



Experimental and numerical investigations of the laminar burning velocities of premixed fuel-rich methane oxy-fuel and oxygen-enhanced flames

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ABSTRACT

In the context of Oxy-fuel combustion, there is a strong industrial interest in highly fuel-rich flames, characterized by an equivalence ratio (Φ) exceeding 2.5, for the production of H₂-CO-rich synthesis gas. The validation of existing chemical reaction mechanisms for this specific regime pose a significant challenge due to the scarcity of experimental data for this particular range of equivalence ratio.

The scope of this study was therefore the determination of the laminar burning velocity s_L of ultra-rich CH₄-O₂ flames under varying conditions, such as high equivalence ratios and preheating temperatures using the heat flux burner method. The laminar burning velocity was determined for equivalence ratio within the range of $2.3 < \Phi < 3.6$ and preheating temperature ranging from 300 K to 455 K. Additionally, the impact of the oxygen content in the oxidizer on s_L was investigated by argon addition in molar percentages ranging from 40 % to 100 %.

The results of our study reveal laminar burning velocities ranging from 5 cm/s to 45 cm/s for pure oxy-fuel CH₄ flames. Preheating is shown to increase s_L and this effect can be represented by a power law correlation $s_L = s_{L,0}(T/T_0)^\alpha$ with $\alpha = 1.53$. Furthermore, the dilution of the oxidizer with argon leads to a significant decrease in s_L of approximately 50 % compared to pure oxy-fuel flames. It is worth noting that detailed reaction mechanisms in combination with molecular transport data are typically not validated within the selected equivalence ratio range.

To assess the performance of such reaction schemes in predicting laminar burning velocity under the specified selected conditions, we evaluated 13 different reaction mechanisms sourced from the literature. We compared the laminar burning velocities obtained through calculations of laminar premixed 1D flames and, additionally compared these with experimental data. A sensitivity analysis of the laminar burning velocity were carried out for selected mechanisms. Among the mechanisms, the CalTech2.3 mechanism exhibited the most consistent and accurate performance, particularly at high equivalence ratios.

1. Introduction

The production of synthesis gas with varying compositions through the combustion of premixed, fuel-rich methane-oxygen mixtures in the absence of a catalyst, a process known as thermal partial oxidation (T-POX), has been an industrial practice since the 1950 s [1]. These T-POX processes are typically characterized by their nitrogen-free nature and are operated under highly fuel-rich conditions to generate undiluted synthesis gas and higher hydrocarbon species for subsequent industrial

applications. In the theoretical and technical development of such reactors, the laminar burning velocity stands out as a critical parameter. It plays a fundamental role in describing the physicochemical interactions at the molecular level, forming the foundation for understanding turbulent combustion. Consequently, this parameter finds extensive application in various models for turbulent combustion [2].

A review of the literature reveals that there is limited experimental data published for T-POX conditions. Laminar burning velocities of pure CH₄-O₂ mixtures were investigated in several publications spanning

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from the 1930 s to the 1970 s [3–9]. The experiments to determine these burning velocities were typically conducted by studying a Bunsen flame [3,6,9] or by observing the transient flame propagation in a closed explosion vessel [4,8]. Many of these atmospheric experiments primarily focused on determining the laminar burning velocity s_L for stoichiometric mixtures, which, according to these publications, falls within the range of approximately 320 cm/s to 640 cm/s.

A recent study was published by Mouze-Mornettas et al. [10], where the laminar burning velocity of CH_4/O_2 flames was investigated with isochoric combustion method for rocket engine application. The measurements and analysis were carried out for equivalence ratios of $0.5 < \Phi < 2.5$, preheat temperatures up to about 500 K and pressures up to about 18 bar. However, it is noteworthy that experimental data for premixed flames involving fuel-rich mixtures with equivalence ratios exceeding $\Phi > 2.5$ are predominantly lacking in the available literature [11].

In 1932, Jahn [3] conducted an extensive examination of flames, encompassing a wide range of equivalence ratios ($0.2 < \Phi < 2.64$) for premixed $\text{CH}_4\text{-O}_2$ mixtures, extending into the partial oxidation (POX) regime of industrial relevance. Jahn's measurements based on investigations of premixed laminar flames using a Bunsen burner and deriving the laminar burning velocity from measurements via visually determined flame heights. However, it is worth noting that due to inherent deviations from the ideal 1D setup imposed by the flow field within such a system, along with systematic challenges associated with measuring laminar burning velocity, particularly at the flame tip and edges, the accuracy of this method is limited [12].

Presently, precise methods have become available for determining the laminar burning velocity, which show a high degree of consistency in terms of reproducibility. In 1993, de Goey et al. [13] introduced a method based on a flat flame burner that balances the heat flux between the flat flame and a temperature-conditioned burner plate. The heat-flux burner arrangement enables precise determination of the laminar burning velocity within a range of 5 cm/s to 60 cm/s. It is important to note that this range is influenced by factors such as flame instabilities at low inlet velocities and enhanced wake effects, which can disrupt the homogeneity of the flame flatness at higher inlet velocities. Consequently, these effects impose constraints on the range of operating conditions that can be explored in terms of equivalence ratio and preheating temperature.

