conditions.

The rising popularity of Computational Fluid Dynamics (CFD) methods underscores a notable gap in the literature, particularly the limited research on employing machine learning techniques to analyze the laminar burning velocity of CH₄–air mixtures [25]. This review chapter reveals that, while studies on flammability and fire safety frequently address combustible mixtures or fuel blends that may include methane, focused investigations on pure methane–air mixtures remain relatively scarce.

2. Materials and Methods

2.1. Experimental Setup and Method Description

This study utilized a range of materials and tools, encompassing both physical laboratory equipment, such as the test apparatus, and computational resources, notably, the CANTERA and GRI-Mech 3.0. To calculate the laminar burning velocity (LBV) of methane–air mixtures, we employed some distinct numerical models: Manton, Lewis et al., Bradley, Mitcheson, and Dahoe. The effectiveness of these models in determining methane combustion's laminar velocity is attributed to their precision in predicting combustion dynamics. This precision provides a robust basis for understanding the core mechanisms of combustion, enabling researchers and engineers to refine the design and operation of methane-fueled systems. Our goal is to improve system efficiency, ensure safety, and minimize emissions. As for the experimental setup, it comprised the following components:

- combustion chamber;
- ignition initiation system;
- pressure determination system that included a pressure transducer, an amplifier, and a recording device to measure the explosion pressure;
- mixture preparation device using the partial pressure method;
- temperature-measuring system;
- safety instrumentation.

The combustion chamber was designed as a spherical container made of stainless steel, with a capacity of 20 dm³. The selection of stainless steel as the material was strategic, intended to withstand corrosion from reactive substances and by-products of

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combustion. Furthermore, the instrumentation of the test apparatus was meticulously crafted to withstand pressures as high as 15 bar, ensuring durability and reliability under demanding conditions.

The spherical chamber was equipped with dedicated ports that served dual purposes: the introduction and extraction of test gases, as well as the injection and expulsion of a methane—air mixture. This configuration enabled meticulous control over the internal gas composition, a crucial factor for achieving accurate and consistent experimental results [26]. The temperature within the chamber was monitored by a thermocouple placed in an optimal location to avoid interfering with the flame's path, with the temperature readings available on a display at the apparatus's base for immediate observation. To mitigate thermal losses and ensure stable temperature conditions, the chamber incorporated a water jacket, effectively sustaining a uniform temperature and enhancing the experiments' precision and reliability.

The ignition mechanism, situated at the center of the test volume, as shown in Figure 1, utilized a thin Nickel-Chromium (Ni-Cr) wire, 0.2 mm in diameter, ignited by an electric arc to initiate combustion. A mechanical stirrer within the chamber, employing the partial pressure technique for mixing, ensured the uniformity of the test mixture. An observation window at the front of the chamber permitted direct visual inspection of the combustion process.

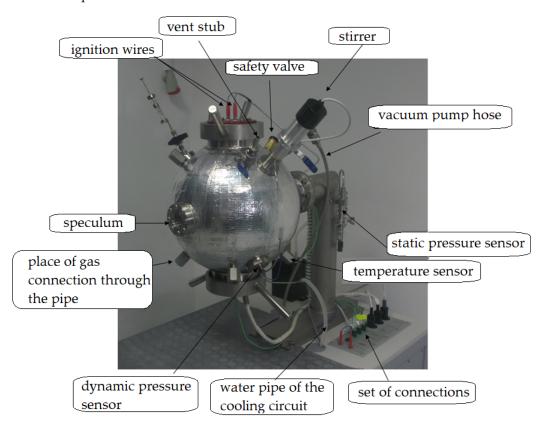


Figure 1. Testing stand with the arrangement of 20 L combustion vessel provided by ANKO [23].

A sophisticated data acquisition system was installed to collect the key parameters during the explosion, comprising a pressure transducer, a recording unit, and a signal amplifier. The gathered data were then relayed to a connected computer, equipped with specialized software for comprehensive analysis. This setup allowed for an in-depth examination and interpretation of the combustion dynamics, facilitating a thorough understanding of the experiment's outcomes.

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The combustion chamber was a spherical container with a capacity of 20 dm³ (20 L). Given that it was spherical, its internal dimensions can be determined using the volume formula for a sphere:

$$V = \left(\frac{3V}{4\pi}\right)^{\frac{1}{3}} \tag{1}$$

The radius was calculated: $r \approx 17.88$. The diameter (D) was twice the radius. Therefore, the internal diameter of the combustion vessel was approximately 35.76 cm.

