https://doi.org/10.1007/s11630-022-1621-x

Measurements of Laminar Burning Velocities of Alternative Fuels: Application in Transport and Aerospace

RICHTER Sandra^{*}, BRAUN-UNKHOFF Marina, NAUMANN Clemens

German Aerospace Center (DLR), Institute of Combustion Technology, Department of Chemical Kinetics and Analytics, Stuttgart 70569, Germany

© The Author(s) 2022

Abstract: The laminar burning velocity belongs to the fundamental combustion properties of fuels being a measure for their heat release, flame length, as well as reactivity and combustion stability, and thus, may impact the design of burners and combustion chambers. Also, these experimental data are needed for the validation and optimization within the construction and development of detailed chemical kinetic reaction mechanisms. Within this study, an overview of the different applications of fuel characterization regarding the specific area of interest (road transport, aviation, and aerospace) will be given. Depending on the application, effects of different molecular characteristics on the laminar burning velocity are evaluated: the presence of oxygen atoms and the grade of branching in a specific fuel molecule as well as the difference in the type of a chemical bond, here, single and double bonds. Examples of alternative fuels being discussed in the present study are: (I) oxymethylene ether (OME_n) in the field of road transport; (II) a paraffinic Alcohol-to-Jet fuel as sustainable aviation fuel; and (III) mixtures of ethane or ethene with nitrous oxide as green propellants for rocket propulsion applications.

Keywords: laminar burning velocity, alternative sustainable fuels, road transport, aviation fuels, green propellants

1. Introduction

The use of alternative and renewable advanced fuels is attracting much interest, to counteract climate change arising due to the burning of fossil fuels. To achieve carbon-neutrality till 2050, efforts are essential within all sectors, industrial and chemical production processes, energy supply in general including heating, with the mobility sector turned out to be a very demanding one. This accounts for all fields of transport: Road transport [1], aviation [2], and maritime shipping [3, 4]. Even in the area of space flight alternative fuels are considered as so called "green propellants".

To evaluate the performance and compatibility of any alternative fuels, information about their physical and thermo-chemical properties are necessary. Here, the laminar burning velocity (LBV) belongs to the fundamental combustion properties of fuels being a measure for their heat release, flame length as well as reactivity and combustion stability, and thus, may impact the design of burners and combustion chambers. Furthermore, the knowledge of the values of the laminar burning velocity of a molecule is needed for the numerical calculation of the values of the turbulent flame speed having a higher relevance for technical combustion processes. For the development of reaction mechanisms,

Corresponding author: RICHTER Sandra

Article Type: Contributed by The 3rd International Discussion meeting on Chemistry and Technology of Combustion Application GE: TIAN Zhenyu Received: Sep 14, 2021

these experimental data are needed for validation and optimization.

Depending on the area of interest, this work gives an overview about different kinds of renewable fuels, i.e., fuels not produced from fossil feedstocks, being studied at the same experimental conditions using the cone angle method. In order to build a data base suitable for the validation and further optimization of kinetic reaction mechanisms, the measurements were performed for equivalence ratios as wide as possible, fuel-lean and fuel-rich. In the field of road transport, oxygenated fuels are currently in the focus due to their potential to reduce not only the carbon dioxide (CO_2) emission but also the emission of harmful exhaust gas components like particulate matter (soot). In the recent years, oxymethylene ethers (OME_n) have attracted major interest, e.g. Refs. [1, 5-9] besides other oxygenated components like alcohols.

The reduction of soot emissions is also playing a major role in the research of alternative jet fuels. However, oxygenated components are not allowed according to the worldwide specification in force due to their risk of a lower storage stability; thus, consequently, fuels such as OME_n, alcohols, and further oxygen-atoms containing fuels are not allowed to serve as sustainable aviation fuels (SAF). Here, in the aviation sector, the remedy is to use paraffinic jet fuels to reduce the formation of soot precursor. In this study, as an example, an AtJ-SPK (Alcohol-to-Jet Synthetic Paraffinic Kerosene) will be discussed being already approved for the use as drop-in fuel to Jet A-1 up to an admixture of 50 vol% according to ASTM D7566 [10].

The research of alternative fuels in the space sector is mainly driven by the efforts to replace the highly toxic hydrazine and hydrazine derivatives as rocket propellants. Here, the reaction systems of ethane + nitrous oxide $(C_2H_6 + N_2O)$ and ethene + nitrous oxide $(C_2H_4 + N_2O)$ are of interest as green propellants.