Historically, the validation of reaction mechanisms for ultra-rich premixed oxy-fuel flames has been somewhat limited. Prior investigations primarily focused on achieving accurate concentration profiles rather than specifically targeting laminar burning velocities. For instance, Albrecht et al. [14] conducted a numerical study on the burning velocities of $\text{CH}_4\text{-O}_2$ flames under ultra-rich conditions, considering elevated pressure and preheating temperature. The primary objective of their work was to determine the necessary residence times for the production of $\text{H}_2\text{-CO}$ -rich synthesis gas. However, the calculations were performed using the GRI3.0 mechanism [15], which is limited in the description of detailed chemistry for higher hydrocarbons. In a similar vein, Li et al. [16] examined specific gas species along the downstream axis of flat, burner stabilized ultra-rich $\text{CH}_4\text{-O}_2$ flames. They compared their experimental results against numerical calculations employing three distinct reaction mechanisms. Their findings revealed that calculations using the mechanisms developed by Curran [17] and Wang-Frencklach [18] satisfactorily reproduced concentration profiles, whereas less agreement in comparison has been achieved using the GRI3.0 mechanism under the studied conditions. Cao et al. [19] explored the influence of species addition on speciation data in POX of natural gas. Their conclusions aligned with previous research, with the Curran mechanism being identified as the most suitable for predicting species profiles. These studies collectively do not consider further parameter, such as laminar burning velocity or ignition delay times for the selection of an appropriate reaction mechanism. In terms of a further use of reaction mechanisms in the engineering or modelling of reactors

operating under fuel-rich oxy-fuel conditions, this parameter have a significant role in the description of flame dynamics.

The present study is centred on the experimental determination of the laminar burning velocity in fuel-rich oxy-fuel methane flames. The further investigations are structured in a multi-step procedure for the identification of suitable detailed reaction mechanism, which are grouped in four subsections:

- The identification of an appropriate reaction mechanism available in the literature; specifically validated for the conditions under investigation, and its comparison to experimental data for the reproduction of the laminar burning velocity and sensitivity analysis on the laminar burning velocity for selected mechanism.
- The analysis of the flame structure using speciation data obtained from experimental results from the existing literature compared to numerical calculations using appropriate reaction mechanisms identified in a).
- The investigation of the impact of preheating of the unburned gas mixture on laminar burning velocity via comparison of experimental results to numerical calculations employing the most suitable mechanism from b).
- The investigation of how the oxygen content in the oxidizer influences the laminar burning velocity of the investigated premixed flames and comparison to the numerical calculations with the same mechanism as in c).

Premixed flames were examined at atmospheric pressure, spanning a broad range of very fuel-rich mixtures with equivalence ratios from $\Phi = 2.3$ to $\Phi = 3.6$. Additionally, the preheating temperature of the unburned gas mixture was varied from 298 K to 455 K. Furthermore, the oxygen content in the oxidizer underwent gradual dilution with argon, transitioning from pure oxy-fuel with 100 % O_2 to 40 % O_2 content (molar-based).

2. Numerical approach

In this study, numerical calculations were conducted using the PREMIX program within the Chemkin package. This program, originally developed by Kee et al. [20,21], was applied to analyze both freely propagating and burner-stabilized flames of premixed gas mixtures. To ensure the attainment of a convergent and mesh-independent solution, the mesh refinement process involved selecting the largest relative gradient and curvature for convergence criteria, which were set at 0.05 and 0.1, respectively. The reactor length used for flame solutions was 22 cm, and all calculations incorporated a mixture-averaged diffusion model for consistency reasons between freely propagating and burner stabilized flame calculations.

For the freely propagating flames: Investigations involved variations in equivalence ratio, preheating temperature, and oxidizer dilution ratio, at ambient pressure conditions. On the other hand, burner-stabilized flame investigations used the inlet conditions and are based on given temperature profiles obtained from experimental investigations [16].

To account for the significance of higher hydrocarbons in rich partial oxidation (POX) flames [22,23], reaction mechanisms characterized by varying maximum C-chain lengths of considered hydrocarbon species was selected for calculating pure oxy-fuel flames. An overview of the investigated mechanisms is provided in Table 1.

3. Experimental setup

The laminar burning velocity is experimentally determined via stationary planar flame studies according to the heat flux method (HFM).