2.2. Methodology

In this study, the experimental procedures were meticulously followed using the equipment detailed in Section 2.1 to ensure the collection of reliable and precise data, thereby laying a robust foundation for our observations and subsequent analyses [23]. The sequence of actions taken is detailed in Figure 2.

STAGE 1

Open the test chamber, wrap the flux wire around the electrodes and then seal the experimental tank, adjust the initial temperature of the chamber. Blow out the tank with compressed air. Close the outlet valve.



STAGE 2

Drain the air from the tank using a pump, creating a vacuum in the chamber. Connect a cylinder of flammable gas (hydrogen or methane) to a specially adapted connector, then unscrew it to introduce the gas into the chamber. Calculate and inject the exact amount of fuel into the tank based on the partial pressure. Cap and disconnect the combustible gas cylinder from the test device.



STAGE 3

Connect and unscrew the air cylinder (acting as an oxidiser). Feed the correct amount of air into the tank, determined by the partial pressure. Turn off and disconnect the oxidising gas cylinder. Close all valves to seal the system. Turn on the mechanical mixer to thoroughly mix the fuel and oxidiser for 3 to 5 minutes, ensuring a homogeneous mixture.



STAGE 4

After switching off the agitator, wait 5 minutes for the combustible mixture to stabilise. Connect the ignition system (electrodes). Use a computer connected to the test apparatus to set up and run a programme to record reaction parameters such as the overpressure created by the explosion. Check that all valves are securely closed. Start the ignition system to initiate the combustion process during which the explosion parameters are recorded.

Figure 2. Sequence of actions when studying the laminar velocity of methane combustion using a spherical sphere.

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3. LBV Numerical Models

To accurately determine the velocity of methane combustion, experiments must strive to produce a flame front that is as uniform and flat as possible. This requires maintaining consistent parameters, unaffected by heat dissipation to nearby solids or interference from the surrounding atmosphere.

3.1. Manton, Lewis, and von Elbe

The Manton, Lewis, and von Elbe [27] method for determining laminar burning velocity relies on extrapolating experimental data obtained from deflagration processes conducted within a rigid, spherical combustion chamber. A key aspect of this method is the analysis of how a flame propagates from the center of the chamber towards its walls, leading to an increase in the chamber pressure due to the thermal expansion of the combusted gases.

In this process, a flame is ignited at the center of a spherical test chamber, causing it to propagate outward towards the chamber walls. This spherical propagation of the flame leads to an increase in the pressure within the chamber, resulting from the thermal expansion of the combusted gases. Simultaneously, the remaining unburned mixture undergoes adiabatic compression, resulting in a temperature increase from the initial T_0 [K] to a final temperature T_u [K].

The formula they developed allows for the calculation of the burning velocity S_l by extrapolating the final explosion pressure data P_e , which corresponds to the combustion pressure occurring at constant volume, assuming the constancy and consistency of the average specific heat and dissociation equilibrium values within the temperature range from 0 to n. The pressure value P_e then corresponds to the final explosion pressure.

The equation used in the Manton, Lewis, and von Elbe [27] method is presented as follows:

$$S_{l} = \frac{d(rb)}{dt} \times \left(1 + \frac{1}{\gamma_{u}} \times \frac{P_{e}}{P} - 1\right) \tag{2}$$

where:

 S_1 is the laminar burning velocity,

d(rb)/dt represents the change in the radius of the sphere formed by combustion products over time,

 γ_u is the ratio of specific heat at a constant pressure to specific heat at a constant volume for a mixture of unburned gases,

 P_e corresponds to the combustion pressure at constant volume, P is the final pressure.

This method provides a significant contribution to understanding the dynamics of flame propagation and allows for the accurate determination of laminar burning velocity, which is crucial for the study of combustion processes, including the combustion of methane and hydrogen [27].

3.2. Bradley and Mitcheson

The Bradley and Mitcheson [28] method for investigating the laminar burning velocity of methane involves a mathematical model based on several critical assumptions. Firstly, they hypothesize that the combustion of the mixture can begin at a central point within a rigid, spherical test chamber. This model further assumes that the laminar flame maintains a smooth, spherical shape, propagating uniformly without being influenced by convective currents. Additionally, it presumes that the pressure distribution throughout the chamber remains uniform and that the unburned combustible mixture undergoes an isentropic compression process.

This approach focuses on the dynamics of pressure changes within the chamber as the flame propagates, considering the specific properties of methane as the combustible gas. The method is particularly noted for its application to situations where precise control over

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> the combustion environment is possible, and where accurate measurements of pressure changes can provide insights into the combustion characteristics of methane.