2. Experimental Measurement of the Laminar Burning Velocity

The laminar burning velocities (LBV, symbol: S_u) of different premixed flames were measured by the use of a Bunsen burner and with the application of the cone angle method [11, 12]. The experiments were conducted at atmospheric (p=0.1 MPa) as well as at elevated pressures with p=0.3 MPa and p=0.6 MPa while the preheat temperature of T=200°C (473 K) was kept constant. The fuel-air equivalence ratio (φ) was varied during the measurements for each fuel and at each pressure. Depending on the fuel and the pressure, the possible φ range was adjusted at the fuel lean as well as at the fuel rich side with a limit for fuel lean mixtures between φ =0.5 and φ =0.8. The stabilization of fuel rich flames was possible in the range from φ =1.5 up to φ =2.0.

The previous studies, where this method was used for the measurements, comprise different kinds of fuels including oxygenated fuels [13–16] and alternative aviation fuels [17–20] as well as gaseous fuels [21, 22].

2.1 Measurement of liquid fuels

A scheme of the experimental set-up for the measurement of liquid fuels is presented in Fig. 1. The different types of fuels considered within this study are listed in Table 1. First, the fuel is vaporized at a temperature depending on the (final) boiling point of the fuel at the considered pressure. The vaporizer is fed with the fuel using an HPLC pump of type LC-20AD (Shimadzu) having a flow rate accuracy of $\pm 1\%$ and a precision of $\pm 0.3\%$. To avoid fractionation during the vaporization of fuel mixtures due to the different

 Table 1
 Overview of the measured liquid fuels and fuel components used for surrogate preparation

Fuels / Fuel Components		Purity	Supplier
n-Butanol		\geq 99.00%	AppliChem
OME1		99.00%	Sigma-Aldrich
OME ₄		98.25%	ASG
	Diesel Surrogate		
50% (molecule fraction)	n-Dodecane	\geq 99.00%	Sigma-Aldrich
30% (molecule fraction)	Farnesane (2,6,10-trimethyldodecane)	\geq 98.00%	Sigma-Aldrich
20% (molecule fraction)	1-Methylnaphthalene	\geq 94.00%	Merck
	Primary Reference Fuel 90 (PRF9	90)	
90 vol%	iso-Octane	≥ 99.80%	Merck
10 vol%	<i>n</i> -Heptane	$\geq 99.00\%$	Merck
Alcohol-to-Jet Synthetic Paraffinic Kerosene (AtJ-SPK)		not applicable	Gevo
Jet A-1		not applicable	*

*The used Jet A-1 was delivered within former projects [23, 24]

RICHTER Sandra et al. Measurements of Laminar Burning Velocities of Alternative Fuels: Application



Fig. 1 Scheme of the experimental set-up for the measurement of the laminar burning velocity of liquid fuels (neat and mixture) using a conical shaped flame; the temperature of the nitrogen preheating depends on the (final) boiling of the fuel/fuel mixtures but is at least 200°C (473 K); HPLC: high performance liquid chromatography, MFC: mass flow controller, *T*_{B,fuel}: (final) boiling point of the fuel/fuel mixture [13–20]. Reprinted by permission of Elsevier Science from "A combined experimental and modeling study of combustion properties of an isoparaffinic alcohol-to-jet fuel", by Richter et al., Combustion and Flame, Volume 240, Copyright 2022 by The Combustion Institute

molecule sizes, the temperature of the vaporizer is set about 30°C to 40°C higher than the final boiling point. For the preparation of the fuel-air mixture the vaporized fuel is first mixed with nitrogen (N₂, supplied by Linde, purity 99.999%), being preheated according to the temperature of the vaporizer. This fuel-N2 mixture is homogenized and adjusted to the set temperature of T=200°C (473 K). In the second mixing step, oxygen (O₂, supplied by Linde, purity 99.95%), being preheated to the set temperature of 200°C (473 K), is added. Due to the mixing with (I) N₂ and, (II) O₂, the partial pressure of the fuel is reduced resulting in the stabilization of fuels with a high (final) boiling point (and a low vapor pressure) in the gaseous phase at 200°C (473 K). Hence, no condensation occurs when the temperature is reduced from the vaporization temperature to the set temperature of 200°C (473 K). The gas flows of N_2 and O_2 are adjusted according to their ratio in air. Thus, after the second homogenizer, the specific fuel-air mixture for the determination of the LBV is prepared.

For the determination of the LBV applying the cone angle method, stable conical-shaped flames are an inevitable requirement. The premixed flames have been stabilized above a nozzle with the help of a coflow. For fuel rich flames ($\varphi \ge 1.0$) air is used as coflow whereas fuel lean flames ($\varphi \le 1.0$) were stabilized using a mixture of 5%CH₄ + 5%H₂ + 90%N₂ (volume fractions). For fuel rich flames, the air coflow enables the post-combustion of unburned hydrocarbons in the exhaust gas. At fuel lean conditions, excess oxygen occurs in the exhaust gas being converted by the CH₄ and H₂ components of the CH₄/H₂/N₂ coflow. Without the post-combustion, the range of measurable φ values is limited, especially for fuel lean mixtures, due to an increasing quenching distance to the nozzle leading to unstable flames. To make sure that the different coflows did not influence the experimental results, the measurements were performed with an overlap of both coflows around stoichiometric conditions. It was found that the LBV data measured within this overlap range were in accordance with the experimental uncertainties.