The experimental setup for the HFM was designed following the specifications detailed in [13], with further elaboration available in [36]. Fig. 1 provides a visual representation of this experimental

Table 1
Selected reaction mechanisms.

mechanism	chain-length	# of species	# of reactions	Ref.
FFCM1	C2	38	291	[24]
GRI3.0	C3	53	325	[15]
Aramco 3.0	C3	581	3037	[25]
Leeds 1.5	C4	37	175	[26]
Curran	C5	132	821	[27]
Princeton	C6	92	621	[28]
HPMech 3.3	C6	92	615	[29]
Konnov 0.5	C6	127	1207	[30]
USC II	C7	111	784	[31]
CalTech 2.3	C16	192	1156	[32]
LLNL	C16	147	664	[33]
ABF	C16	101	544	[34]
MIT	C16	157	872	[35]

arrangement. For the measurement of the temperature profile, eight T-type thermocouples were defined positioned in a spiral configuration centered in the cross section in flow direction through the burner plate. This thermocouple placement design was adopted from Hermanns [37]. The burner plate, fabricated from brass, features a grid of evenly spaced holes, each measuring 0.2 mm in diameter and spaced 0.7 mm apart. For temperature conditioning, the burner plate was integrated into a heating circuit with a temperature range spanning from 380 K to 535 K, achieving a temperature 80 K above the preheating temperature of the unburned gas mixture. Precise control of the inlet flow rates was achieved through thermal mass flow controllers (MFC, Bronkhorst High-Tech). Both, the premixed gas mixture and the burner were preheated from 298 K to 455 K using a secondary heating circuit. To ensure the high purity of the methane, oxygen, and argon components, their compositions were verified to exceed 99.5 % by volume.

The estimation of experimental error of the laminar burning velocity was carried out, accounting for the uncertainties associated with the thermal mass flow controllers (MFCs), thermocouples, and their respective positions. The error bar of the equivalence ratio is calculated based on uncertainty of the mass flow controllers. We considered the most unfavorable case, which leads to the largest errors at very fuel-rich conditions. However, the mass flow controllers were calibrated before the measurement campaign.

It should be noted that the absence of thermal ballast, such as nitrogen or argon, in oxy-fuel flames results in higher heat load, leading to increased heat transfer between the burner plate and the flame. In addition, the radiation of hot soot particles increases the heat transfer. To compensate for these effects, the temperature difference between the incoming gas flow and the burner plate had to be elevated compared to

conventional air flames. The influence of the plate temperature on the laminar burning velocity was investigated in a preliminary study [38]. The chosen plate temperature shows a low sensitivity on the measured burning velocity without influencing the preheat zone. The experimental setup was validated by investigating CH₄/air flames at ambient inlet temperature and pressure. The experimental results can be found in the [supplementary material S1](#) in comparison with data from the literature.

4. Results and discussion

To assess the available data concerning laminar burning rates in fuel-rich oxy-fuel mixtures, extend the existing knowledge boundaries, and gauge the performance of published reaction mechanisms in predicting such data, we undertake a comprehensive comparison between experimental and calculated results. Initially, we compare and evaluate the outcomes derived from a range of detailed reaction mechanisms without restricting them to their intended validity domains.

Given the industrial necessity to modulate process temperatures, which hinges on a deep understanding of both preheating and dilution, we proceed to examine the CalTech2.3 mechanism. This mechanism, exhibiting superior overall performance in our initial comparison, undergoes further scrutiny in the subsequent section. Here, we compare its calculation results with experimental data for preheated and diluted mixtures.

a) Identification of detailed reaction mechanism via comparison of laminar burning velocity

We employed the reaction mechanisms, as listed in [Table 1](#) from various sources found in the literature, in a first overview we compute the laminar burning velocities of pure fuel-rich CH₄-O₂ flames at an initial gas mixture temperature of $T_0 = 473$ K. The calculated laminar burning velocity over equivalence ratio is depicted in [Fig. 2](#), revealing a broad spectrum of calculated laminar burning velocities across the entire range of investigated equivalence ratios for the different reaction mechanisms. The results based on the Curran, Konnov0.5, MIT and GRI3.0 mechanism is in the upper range of laminar burning velocity depending on the equivalence ratio while Leeds1.5 and CalTech2.3 are at the lower value range.

In the following, the laminar burning velocity at an unburned mixture temperature of 300 K is compared to experimental data from literature and this work. This comparative analysis of numerical and experimental results is depicted in [Fig. 3](#).