> The equation derived by Bradley and Mitcheson [28] to calculate laminar burning velocity is as follows:

$$\frac{dP}{dt} = 3S_l \times \left(\frac{R}{P_e - P_0}\right) \times \left(\frac{P}{P_0}\right)^{\frac{1}{\gamma_u}} \times \left[1 - \left(\frac{P_0}{P}\right)^{\frac{1}{\gamma_u}}\right] \times \left(\frac{P_e - P}{P_e - P_0}\right)^2 \times \left(\frac{3}{P_e - P_0}\right) \tag{3}$$

where:

 $\frac{dP}{dt}$ is the rate of pressure change within the chamber, S_l is the laminar burning velocity,

R represents the chamber radius,

 P_0 is the initial pressure,

P is the pressure at a given moment during the combustion process,

 P_e is the final explosion pressure,

 γ_u is the ratio of specific heats (at constant pressure and constant volume) of the unburned gas mixture.

This model and its associated equation allow for a detailed analysis of the laminar burning velocity of methane, taking into account the specific conditions under which combustion occurs. It provides a valuable tool for understanding the fundamental aspects of methane combustion, particularly in controlled experimental settings.

3.3. The "Thin Flame" Model by Dahoe

The "thin flame" model developed by Dahoe [29] focuses on investigating the laminar burning velocity of methane-air mixtures by examining changes in the pressure profile within a combustion chamber. This model simplifies the combustion process by considering the flame to be infinitely thin, which allows for a more straightforward mathematical description of the flame propagation and its effects on the surrounding gas mixture.

The key assumption of the "thin flame" model is that, despite the flame's negligible thickness, it can still significantly influence the temperature, pressure, and velocity of the gas ahead of and behind the flame front. This simplification enables the model to focus on the essential characteristics of laminar flame propagation, such as the relationship between the laminar burning velocity, temperature, and pressure.

Dahoe utilized this model to derive equations that relate the laminar burning velocity of methane to measurable quantities like pressure and temperature changes within the combustion chamber. The model takes into account the properties of methane-air mixtures and employs coefficients that accurately represent the behavior of these mixtures under combustion conditions.

One of the key equations derived from the "thin flame" model to calculate the laminar burning velocity (S_l) for methane–air mixtures is given by:

$$\frac{dP}{dt} = \frac{3(P_{max} - P_0)}{4\pi V_k \left(\frac{1}{3}\right)} x \left(1 - \left(\frac{J_{10}}{\overline{D}_1}\right)^{\frac{1}{\gamma}}\right) \times \left(\frac{P_{max} - P}{P_{emax} - P_0}\right)^2 \times \left(\frac{P}{P_0}\right)^{\frac{1}{\gamma}} \times S_{uL} \tag{4}$$

In this equation:

dP/dt represents the rate of pressure change over time,

 P_{max} is the maximum pressure reached during the combustion,

 P_0 is the initial pressure,

 V_k is the volume of the combustion chamber,

 γ is the specific heat ratio of the gas mixture,

 S_{uL} is the laminar burning velocity being determined.

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Furthermore, Dahoe [29] explored the impact of temperature and pressure on the laminar combustion velocity through additional equations, incorporating coefficients specific to methane–air mixtures as proposed by Iijima and Takeno [30].

The "thin flame" model offers a valuable approach for studying the dynamics of flame propagation, particularly in gases like methane, by simplifying the complex processes involved in combustion. It provides a framework for understanding how various factors, including pressure and temperature, influence the laminar burning velocity, which is crucial for the design and optimization of combustion systems.

3.4. Three-Layer Model (Dahoe—2013)

In their 2013 study [31], Dahoe and colleagues focused on measuring the laminar burning velocity (S_U) by observing the evolution of explosion pressure curves within a rigid spherical combustion chamber. To calculate the combustion velocity, they utilized a combination of the Levenberg–Marquardt optimization algorithm and the finite Runge–Kutta numerical integration method [32–37]. This integrated methodology was rigorously validated against three distinct test patterns and applied in simulations using two models that described the pressure increase dynamics during explosions in confined spaces, specifically for hydrogen and methane–air mixtures.

The "three-layer model" introduced by Dahoe in later research represents a significant advancement in the study of laminar burning velocity, particularly for methane combustion. This model provides a more detailed and nuanced understanding of flame propagation by dividing the combustion process into three distinct zones:

Unburned Gas Mixture Zone: The area ahead of the flame where the gas mixture remains unburned and is at its initial state.