For the experimental determined LBV data of liquid fuels, the uncertainties range from 2 cm/s to 5 cm/s resulting from the law of error propagation. Mainly due to the difficult flame stabilization and the determination of the cone angle, the highest uncertainty values were found for the measurements at elevated pressures and for fuel rich mixtures. The resulting relative uncertainties are in the range from 3% to 6% for most of the experimental data with up to 10% for some single points at ambient pressure and up to 14% at elevated pressures, respectively. Besides the flame stabilization and cone angle determination, the precision of the measurements are also influenced by fluctuations of the pressure and the temperature as well as by the accuracy of the mass flow controllers (for more information see Refs. [13–20]).

2.2 Measurement of gaseous fuels

As shown in Fig. 2 [21, 22], the set-up for the measurement of gaseous fuels is similar to the set-up used for liquid fuels. The main difference belongs to the mixture preparation because for gaseous fuels, vaporization or preheating is not required. Furthermore, the temperature of the nozzle was monitored at the tip during the measurements of the ethane (C_2H_6) / ethene (C_2H_4) + nitrous oxide (N₂O) reaction system using a type K thermocouple showing that the set temperature of 473 K varies only in a range of ±5 K. The burning gases as listed in Table 2 were delivered by Linde AG.



Fig. 2 Scheme of the experimental set-up for the measurement of the laminar burning velocity of gaseous fuels using a conical shaped flame [21, 22]. Here, the mixture preparation for the reaction systems ethane (C₂H₆) or ethene (C₂H₄) + nitrous oxide (N₂O) with dilution of nitrogen (N₂) is shown

2.3 Determination of the laminar burning velocity from the cone angle

The cone angle detection was performed at every measurement by recording pictures with a CCD-camera from LaVision of the type Imager Intense at the liquid burner system and Imager pro at the gaseous burner system, respectively. The laminar burning velocity (S_u) is calculated from the cone angle (α) of the flame and the gas velocity (v_u) of the unburned fuel-air mixture according to the relation $S_u=v_u \cdot \sin \alpha$ [11, 12] and Fig. 3. In the ideal case, the cone angle has a value of about 40°.



Fig. 3 Relation between the cone angle α , the velocity v_u of the unburned gas, and the laminar burning velocity S_u [13–20]. Reprinted by permission of Elsevier Science from 'A combined experimental and modeling study of combustion properties of an isoparaffinic alcohol-to-jet fuel', by Richter et al., Combustion and Flame, Volume 240, Copyright 2022 by The Combustion Institute [20].

To achieve a better flame stabilization for fuel rich flames, in particular for $\varphi \ge 1.7$, this angle is reduced with increasing φ values to 30° whereas for fuel lean flames ($\varphi \le 0.7$) the cone angle is increased to 55°.

3. Road Transport Fuels

3.1 Oxymethylene ethers

In road transport, oxymethylene ethers (OME_n: H₃CO(H₂CO)_nCH₃) are of interest as alternative fuel compounds for diesel engines due to several reasons: (I) They show nearly no soot formation [5] compared to the conventional as well as other oxygenated fuels like alcohols or conventional biodiesel since they contain no C-C bonds (as example, the molecular structures of OME₁ and OME₄ are shown in Fig. 4). Thus, with the use of OME_n as a blending component to a diesel fuel a distinct reduction of the soot emissions can be achieved. Moreover, this enables also the reduction of the emissions of nitrogen oxides (NO_x) due to the possible escape from the trade-off in the exhaust gas treatment between soot and NO_x . (II) The Power-to-Liquid (PtL) process can be applied for the production of OME_n . Besides the use of renewable energies also biomass, being converted in a gasification or fermentation processes, is a possible resource. (III) OME_n are fully miscible with a conventional diesel fuel. Especially OME_n with $n \ge 2$ comply with some required properties of a diesel fuel: According to the standard EN 590 [25] the upper limit of the boiling range of conventional diesel fuels is 360° C (633 K). The OME_n are conform with this

limit since their boiling temperatures ranges from 105° C (378 K) for OME₂ to 280°C (553 K) for OME₅ [1]. With the cetane number (CN) as a measure for the ignition, the admixture of higher OME_n can improve the ignition behavior of a diesel fuel, requiring a minimum CN of 51 [25]. The cetane numbers of OME_n increase from OME₂ to OME₅ with CN=63 for OME₂ and CN=100 for OME₅ [1].

Besides the fuel properties, also the compatibility with current engine technologies and materials has to be considered. Here, it is foreseeable that modifications of the engine and the sealing material are necessary for the use of diesel-OME_n blends as studied by Omari et al. [5] and Pélerin et al. [6].