In a general context, the laminar burning velocities obtained

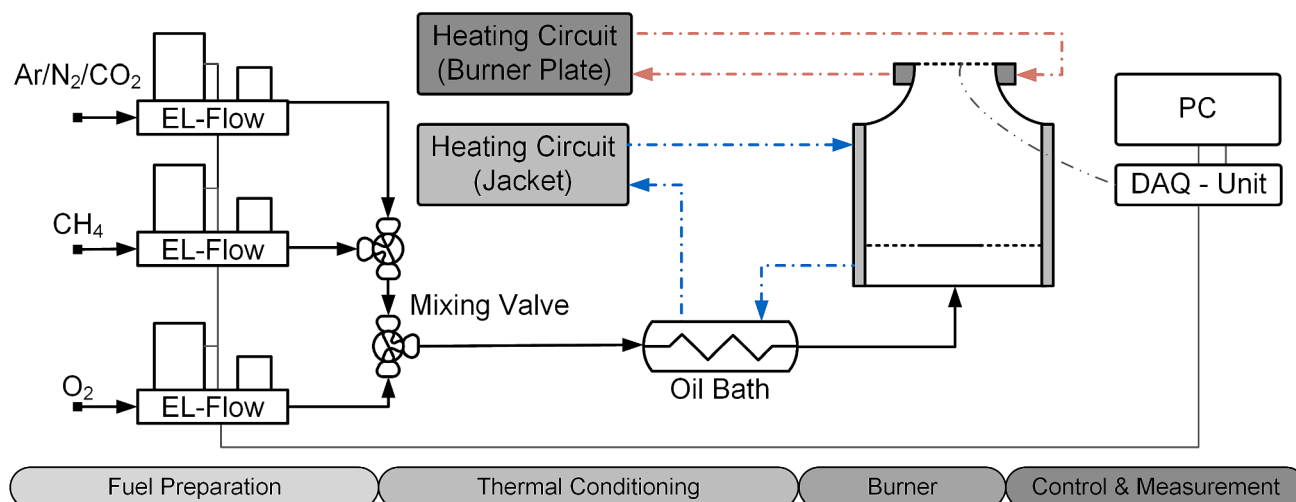


Fig. 1. Schematic flow diagram of the heat-flux burner experimental setup.

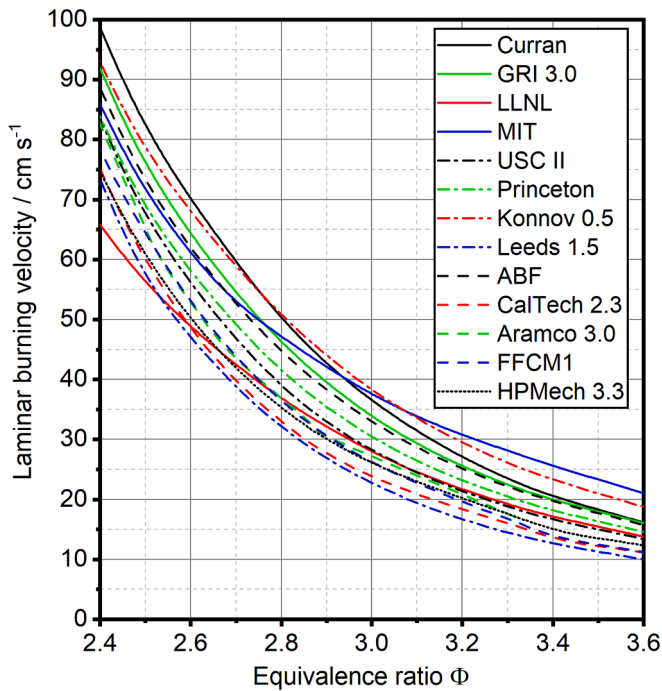


Fig. 2. Calculated laminar burning velocities of fuel-rich $\text{CH}_4\text{-O}_2$ -flames at initial temperature of 473 K at ambient pressure.

experimentally with the HFM are approximately 25 % lower than those reported by Jahn [3]. Specifically, at an equivalence ratio of $\Phi = 2.3$, the HFM result is at $s_L = 42$ cm/s, while when the oxygen content is reduced to an equivalence ratio of $\Phi = 3.63$, the laminar burning velocity decreases to $s_L = 5.3$ cm/s.

For comparative purposes with numerical simulations, we selected the GRI3.0 and CalTech2.3 mechanisms [32] as depicted in Fig. 3. In comparison, the values from experimental data of Jahn [3] are trending close to calculations using the GRI3.0 mechanism towards increasing

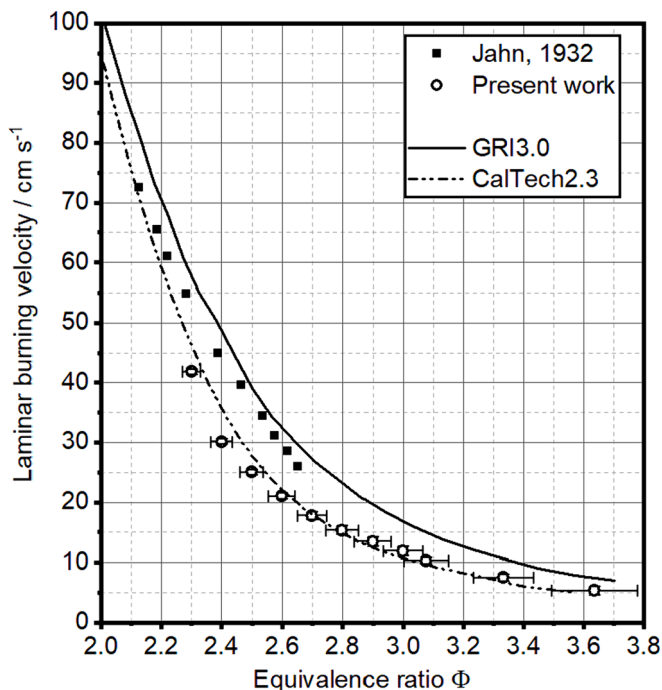


Fig. 3. Comparison of numerical and experimentally determined laminar burning velocities of pure fuel-rich $\text{CH}_4\text{-O}_2$ -flames at $T = 300$ K.

equivalence ratio and close to the CalTech2.3 towards decreasing equivalence ratio. The data from Jahn [3] exhibit favourable agreement with the CalTech2.3 mechanism, particularly at low equivalence ratios (Φ). For Φ values greater than 2.65, there is a gap in the literature data. However, our present work offers a valuable extension to the validation range, revealing excellent agreement of the CalTech2.3 mechanism with the experimental data for Φ values above 2.65. Based on these findings mechanisms in the lower value range of laminar burning velocity (as seen in Fig. 2) are qualified for the further step of investigation. Several research groups have indicated the Curran mechanism to perform well in terms of main species profiles for such flames [16,19]. In contrast, this mechanism did not provide a suitable prediction for the laminar burning velocity.