Reaction Zone: The thin layer where the actual combustion takes place. This is the area of interest where the chemical reaction of methane with oxygen occurs, leading to the production of combustion products.

Post-combustion Zone: The area behind the flame front where the combustion products reside, having a higher temperature and different composition compared to the unburned gas.

Unlike the "thin flame" model, which simplifies the flame as having a negligible thickness, the "three-layer model" assigns a non-zero thickness to the flame, $\delta \neq 0$, allowing for a more comprehensive analysis of the flame's impact on the surrounding gas mixture. This thickness accommodates variations across the combustion front, enabling a detailed study of the physical and chemical transformations that occur during combustion.

The mathematical formulation of the "three-layer model" captures the dynamics of flame propagation by considering the interactions between these zones. It accounts for the thermal and compositional changes that the gas mixture undergoes as it moves from the unburned zone, through the reaction zone, and into the post-combustion zone.

One of the key aspects of the "three-layer model" is its ability to provide insights into the effects of various parameters, such as the initial temperature, pressure, and mixture composition, on the laminar burning velocity. By analyzing the pressure and temperature changes within the combustion chamber, the model can accurately predict the laminar burning velocity (*LBV*) for methane–air mixtures.

The "three-layer model" offers a robust framework for quantitatively assessing the flame characteristics and propagation dynamics within the combustion process. It has been rigorously validated against experimental data and applied in simulations to describe the pressure increase dynamics during explosions in confined spaces, specifically for hydrogen and methane—air mixtures.

This model's detailed representation and division into three zones make it an invaluable tool for understanding the complex interactions and transformations that occur during the combustion of methane, providing a solid foundation for further research and development in combustion science.

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3.5. Cantera and GRI-Mech 3.0

Cantera v. 3.0.0. and GRI-Mech 3.0 are both advanced computational tools utilized in the study of combustion processes, including the laminar burning velocity of methane. These models provide comprehensive frameworks for simulating the chemical kinetics and thermodynamics of combustion, allowing researchers to analyze and predict the behavior of methane flames under various conditions.

Cantera is an open-source suite of tools for modeling the thermodynamics, chemical kinetics, and transport processes of gases and reacting flows. It is designed to solve problems in combustion, chemical propulsion, and environmental science, among other fields. Cantera is particularly useful for studying the laminar burning velocity of methane, due to its ability to accurately model the chemical kinetics involved in methane combustion. Researchers can use Cantera to simulate one-dimensional flames, including freely propagating flames, to measure the laminar burning velocity directly from simulations. Cantera's flexibility in defining and manipulating chemical reaction mechanisms makes it an invaluable tool for investigating how various factors affect the laminar burning velocity of methane.

GRI-Mech 3.0 (Gas Research Institute Mechanism 3.0) is a widely recognized and utilized chemical kinetic mechanism for modeling the combustion of natural gas, primarily methane. Developed through extensive validation against experimental data, GRI-Mech 3.0 includes a comprehensive set of reactions and species that are crucial for accurately predicting the combustion of methane and its derivatives. The model is especially noted for its ability to replicate the chemical kinetics of methane combustion across a wide range of conditions, making it a cornerstone for studies related to methane combustion kinetics, including the determination of laminar burning velocities. Researchers often use GRI-Mech 3.0 as a basis for their simulations in Cantera or other computational fluid dynamics (CFD) software to explore the intricacies of methane combustion.

Both Cantera v. 3.0.0. and GRI-Mech 3.0 can be integrated into larger computational frameworks to conduct detailed simulations of methane combustion processes. By combining Cantera's capabilities for modeling reacting flows with the detailed chemical kinetics provided by GRI-Mech 3.0, researchers can achieve highly accurate predictions of the laminar burning velocity of methane. This integrated approach allows for the exploration of how changes in temperature, pressure, and mixture composition influence the combustion process, providing insights that are critical for the development of more efficient and cleaner combustion technologies.

In summary, Cantera and GRI-Mech 3.0 offer powerful and flexible platforms for the advanced study of methane combustion, enabling researchers to delve into the complex dynamics of laminar flame propagation and optimize combustion processes for practical applications.

4. Results

Measurements were conducted on the explosive–stoichiometric attributes of methaneair mixtures across five distinct initial temperatures. For each temperature point, denoted as T_0 , a set of five measurements were meticulously executed in accordance with the prescribed test protocol. Throughout these assessments, the recording frequency for the explosion parameters remained consistent at 150 kHz, while the initial pressure for every trial was fixed at $P_0 = 1$ bar.