So far, there are only a few studies available in the literature focusing on the combustion properties of higher OME_n ($n\geq 2$). Regarding the LBV, Sun et al. [7] have measured OME₃ at 1 atm (0.101 325 MPa) and 135°C (408 K) and OME₂ were measured by Eckart et al. [8] as well as by Ngugi et al. (2021) [15] at various temperatures and pressures. Considering OME₁, more studies about the combustion properties are available. An overview is given by Ngugi et al. (2020) [14] as well as by Fenard and Vanhove [9]. To gain more information about these fundamental combustion characteristics, the LBV measurements of OME₁ and OME₄ were presented in this work. The results are compared with data for PRF90 and *n*-butanol in the case of OME₄ [16].

$$OME_{1} H_{3}C \xrightarrow{O} CH_{2} CH_{3}$$
$$OME_{4} H_{3}C \xrightarrow{O} CH_{2} CH_{2} CH_{2} CH_{2} CH_{2} CH_{2} CH_{2} CH_{3}$$



3.2 Laminar burning velocities of oxymethylene ethers

The results of the measured laminar burning velocities of OME₁ and OME₄ are shown in Fig. 5. Considering OME₄, the measurements are compared with a diesel surrogate and a mixture of diesel surrogate + 30 wt% OME₄ (Fig. 5(a)) at pressures of 0.1 MPa, 0.3 MPa, and 0.6 MPa. For the sake of a better clarity, the comparison of OME₁ to *n*-butanol and PRF90 are only shown for 0.1 MPa and 0.6 MPa.

The diesel surrogate used for the comparison with OME₄ as well as the base fuel for the mixture consists of 50%n-dodecane + 30%farnesane (2,6,10-trimethyldodeca ne) + 20%1-methylnaphthalene (molecule fraction). The composition of the surrogate was chosen in order to mirror major physical properties of a typical diesel fuel. For the neat surrogate, the maximum LBV at 0.1 MPa is located at $\varphi=1.1$ with $S_u=83$ cm/s (± 2 cm/s). In contrast, for OME4 was a distinct higher LBV obtained with a maximum of $S_u = 108 \text{ cm/s} (\pm 5 \text{ cm/s})$ and a shift of the corresponding φ value to φ =1.2. The maximum of the LBV follows the maximum of the adiabatic flame temperature. It is assumed that the maximum LBV for OME_n at about $\varphi = 1.2$ is caused by the formed reactions products being different to the reaction products of hydrocarbons. This could be a result from both the oxygen content within the OME_n molecules as well as the fact that no C-C bonds occur in OME_n molecules.

The maximum LBV of the mixture diesel surrogate + 30 wt%OME₄ is located at φ =1.1 as well and shows only a slight increase by about 4 cm/s to 87 cm/s (±2 cm/s) compared to the pure diesel surrogate. At elevated pressures, similar results were obtained regarding the comparison of the different fuels (see Fig. 5) with lower values being measured for the LBV [16].



Fig. 5 Results of the measured laminar burning velocities of road transport fuels in mixture with air: (I) OME₄ in comparison with a diesel surrogate (= 50%n-dodecane + 30%farnesane (2,6,10-trimethyldodecane) + 20%1-methylnaphthalene (molecule fraction)) and a mixture of the diesel surrogate + 30 wt%OME₄ (a) [16], and (II) OME₁ in comparison with PRF90 and *n*-butanol (b) [14].

Regarding the comparison of OME₁ to PRF90 (Fig. 5(b)) similar results were obtained as for OME₄ and the diesel surrogate. In detail, the maximum of OME₁ is located at φ =1.2 with S_u =103.1 cm/s at 0.1 MPa and with S_u =64.8 cm/s at 0.6 MPa. For PRF90, the maximum LBV amount to S_u =80 cm/s at 0.1 MPa and to S_u =51 cm/s at 0.6 MPa, each at φ =1.1. Interestingly, the values of the LBV of *n*-butanol are for the most conditions between the values of OME₁ and PRF90, with the peak value at φ =1.1 and S_u =91 cm/s at 0.1 MPa and S_u =59 cm/s at 0.6 MPa [14].

The results for the LBV measurements of OME_1 and OME_4 in comparison to other fuels show that the amount of oxygen in fuel molecules is of high importance leading to an increased LBV and therefore to a higher reactivity as well.