A sensitivity analysis on laminar burning velocity for rich CH_4/O_2 mixtures at different equivalence ratios using GRI3.0 and Caltech2.3 are shown in Fig. 4 and Fig. 5, respectively. The most promoting reaction on the laminar burning velocity is the radical chain branching reaction $\text{H} + \text{O}_2 = \text{O} + \text{OH}$, followed by the oxidation of ethyleneyel via $\text{C}_2\text{H}_3 + \text{O}_2 = \text{CH}_2\text{CHO} + \text{O}$ and acetylene via $\text{C}_2\text{H}_2 + \text{O} = \text{HCCO} + \text{H}$. In general, the influence of the oxidation reactions decreases as the the equivalence ratio increases. The decomposition of methane has a strongly inhibiting effect on the laminar burning velocity show via $\text{CH}_4 + \text{H} = \text{CH}_3 + \text{H}_2$, $\text{CH}_4 + \text{OH} = \text{CH}_3 + \text{H}_2\text{O}$ and via $\text{CH}_3(+\text{M}) + \text{H} = \text{CH}_4(+\text{M})$. These results are consistent with [10] for fuel-rich CH_4/O_2 flames.

The formation of higher hydrocarbons, especially C_2 -species, is inhibited. The reaction $2\text{CH}_3(+\text{M}) = \text{C}_2\text{H}_6(+\text{M})$ shows a strong effect and the reaction $\text{C}_2\text{H}_2(+\text{M}) + \text{H} = \text{C}_2\text{H}_3(+\text{M})$ less pronounced one, but both increase with increasing the equivalence ratio. The analysis indicates that the formation pathway to higher hydrocarbons, especially the C_2 -chemistry, plays, as expectable a significant role on the laminar burning velocity of rich $\text{CH}_4\text{-O}_2$ flames.

Dubey et al. [39] reported about large discrepancy of the prediction of C_2 -species in fuel-rich premixed CH_4/air weak flames using different reaction mechanism. They stated that the reactions of the CH_3 radical is one of the most important species in the formation and consumption of higher hydrocarbons. Our analysis indicates that the formation pathway to higher hydrocarbons, especially the C_2 -chemistry, plays a significant role on the laminar burning velocity of rich $\text{CH}_4\text{-O}_2$ flames, which explain the large discrepancy of the calculated laminar burning velocities shown in Fig. 2.

b) Flame structure analysis

We examined the structure of burner-stabilized laminar premixed flames by comparing species mole fractions at different heights above the burner for three specific equivalence ratios: $\Phi = 3.08$, $\Phi = 3.33$ and $\Phi = 3.64$. Our reference data were extracted from the research of Li et al.

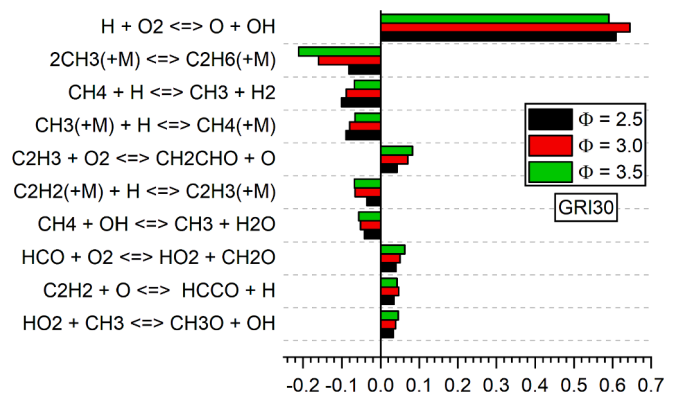


Fig. 4. Sensitivity analysis on laminar burning velocity for rich CH_4/O_2 mixtures at different equivalence ratios using GRI3.0 (300 K, 1 atm).

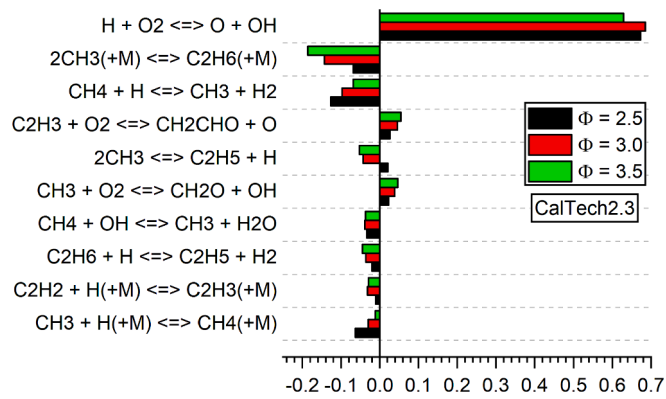


Fig. 5. Sensitivity analysis on laminar burning velocity for rich CH_4/O_2 mixtures at different equivalence ratios using CalTech2.3 (300 K, 1 atm).