Measurements to determine the explosive–stoichiometric properties of methane–air mixtures were carried out at five distinct initial temperatures. For each specified initial temperature, noted as T_0 , a series of five meticulous measurements followed a predefined test protocol. During these evaluations, the data-recording frequency for capturing the explosion parameters was uniformly maintained at 150 kHz. Additionally, the initial pressure for each measurement was consistently set at $P_0 = 1$ bar.

The result of each trial is visually represented by a curve that illustrates the progression of the explosion pressure over time. Aggregated curves, summarizing the outcomes

of the five measurements conducted at each specific initial temperature (T_0 = 298.15 K, T_0 = 323.15 K, and T_0 = 348.15 K), are depicted separately in Figures 3–5.

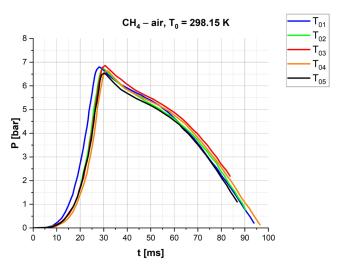


Figure 3. P(t) curves for methane–air mixtures, T_0 = 298.15 K.

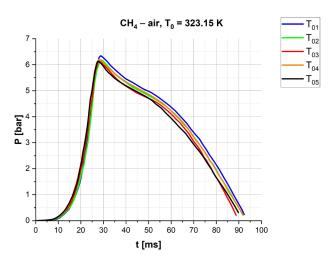


Figure 4. P(t) curves for methane–air mixtures, $T_0 = 323.15$ K.

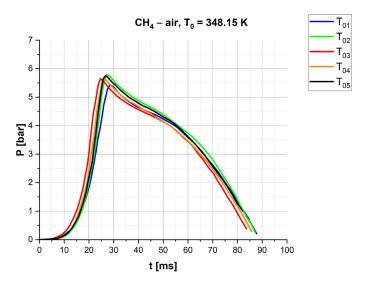


Figure 5. P(t) curves for methane–air mixtures, T_0 = 348.15 K.

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The selection of these temperatures for the laminar burning velocity (LBV) tests was intentional, aiming to mimic the common operational temperatures found in many methanefueled systems [38]. Furthermore, these temperatures were chosen due to their ease of attainment and the ability to precisely control them, making them ideal for experiments conducted in a laboratory setting.

From the five experimental tests conducted at varying initial temperatures with the stoichiometric mixture of methane and air, we computed the average values for two critical parameters: the maximum explosion pressure (P_{max}) and the peak rate of explosion pressure rise. These averages were derived from the data collected across all temperature conditions tested, providing insights into the combustion characteristics under different thermal environments. These calculated values are presented in Table 1.

Table 1. Maximum explosion pressure and maximum rate of explosion pressure rise values for methane–air mixtures.

	$T_0 = 298.15 \text{ K}$		$T_0 = 323.15 \text{ K}$		$T_0 = 348.15 \text{ K}$	
Nr	P_{max} [bar]	$\left(\frac{dp}{dt}\right)_{max} \left[\frac{bar}{s}\right]$	P _{max} [bar]	$\left(\frac{dp}{dt}\right)_{max}\left[\frac{bar}{s}\right]$	P _{max} [bar]	$\left(\frac{dp}{dt}\right)_{max} \left[\frac{bar}{s}\right]$
1	6.802405	675.04	6.34	747.21	5.44	538.87
2	6.754296	720.31	6.19	712.08	5.79	703.36
3	6.861446	705.6	6.16	734.1	5.65	740.93
4	6.644578	711.6	6.2	688.56	5.64	683.72
5	6.537801	661.87	6.14	687.34	5.76	727.79
Average	6.720105	694.884	6.206	713.858	5.656	678.934

4.1. Results of LBV Numerical Calculations

A numerical simulation was carried out, incorporating all the models described alongside Equations (2)–(4). This simulation generated experimental plots that illustrate the pressure–time relationship, represented as P(t). From these plots, we were able to extract critical values, including the maximum explosion pressure (P_{max}) and the time interval from the reaction's initiation to the point where this maximum pressure was reached.

4.1.1. Results of Manton, Lewis, and Von Elbe Model

Table 2 presents the data obtained from applying Equation (2) for three different initial temperatures (T_0). Additionally, it details the calculations of the laminar burning velocity (S_U) that were extrapolated from these specific values.

Table 2. The necessary data for computing S_U using the Manton, Lewis, and von Elbe model with three initial temperatures.