4. Aviation Fuels

4.1 Alcohol-to-Jet Synthetic Paraffinic Kerosene

Currently, Alcohol-to-Jet Synthetic Paraffinic Kerosene (AtJ-SPK) is one of the few certified sustainable aviation fuels (SAF) being produced in industrial scale and applied in regular flights. As defined within international standard ASTM D7566 [10] the usage is allowed in blends with fossil Jet A-1 up to 50 vol%. The production AtJ-SPK based on iso-butanol originating from a well-established fermentation process [26]. As displayed by the gas chromatograms (GC) in Fig. 6(b) it consists mainly of the two highly branched 2,2,4,6,6-pentamethyl heptane (*i*-C₁₂H₂₆, iso-alkanes iso-dodecane) and 2,2,4,4,6,8,8-heptamethyl nonane (i-C₁₆H₃₄, iso-cetane). In this fuel the percentages of the components amount to 83% for iso-dodecane and to 17% for iso-cetane (molecule fraction) [20]. In Fig. 6, also the gas chromatogram of a Jet A-1 fuel is presented showing that a conventional jet fuel, i.e., stemming from fossil crude oil, is a multi-component mixture with many linear *n*-paraffins as main component. Other structures include iso-paraffins and aromatics. The group of aromatics play

an important role in the formation of polyaromatic hydrocarbons and of particulate matter and thus, in the emission pattern in the exhaust gas since they act as precursors for soot particles [17, 27]. The reduction of the number of aromatics in a jet fuel is a promising strategy aiming at the reduction of soot emissions. Besides the market launch of carbon neutral fuels, this is the main motivation in the development of SAF.

4.2 Laminar burning velocities of AtJ-SPK

The results of the measured LBVs of AtJ-SPK are given in Fig. 7(a), in comparison to measurements of Jet A-1. The peak values of the LBVs of AtJ-SPK are located at $\varphi=1.05$ to 1.1, depending on pressure, with 78.4 cm/s at p=0.1 MPa, 63.3 cm/s at p=0.3 MPa, and 51.0 cm/s at p=0.6 MPa. According to the results, Jet A-1 has a slightly higher LBV, especially at fuel rich mixtures with a difference to AtJ-SPK of about 2 cm/s at φ =1.05 which increases to about 8 cm/s between $\varphi = 1.25$ and φ =1.45. Hence, although AtJ-SPK and Jet A-1 contain different fuel molecules regarding amount and size of the specific components (see Fig. 6), the measured LBVs exhibit only small differences [18, 20]. From these results, a systematic trend to smaller LBV values for AtJ-SPK emerges, being caused by the highly branched structure of the AtJ-SPK molecules: It is generally known that linear (fuel) molecules have a higher reactivity and lead therefore to higher LBV values than in the case of branched (fuel) molecules [28]. Regarding AtJ-SPK, mainly the occurrence of the tert-butyl radical during the oxidation process governs the reactivity and magnitude of the specific combustion properties [20]. Since conventional jet fuels contain mainly n-paraffins (see Fig. 6), the β -scission leads mainly to the formation of primary or secondary radicals being less stable than the tertiary tert-butyl radical.

Similar results were obtained for the comparison of the LBVs of iso-octane and n-dodecane as presented in Fig. 7(b). These fuel components were measured using the same experimental set-up at an initial preheat



Fig. 6 Gas chromatogram of Alcohol-to-Jet Synthetic Paraffinic Kerosene (AtJ-SPK) (b) compared to Jet A-1 (a)

temperature of 200°C (473 K) at p=0.1 MPa. Here, the peak value of iso-octane is located at $\varphi = 1.05$ with $S_u = 74.8 \text{ cm/s}$ whereas the one of *n*-dodecane is higher, by about 10 cm/s [27]. The results are further compared to literature data from Kumar and Sung [29], Kumar et al. [30], and Galmiche et al. [31] confirming the expected difference between the branched iso-octane and the linear n-dodecane. The difference between the data, being observed especially in the fuel rich regime ($\phi > 1.0$), may partially be caused by the different methods used for the measurements. In the studies from Kumar and Sung [29] and Kumar et al. [30] the counterflow method was applied leading to slightly higher values for the LBV. In contrast, Galmiche et al. [31] have used a spherical flame vielding lower LBV values for stoichiometric and fuel rich mixtures. Interestingly, for both methods being used a correction of the stretch effect was done; however, this is not possible for LBV measurements using the cone angle method as shown in the present work. But



Fig. 7 Results of the measured laminar burning velocities of jet fuels and components in mixtures with air: (I) Alcohol-to-Jet Synthetic Paraffinic Kerosene (AtJ-SPK) in comparison with Jet A-1 (a) [18, 20], and (II) *n*-dodecane and iso-octane with comparison to literature data from Kumar and Sung [29], Kumar et al. [30], and Galmiche et al. [31] (b) [27].

nevertheless, this does not lead to inaccurate results as the results from Kumar et al. [30] and Galmiche et al. [31] differ as well. Hence, LBV data obtained from measurements using the cone angle method are in the overall uncertainty range of the LBV data.