[16]. The analyzed species encompassed methane as the primary fuel, water and carbon dioxide as complete combustion products, hydrogen and carbon monoxide as principal products of partial oxidation (POX), and acetylene as an intermediate species. Li et al. [16] indicate a 10 % uncertainty in their measurements of the major species.

For the purpose of our evaluation, we utilized the CalTech2.3 and Leeds1.5 mechanism. These mechanisms were selected due to their consistent correlation with a lower laminar burning velocity (as illustrated in Fig. 2), which was further validated through comparison with experimental data shown in Fig. 3. An additional comparison with the GRI3.0, Curran, and Wang-Frenklach mechanisms can be found in [16], where the Curran mechanism exhibited superior performance.

Fig. 6 and Fig. 7 showcase the comparison between calculated (with Leeds1.5 and CalTech2.3) and experimentally obtained species mole fractions at various heights above the burner for an equivalence ratio of $\Phi = 3.33$. It should be noted that the hot mixture is not yet in equilibrium at this height above the burner and synthesis gas is still formed. It is evident that the Leeds 1.5 mechanism accurately predicts methane but

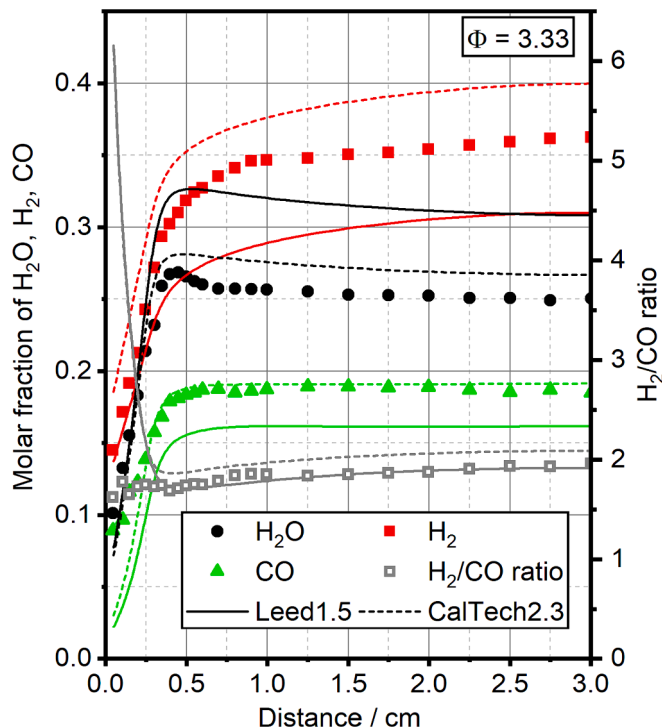


Fig. 6. Comparison of species profiles between experimental results [16] and Leeds1.5 and CalTech2.3 at $\Phi = 3.33$ and inlet temperature of $T = 300$ K.

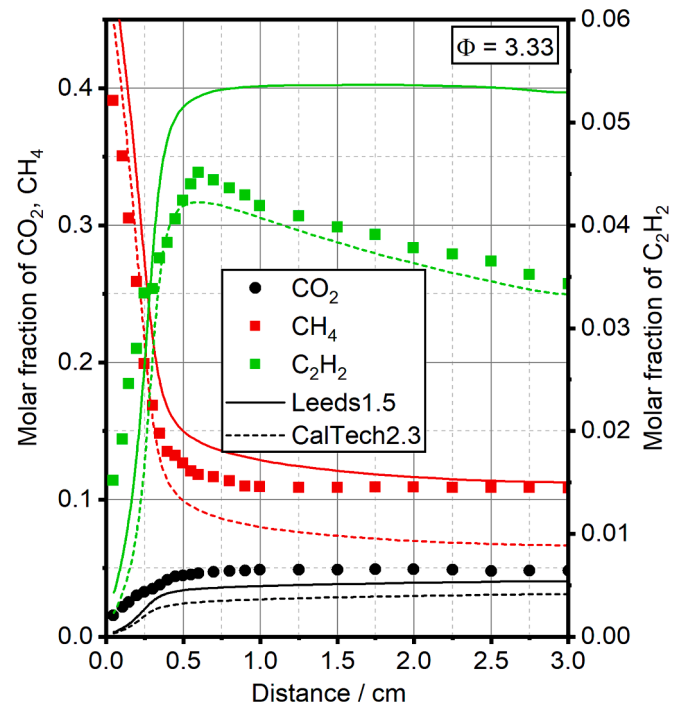


Fig. 7. Comparison of species profiles between experimental results [16] and Leeds 1.5 and CalTech2.3 at $\Phi = 3.33$ and inlet temperature of $T = 300$ K.

falls short in reproducing the formation of H_2 and H_2O .