$T_i[K]$	d_{rb}/dt [m/s]	T_b [K]	T_e [K]	P_e [bar]	P_{max} [bar]	S_{U} [m/s]
298.15	0.563212	2221	2292.503	7.689092	6.714	0.510277
323.15	0.595745	2243	2320.365	7.180458	6.206	0.535666
348.15	0.629852	2255	2338.278	6.716296	5.656	0.555473

Figure 6 depicts the correlation between the initial temperature and the calculated laminar burning velocity, as derived from the mathematical model developed by Manton, Lewis, and von Elbe.

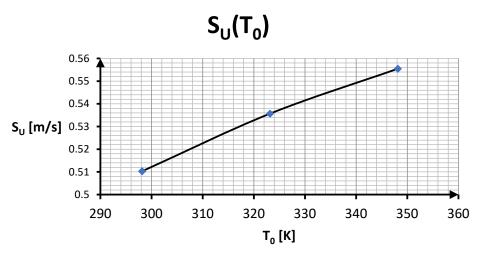


Figure 6. Dependence of the laminar burning velocity (S_U) on the initial temperature for stoichiometric methane–air mixture, based on Manton, Lewis, and von Elbe model.

4.1.2. Results of Bradley and Mitcheson Model

To conduct numerical simulations following Bradley's methodology, we utilized Equation (3), where the pressure variable (P) represents the peak rate of the explosion pressure accumulation. This rate was determined from the experimental curves, P(t), with the ultimate pressure (P_e), considered to be the maximum explosion pressure (P_{max}).

Table 3 presents the values calculated using Equation (3) for three different initial temperatures (T_0), along with the corresponding laminar burning velocities (S_U) derived from these calculations.

Table 3. The necessary data for computing S_U using the Bradley and Mitcheson model with three initial temperatures.

T ₀ [K]	P _{max} [bar]	P [bar]	dp/dt [bar/s]	S _U [m/s]
298.15	6.714	4.9189	69.4884	0.2348
323.15	6.206	4.685567	71.3858	0.273335
348.15	5.656	4.312715	67.8934	0.309474

In Figure 7, the correlation between the initial temperature and the laminar burning velocity is illustrated.

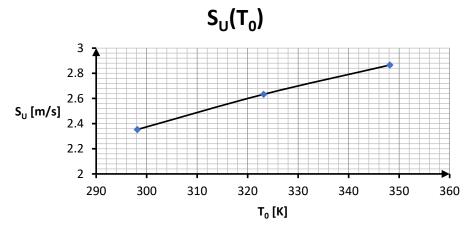


Figure 7. Dependence of the laminar burning velocity (S_U) on the initial temperature for stoichiometric methane–air mixture, based on Bradley and Mitcheson model.

4.1.3. Results of Dahoe 2005 Model

The results obtained from the numerical simulation conducted by Dahoe in 2005 are in accordance with the parameters outlined in Equation (4). Importantly, the formula for determining the laminar burning velocity (S_U) does not account for the flame thickness. This omission is noteworthy, because it suggests the calculation of S_U is designed to focus on other critical parameters of flame propagation, excluding the physical dimension of flame thickness from its considerations ($\delta = 0$). To accurately derive the necessary values, it is essential to determine both the maximum explosion pressure (P_{max}) and the pressure at the point of the maximum rate of explosion pressure rise (dp/dt)_{max}. These critical measurements are fundamental for calculating related parameters effectively. Additionally, it is crucial to highlight that the combustion chamber volume (V_k) is defined as 0.02 m³. Due to the equations' similarities—Equation (4) closely aligns with Equation (3) from the Bradley and Mitcheson model—the outcomes derived from both equations are identical. These findings are elaborated upon in Section 4.1.2.

4.1.4. Results of Dahoe 2013 Model

From the experimental plots that depict the relationship between the explosion pressure and time, we can extract critical values, including the maximum explosion pressure (P_{max}) and the pressure (P) at the point of the maximum rate of explosion pressure rise as $\left(\frac{dp}{dt}\right)_{max}$ or $\frac{dP}{dt}$ in Equation (4). The initial explosion pressure is established at $P_0=1$ bar, and the volume of the test chamber is defined as $V_k=0.02$ m³. In the three-zone flame model, calculating the laminar burning velocity (LBV) requires an estimation of the flame thickness, denoted as δ^0_{uL} . For methane–air mixtures, estimating the unstretched flame thickness necessitates the use of Cantera. Table 4 displays the data obtained from Equation (4) across three different initial temperatures (T_0) , together with the laminar burning velocities (S_U) that were calculated based on these data.