5. Fuels for Aerospace - Space Flights

5.1 Green propellants

As green propellants for application in space, ethane-nitrous oxide $(C_2H_6 + N_2O)$ or ethene-nitrous oxide (C₂H₄ + N₂O) mixtures are considered to replace the highly toxic and carcinogenic hydrazine including its derivatives as a consequence of the REACH regulative [33]. Their high long-term stabilities as well as their high specific impulse are required and advantageous properties for propellants. Hence, in spite of their toxicity, hydrazines are still used in different propulsion applications, e.g. in attitude control systems for satellites where the propellant is only occasionally used [32]. As hydrazine and its derivatives were defined as "substances of very high concern" in 2011 by the framework legislation of the European Commission for the Registration, Evaluation, Authorization and Restriction of Chemicals (REACH) [33], it is expected that their use will be restricted and become expensive as well as impractical. To cope with this challenge, so-called green propellants [34, 35] were investigated as possible alternatives for hydrazine within the DLR Future Fuels initiative. In detail, the study has focused on hydrocarbon-nitrous oxide mixtures due to several reasons: (I) these mixtures are less or even non-toxic; (II) they have a similar high specific impulse, and (III) they are cost-efficient. On the other hand, the reaction systems of hydrocarbon-nitrous oxide mixtures, being only usable as premixed propulsion systems, are characterized by higher flame temperatures and an increased risk of flashback. In order to handle and control these disadvantages, a deeper knowledge about the combustion behavior of these mixtures, $C_2H_6 + N_2O$ or $C_2H_4 + N_2O$, respectively is necessary. Therefore, the values of their LBVs were measured in this study-for each reaction system in dilution with 40%, 50%, and 60% nitrogen (N₂) [22].

5.2 Laminar burning velocities of C₂H₆/C₂H₄+N₂O in dilution with N₂

The results of the measured laminar burning velocities are displayed in Fig. 8. When comparing both reaction systems, $C_2H_6 + N_2O$ and $C_2H_4 + N_2O$, a similar dependency on pressure variation and nitrogen dilution is revealed. The main differences are obtained for the height and location of the peak φ value of the LBV. Summarizing all conditions studied, the maxima of the burning velocity for the $C_2H_6 + N_2O$ system ranges from



Fig. 8 Results of the measured laminar burning velocities of the reactions systems C₂H₆+N₂O (a) and C₂H₄+N₂O (b), each diluted with varying percentages of N₂ [22]

 φ =1.05 to φ =1.15 whereas the ones of C₂H₄ + N₂O are shifted to slightly fuel richer mixtures, with a φ range from about 1.15 to 1.25.

Regarding the height of the laminar burning velocities, for the system $C_2H_4 + N_2O$, distinct higher values were obtained than for the $C_2H_6 + N_2O$ system being equivalent to a higher reactivity and a more intense heat release on behalf of the $C_2H_4 + N_2O$ system. These findings were expected due to the double bond existing in the C₂H₄ molecule. The difference between the maxima of both systems is up to about 25 cm/s at p=0.1 MPa with 40% nitrogen dilution. With 60% nitrogen dilution, this difference is reduced to about 10 cm/s. Similar results are obtained comparing the values of the burning velocity at elevated pressures. Considering the range of the peak values for both systems, the difference between 0.1 MPa and 0.3 MPa is about 10 cm/s with 40% nitrogen dilution, and merely 5 cm/s with 60% nitrogen, respectively. Since both parameters: high nitrogen dilution and elevated pressures, lead to lower laminar burning velocities where in general flame stabilization is more difficult, measurements at 0.6 MPa with 60% nitrogen could not be conducted [22].

6. Conclusions

This paper gives an overview of different applications for the measurement of the laminar burning velocity (LBV) in transport (OME_n), aviation (AtJ), and rocket propulsion ($C_2H_{6(4)}+N_2O$) demonstrating that the LBV is a useful tool to obtain valuable information about the combustion behavior and reactivity of liquid as well as gaseous fuels. It is not only a measure for heat release, flame length, and reactivity but also an indicator for the propagation of turbulent flames. Due to this, the information about LBV has an impact on design of burners and combustion chambers; in addition, these data are required as validation data for the development of reaction mechanisms.

With the examples given in the present work, different effects of typical structure characteristics existing in fuel molecules on LBV were investigated. The study on OME_n , being of interest as alternative fuels in road transport, shows the influence of oxygen atoms in the molecular structure leading to higher LBV for highly oxygenated fuels compared to pure hydrocarbons. The comparison of the sustainable aviation fuel AtJ-SPK, consisting of highly branched molecules, to Jet A-1 clearly reveals that branched fuel molecules (iso-alkanes) lead to lower LBVs than fuels containing (mostly) linear molecules. Lastly, the effects of different type of bonds (single and double bond) within a fuel molecule on LBV have been studied, by measuring the green propellant mixtures of $C_2H_6 + N_2O$ and $C_2H_4 + N_2O$ systems showing distinct higher LBV values for the mixture containing a C=C bond (ethene).