The CalTech2.3 mechanism demonstrates better agreement for H_2O and CO and less for H_2 , CH_4 and CO_2 . Interestingly, the intermediate species C_2H_2 exhibits excellent agreement. It should be noted that in all cases (experiments and simulation) the sum of the species presented is almost 99 % behind the flame front, with the remainder being assumed to be higher hydrocarbons. This trend persists for equivalence ratios of $\Phi = 3.08$ (see Fig. S2 and Fig. S3) and $\Phi = 3.64$ (see Fig. S4 and Fig. S5) for both mechanisms.

While the context of this study is on the specific products of T-POX processes of methane as higher hydrocarbons and synthesis gas. The CalTech2.3 mechanism has been assessed to be the most accurate among the investigated mechanisms in terms of laminar burning velocity. Deviations of the main species were found in both calculations; however, in this case the Leeds1.5 mechanism predicts the H_2/CO -ratio in excellent agreement.

c) Effect of Preheating on laminar burning velocity

In the subsequent step, we evaluated the laminar burning velocities of fuel-rich methane-oxygen mixtures across a range of equivalence ratios, spanning from $\Phi = 2.38$ to $\Phi = 3.63$, while also varying the preheating temperatures from $T = 300$ K to $T = 455$ K. As anticipated, the introduction of preheating resulted in higher laminar burning velocities. Notably, elevating the preheating temperature from 300 K to 455 K led to a significant boost in laminar burning velocities, reaching approximately a 200 % increase.

To examine the temperature dependency of s_L for fuel rich methane oxygen mixtures, we calculated the coefficient α in the power law correlation $s_L = s_{L,0}(T/T_0)^\alpha$ [40,41] using data obtained from the Heat Flux Method (HFM). This analysis incorporated results from five measurement series, with only three of them displayed in Fig. 8, covering a range of preheating temperatures from 300 K to 455 K. Additionally, we utilized the CalTech2.3 calculations for comparison.

Our findings revealed that the resulting coefficient α remains nearly constant within the confidence interval of the measured data, with a mean value of $\alpha = 1.57$. This consistency held true for the investigated

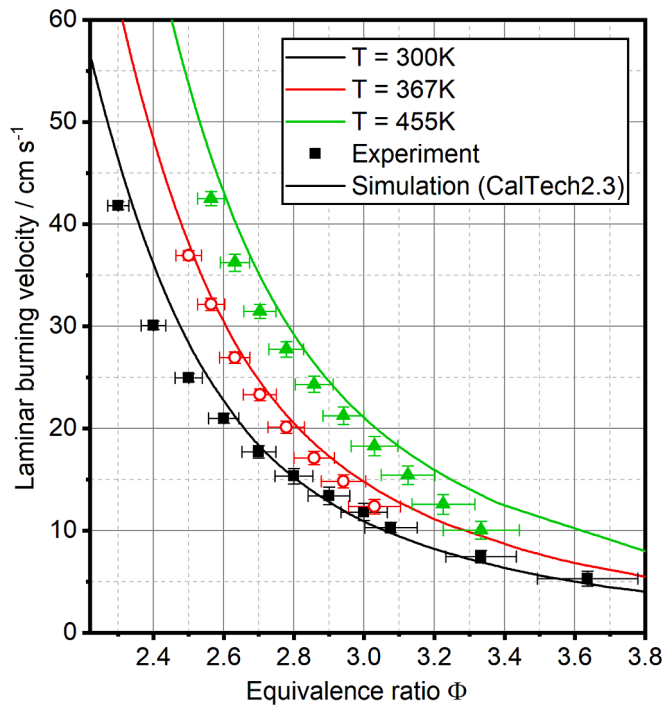


Fig. 8. Laminar burning velocities of pure fuel-rich $\text{CH}_4\text{-O}_2$ -flames at different preheating temperatures.

range of equivalence ratios and preheating temperatures, as visually depicted in Fig. 9. Remarkably, these results exhibited exceptional agreement with the calculations using the CalTech2.3 mechanism, which yielded a coefficient of $\alpha = 1.55$.

d) Effect of Argon-dilution on laminar burning velocity

The experimentally determined laminar burning velocities with

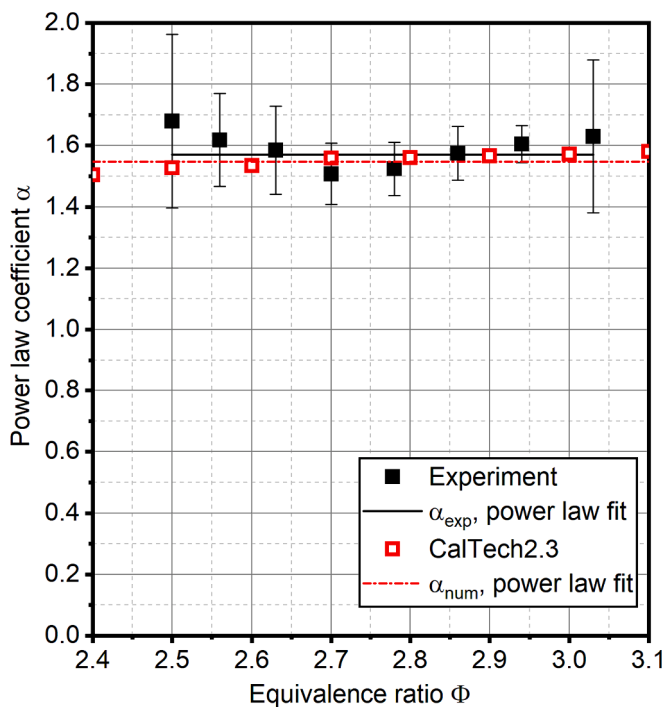


Fig. 9. Determined power law coefficients α for investigated equivalence ratios.