P T_0 dp/dt P_{max} δ S_{U} r_f 298.15 69.4884 6.714 4.9189 0.000523 0.162826 0.162302 0.23484 323.15 71.3858 6.206 4.6856 0.000538 0.16306 0.162523 0.273382 348.15 67.8934 4.3127 0.162233 5.656 0.000555 0.162788 0.309526

Table 4. The necessary data for computing S_U using the Dahoe 2013 model with three initial temperatures.

Figure 8 depicts the correlation between the initial temperature and the laminar burning velocity (S_U), as calculated using the mathematical model introduced by Dahoe in 2013. This visualization highlights how S_U can vary with changes in the initial temperature, according to Dahoe's model.

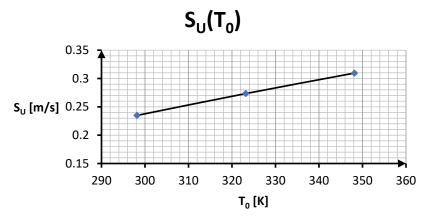


Figure 8. Dependence of the laminar burning velocity (S_U) on the initial temperature for stoichiometric methane–air mixture, based on Dahoe 2013 model.

4.1.5. Results of Cantera Simulations

Figure 9 showcases a script from the Cantera toolkit, which, upon specifying the initial conditions—the temperature, pressure, and composition of the combustible mixture—automatically calculates the laminar burning velocity. Table 5 then lists the computed initial temperatures (T_0) and the corresponding laminar burning velocities (S_U), as determined using the Cantera for stoichiometric methane—air mixtures.

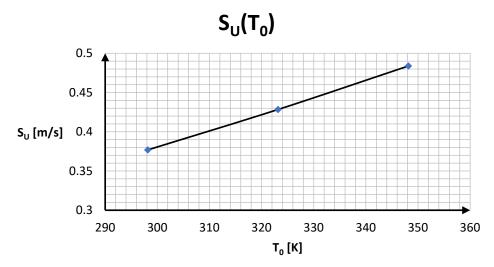


Figure 9. Dependence of the laminar burning velocity (S_U) on the initial temperature for stoichiometric methane–air mixture, based on Cantera simulations.

Table 5. Results of S_U calculation for methane–air mixture using Cantera.

T_0 [K]	S_{U} [m/s]
298.15	0.376829
323.15	0.428361
348.15	0.483786

5. Summary

Laminar burning velocity (S_U) is a pivotal parameter that defines the behavior of combustible mixtures. Given that S_U cannot be measured directly, the deployment of accurate mathematical models is crucial for its numerical determination, relying on well-defined parameters of the combustion process. In pursuit of this, experimental trials were conducted with a specialized apparatus, employing procedures specifically designed for stoichiometric methane—air mixtures. For each experiment, the combustible mixture was ignited at a uniform initial pressure (P_0) of 1 bar, across three selected initial temperatures: 298.15 K, 323.15 K, and 348.15 K. The experimental data, capturing the evolution of the explosion pressure over time P(t), serve as a basis for these analyses.

Figure 10 illustrates the derived laminar burning velocities for the methane–air mixtures, based on the observed temporal pressure profiles, as well as all calculation models, including Manton, von Elbe, and Lewis, Bradley and Mitcheson, and both Dahoe models.

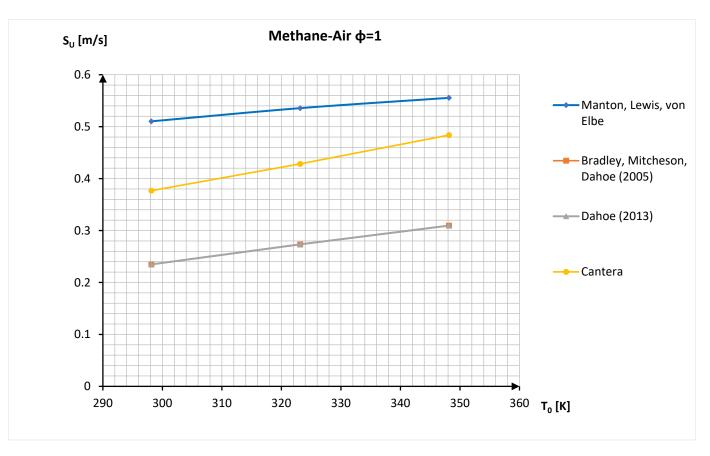


Figure 10. Dependence of laminar combustion velocity (SU) on initial temperature for a stoichiometric mixture of methane and air, for all models.