Since the measurements of the liquid fuels were performed at the same experimental conditions, i.e., at a preheat temperature of 200°C (473 K) and at pressures of 0.1 MPa, 0.3 MPa, and 0.6 MPa using the same oxidator $(21\%O_2 + 79\%N_2),$ burner and method. all LBV experimentally obtained data are directly comparable. Besides the measurements presented here, even more fuels were measured covering a broad range of fuel molecules from gaseous fuels up to high-boiling fuels with vaporization temperatures up to 400°C (670 K).

Acknowledgment

The authors thank N. Ackermann for the performance of the GC analyses.

References

 Schemme S., Samsun R.C., Peters R., Stolten D., Power-to-fuel as a key to sustainable transport systems – An analysis of diesel fuels produced from CO₂ and renewable electricity. Fuel, 2017, 20: 198-221.

- [2] Richter S., Braun-Unkhoff M., Naumann C., Riedel U., Paths to alternative fuels for aviation. CEAS Aeronautical Journal, 2018, 9(3): 389–403.
- [3] DNV GL, Maritime Forecast to 2050 Energy Outlook 2020, available for download at https://eto.dnv.com/2020/maritime (access on March 08, 2022).
- [4] Lloyd's Register (LR), University Maritime Advisory Services (UMAS), Zero-Emission Vessels 2030. How do we get there? 2017, available for download at https://www.lr.org/en/insights/global-marine-trends-2030/ zero-emission-vessels-2030/ (access on March 08, 2022).
- [5] Omari A., Heuser B., Pischinger S., Rüdinger C., Potential of long-chain oxymethylene ether and oxymethylene ether-diesel blends for ultra-low emission engines. Applied Energy, 2019, 239: 1242–1249.
- [6] Pélerin D., Gaukel K., Härtl M., Jacob E., Wachtmeister G., Potentials to simplify the engine system using the alternative diesel fuels oxymethylene ether OME₁ and OME₃₋₆ on a heavy-duty engine. Fuel, 2020, 259: 116231.
- [7] Sun W., Wang G., Li S., Zhang R., Yang B., Yang J., Li Y., Westbrook C.K., Law C.K., Speciation and the laminar burning velocities of poly (oxymethylene) dimethyl ether 3 (POMDME3) flames, an experimental and modeling study. Proceedings of the Combustion Institute, 2017, 36(1): 1269–1278.
- [8] Eckart S., Cai L., Fritsche C., vom Lehn F., Pitsch H., Krause H., Laminar burning velocities, CO and NO_x emissions of premixed polyoxymethylene dimethyl ether flames. Fuel, 2021, 293: 120321.
- [9] Fenard Y., Vanhove G, A mini-review on the advances in the kinetic understanding of the combustion of linear and cyclic oxymethylene ethers. Energy & Fuels, 2021, 35(18): 14325–14342.
- [10] Standard specification for aviation turbine fuel containing synthesized hydrocarbons. ASTM D7566, available at https://www.astm.org/Standards/D7566.htm (access on March 08, 2022).
- [11] Andrews G, Bradley D., Determination of burning velocities, A critical review. Combustion and Flame, 1972, 18(1): 133–153.
- [12] Eberius H., Kick T., Stabilization of premixed, conical methane flames at high pressure, Berichte der Bunsen-Gesellschaft für physikalische Chemie, 1992, 96(10): 1416–1419.
- [13] Methling T., Richter S., Kathrotia T., Braun-Unkhoff M., Naumann C., Riedel U., An investigation of combustion properties of butanol and its potential for power generation. Journal of Engineering for Gas Turbines and Power, 2018, 140(9): 091505-091505-10, GTP-18-1014.
- [14] Ngugi J.M., Richter S., Braun-Unkhoff M., Naumann C.,

Riedel U., An investigation of fundamental combustion properties of the oxygenated fuels DME and OME₁. Proceedings of the ASME Turbo Expo 2020, virtual, online, 2020, 3: GT2020-14702. DOI: 10.1115/GT2020-14702.