argon dilution are illustrated in Fig. 10. When the oxygen content is reduced from 100 % O_2 to 40 % (molar-based), it results in a notable reduction in the laminar burning velocity, approximately 50 % in value.

For the sake of comparison, we conducted numerical simulations employing the CalTech2.3 mechanism with varying O_2 content in the oxidizer, specifically 40 %, 70 %, and 100 % (indicated by the thicker lines). Notably, when high dilution ratios were employed, the mechanism consistently underestimated the laminar burning velocity, while demonstrating excellent agreement in more fuel-rich oxy-fuel mixtures. Naturally, the laminar burning velocity decreases as the Ar-dilution increases. A comprehensive representation of the results from all the conducted experiments with different Ar-dilutions can be found in Figure S6.

5. Conclusions

In the presented study, we conducted experimental and numerical investigations on the laminar burning velocities of rich methane-oxy-fuel flames at high equivalence ratios and various preheating temperatures. Our findings revealed lower laminar burning velocities than those reported by Jahn [3] in 1932. When we compared the results from calculations using 13 different reaction mechanisms, we observed a wide range of variations in the predicted laminar burning velocities, consistently demonstrating a trend of over-predicting the experimental results.

Notably, the CalTech2.3 mechanism outperformed the others in calculating the laminar burning velocity s_L under the specified conditions of fuel-rich oxy-fuel combustion. A sensitivity analysis of the laminar burning velocity showed the importance of the C_2 -chemistry. Analysis of burner-stabilised flames showed that both the CalTech2.3 and Leeds1.5 mechanisms do not accurately reproduce all the main species in the flame structure. However, the CalTech2.3 mechanism accurately predicts acetylene, especially in fuel-rich oxyfuel flames.

With respect to the influence of preheating temperature on s_L in fuel-rich methane-oxygen flames, our results consistently demonstrated an approximately constant power-law coefficient, $\alpha = 1.57$. However, it is

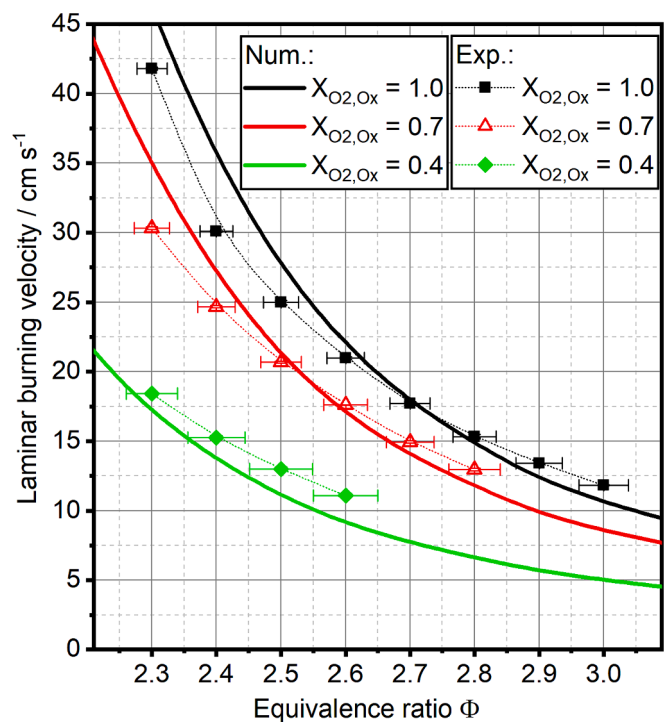


Fig. 10. Calculated and measured laminar burning velocities of fuel-rich methane-argon-oxygen mixtures at $T = 300 \text{ K}$.

important to note that the CalTech2.3 mechanism exhibited a more favorable agreement for lower equivalence ratios compared to higher ones in all cases, including those involving preheating and oxidizer dilution.

CRedit authorship contribution statement

Christof Weis: Writing – review & editing, Writing – original draft, Investigation, Conceptualization. **Matthias Martin Sentko:** Writing – original draft, Visualization, Investigation, Conceptualization. **Björn Stelzner:** Writing – review & editing, Writing – original draft, Visualization, Conceptualization. **Peter Habisreuther:** Writing – review & editing, Writing – original draft, Visualization, Validation, Conceptualization. **Nikolaos Zarzalis:** Writing – review & editing, Supervision, Funding acquisition, Conceptualization. **Dimosthenis Trimis:** Writing – review & editing, Supervision, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.fuel.2024.131601>.

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