6. Discussion

The laminar burning velocity (LBV) is crucial for predicting the behavior of combustible mixtures. Our experimental results demonstrated that the LBV increases with the initial temperature (T_0), indicating a direct relationship between temperature and combustion velocity. This aligns with the existing literature, which suggests that higher temperatures promote faster combustion reactions. Using the Cantera v. 3.0.0., which accounts for the detailed chemical kinetics of combustion, we verified our experimental results. The Cantera-based simulations provided a benchmark for comparing various predictive models. Among the models evaluated, the Bradley and Mitcheson [27,28] and Dahoe [29] models showed the closest agreement with the Cantera results, exhibiting a discrepancy of less than 0.05 m/s. This minimal difference underscores the reliability of these models for predicting the SU in methane–air mixtures.

While the Bradley and Dahoe models demonstrated a high accuracy, the Manton, Lewis, and von Elbe models produced slightly lower SU values (up to 0.3 m/s). These discrepancies can be attributed to the simplifications inherent in these models. Despite this, the thin flame model proposed by Dahoe [29] proved effective, closely aligning with the more sophisticated three-zone flame model [31]. The thin flame model's simplicity and robustness make it a valuable tool for practical applications, where computational resources or detailed kinetic data might be limited.

Understanding the LBV and other combustion parameters at elevated temperatures is essential for designing safer and more efficient energy systems. The data obtained from this study are particularly relevant for the natural gas industry, where methane is a primary component. As an efficient "bridge fuel" in the transition to cleaner energy sources, methane's combustion characteristics must be well understood to optimize its use and mitigate associated risks.

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Methane is widely used in industrial applications, and its safe handling is paramount. Knowledge of combustion parameters such as Pmax and (dP/dt)max helps in designing safety measures to prevent and mitigate explosive incidents in industries such as chemical manufacturing, oil and gas, and power generation. Accurate data on LBV are essential for the design of safety systems, such as venting and suppression mechanisms.

Methane, being a major component of natural gas, is a crucial energy source. Understanding its combustion dynamics at different temperatures enables the optimization of combustion processes, leading to a higher efficiency and lower emissions. This is particularly important in the context of transitioning to cleaner energy sources where methane serves as a "bridge fuel".

An improved combustion efficiency directly correlates with reduced emissions of harmful pollutants such as NOx and CO₂. Detailed knowledge of methane combustion at elevated temperatures can inform the development of technologies that minimize the environmental impact of natural gas usage.

Our experiments were conducted at a standard initial pressure of 1 bar, focusing on temperatures ranging from 298.15 K to 348.15 K. Future studies should explore a broader range of pressures and temperatures to provide a more comprehensive understanding of methane—air combustion dynamics. Additionally, incorporating more complex chemical kinetic models in simulations could further enhance the accuracy of predictive models.

The findings of this study contribute valuable data to the field of combustion science, supporting the advancement of safety protocols and the efficient use of natural gas in energy production. By comparing the experimental results with various predictive models, we identified reliable methods for estimating laminar burning velocities, which are crucial for the safe and effective design of combustion systems.

7. Conclusions

For methane-air mixtures, the laminar burning velocity (S_U) calculated using the thin flame model [29] closely aligns with the S_U velocity derived from the more sophisticated three-zone flame model [31]. As the initial temperature (T_0) increases, so does S_{IJ} , reflecting a direct relationship between temperature and combustion velocity. The literature [34–38] discusses LBV's dependency on the initial pressure and the stoichiometry coefficient of the mixture, with a standard pressure of $P_0 = 1$ bar and temperature of $T_0 = 298$ K, facilitating the verification of the results at the experiment's lower temperature limit ($T_0 = 298.15 \text{ K}$). Cantera, which considers the chemical kinetics of combustion, is deemed as the most reliable for verifying computations. When comparing the numerical models with the Cantera results, the models from Bradley and Mitcheson et al. (2005) and Dahoe (2013) most accurately represent methane–air mixture S_U, with a discrepancy of less than 0.05 m/s for the investigated temperatures. The propagated sphere radius' speed significantly influences the final S_U outcome. The Manton, Lewis, and von Elbe models yield slightly lower S_U values (up to 0.3 m/s) compared to Cantera, likely due to their simplifications. However, the LBVs from the Bradley and Mitcheson models and the 2005 Dahoe model closely match those calculated using the 2013 Dahoe model, with only a 0.003% difference in estimation. Despite the thin flame model's considerable simplifications, it remains effective for predicting S_U in methane-air mixtures. These models, including those proposed by Bradley, Mitcheson, and Dahoe from 2005, demonstrate a robust reliability in their predictions, affirming their utility alongside more complex methods like Cantera.

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