- [15] Ngugi J.M., Richter S., Braun-Unkhoff M., Naumann C., Köhler M., Riedel U., A study on fundamental combustion properties of oxymethylene ether-2. Journal of Engineering for Gas Turbines and Power, 2022, 144(1): 011014.
- [16] Richter S., Kathrotia T., Braun-Unkhoff M., Naumann C., Köhler M., Influence of oxymethylene ethers (OME_n) in mixtures with a diesel surrogate. Energies, 2021, 14(23): 7848.
- [17] Kick T., Herbst J., Kathrotia T., Marquetand J., Braun-Unkhoff M., Naumann C., Riedel U., An experimental and modeling study of burning velocities of possible future synthetic jet fuels. Energy, 2012, 43(1): 111–123.
- [18] Richter S., Naumann C., Riedel U., Experimental study of the combustion properties of an Alcohol-to-Jet fuel. Proc. of 2nd World Congress on Momentum, Het and Mass Transfer, presented at the 2nd International Conference on Combustion Science and Process 2017 (CSP'17), Barcelona, Spain, 2017: CSP 107. DOI: 10.11159/csp17.107. https://avestia.com/MHMT2017_Proceedings/files/list_of papers.html (access on March 08, 2022).
- [19] Richter S., Kathrotia T., Naumann C., Kick T., Slavinskaya N., Braun-Unkhoff M., Riedel U., Experimental and modeling study of farnesane. Fuel, 2018, 215: 22–29.
- [20] Richter S., Kukkadapu G., Westbrook C.K., Braun-Unkhoff M., Naumann C., Köhler M., Riedel U., A combined experimental and modeling study of combustion properties of an isoparaffinic alcohol-to-jet fuel. Combustion and Flame, 2022, 240: 111994.
- [21] Richter S., Ermel J., Kick T., Braun-Unkhoff M., Naumann C., Riedel U., The influence of diluent gases on combustion properties of natural gas, a combined experimental and modeling study. Journal of Engineering for Gas Turbines and Power, 2016, 138(10): 101503-101503-9, GTP-15-1572.
- [22] Richter S., Janzer C., Methling T., Naumann C., Green Propellants for in-space propulsion, experimental and modelling study on the combustion chemistry of ethane/ethene-nitrous oxide mixtures. Proc. of 7th Space Propulsion Conference SP2020+1, virtual, online, 2021, S43: SP202 00524.
- [23] Alfa-BIRD, Alternative Fuels and Biofuels for Aircraft, EUFP7/2007-2013, grant agreement no° 213266; co-ordinator, EU-VRI, (Germany). http://www.alfa-bird.eu-vri.eu (access on March 08,

2022).

- [24] SWAFEA, Sustainable way for alternative fuels and energy for aviation, EU, DG-TREN, final report. http://www.icao.int/environmental-protection/GFAAF/Do cuments/SW_WP9_D.9.1%20Final%20report_released% 20July2011.pdf (access on March 08, 2022).
- [25] Automotive fuels-Diesel-Requirements and test methods. EN 590, German version EN 590,2013+A1, 2017.
- [26] Gevo, Sustainable Aviation Fuel, Whitepaper, 2019, available for download at https://gevo.com/products/sustainable-aviation-fuel (access on March 08, 2022).
- [27] Richter S., Braun-Unkhoff M., Kathrotia T., Naumann C., Kick T., Slavinskaya N., Riedel U., Methods and tools for the characterization of a generic jet fuel. CEAS Aeronautical Journal, 2019, 10(3): 925–935.
- [28] Ranzi E., Frassoldati A., Grana R., Cuoci A., Kelley A.P., Law C.K., Hierarchical and comparative kinetic modeling of laminar flame speeds of hydrocarbon and oxygenated fuels. Progress in Energy and Combustion Science, 2012, 38(4): 468–501.
- [29] Kumar K., Sung C.J., Laminar flame speeds and extinction limits of preheated n-decane/O₂/N₂ and n-dodecane/O₂/N₂ mixtures. Combustion and Flame, 2007, 151(1–2): 209–224.
- [30] Kumar K., Freeh J.E., Sung C.J., Huang Y., Laminar flame speeds of preheated iso-octane/O₂/N₂ and

n-heptane/O₂/N₂ mixtures. Journal of Propulsion and Power, 2007, 23(2): 428–436.

- [31] Galmiche B., Halter F., Foucher F., Effects of high pressure, high temperature and dilution on laminar burning velocities and Markstein lengths of iso-octane/air mixtures. Combustion and Flame, 2012, 159(11): 3286–3299.
- [32] Aggarwal R., Patel I., Sharma P.B., Green propellant, a study. International Journal of Latest Trends in Engineering and Technology, 2015, 6(1): 83–87.
- [33] European Chemicals Agency (ECHA), General Report 2011–The Year of Dissemination, 2012.
- [34] Ciezki H., Zhukov L., Werling L., Kirchberger C., Naumann C., Firess M., Riedel U., Advanced Propellants for Space Propulsion – A Task within the DLR Interdisciplinary Project "Future Fuels". Proc. 8th European Conference for Aeronautics and Space Science, Madrid, Spain, 2019.
 DOI: 10.13009 /EUCASS2019-276.
- [35] Werling L., Hörger T., Manassis K., Grimmeisen D., Wilhelm M., Erdmann C., Ciezki H., Schlechtriem S., Richter S., Methling T., Goos E., Janzer C., Naumann C., Riedel U., Nitrous oxide fuels blends, research on premixed monopropellants at the German Aerospace Center (DLR) since 2014. Proc. AIAA Propulsion and Energy Forum, digital, 2020: AIAA-2020-3807. DOI: 10.2514/6.2020-3807.