

Combustion characteristics of synthetics fuels: Determination of the laminar burning velocity of OME 1

S. Eckart*, C. Krasselt, H. Krause

Institute of Thermal Engineering, TU Bergakademie Freiberg, Freiberg, Germany

Abstract

Oxygenated fuel components are known to reduce soot emissions significantly in diesel engines while having little effect on NO_x emissions. The advantage of C₁-oxygenate dimethoxy methane (OME₁) is the lack of C–C bonds in its molecular structure. This fuel was found to have the strongest effect on the reduction of soot and particle number emissions compared to other oxygenated substances [1]. OME_{1b} also belongs to the group of oxymethyleneethers (OME_n) with the molecular structure CH₃–O–(CH₂–O)_n–CH₃ and $n = 1$ (short molecular structure C₃H₈O₂).

The laminar burning velocity is a fundamental property of a reactive fuel-oxidizer mixture, varying with composition, pressure and initial temperature. These values are important for validation of reaction mechanisms and the specific design of industrial burners. There are several experimental methods to measure laminar burning velocity, e.g. the bunsen flame method, the spherically expanding flame method, the stagnation flame method and the flat flame burner method, which also includes the heat-flux burner method. For a lot of fuels, especially synthetic fuel blends, there is a lack of data for fundamental combustion properties. Therefore, we applied the heat-flux burner method to measure laminar burning velocities of OME₁ within a range of equivalence ratios from 0.6 to 1.9 and initial temperatures of 363 K at atmospheric conditions in comparison with different low calorific and hydrogen containing fuels.

Keywords: burning velocity; synthetic fuel; laminar flame, Oxygenate, Combustion, Emission

1. Introduction

Since the beginning of industrialization, the global consumption of fossil fuels in transport and mobility sector has been steadily increased. However, these resources are limited, so in the future fuels should be provided in an alternative way. For this reason, it is important to use existing resources in an environmentally friendly and effective manner. For a sustainable use of these resources, low-emission and high efficiency combustion systems are a key technology to fulfil the requirements. The European Union's steadily tightening CO₂ limits provide for a total elimination of greenhouse gas emissions from the transport sector by 2050. Therefore, combustion systems based on “green” synthetic liquids and gaseous fuels are more environmentally friendly compared to diesel and petrol fired engines. Furthermore, oxygenated fuels should be addressed to reduce carbon dioxide and soot emissions per unit of energy. OME (oxymethylenether) has repeatedly proven to be an excellent alternative to diesel fuel. Technologies based on these fuels for low pollutant emissions are present, but still have to be established in the market.

In the last few years, bio- and synthetic fuels have displaced a small part of conventional fuels, whereas petrodiesel is still the most common type of diesel fuel. Using bio- and synthetic fuels instead of fossil fuels is relevant due to the adverse health effects, environmental degradation and the impact on global warming caused by fossil fuels in the industrial and mobility sector. Therefore, the commitment to reduce fossil fuel use was reinforced when 195 countries agreed to a limitation of global warming in the Paris agreement (December 2015, Paris climate conference (COP21)). Different fuel properties have been used to interpret the changes in exhaust emissions, such as the oxygen content. The presence of long-chain alkyl esters, which have two oxygen atoms per molecule, is an influential factor that distinguishes bio- and synthetic from conventional fossil fuels. Since the presence of oxygen in fuel can reduce emissions, a low volume of a highly-oxygenated fuel additive can significantly reduce emissions.

The laminar burning velocity of an adiabatic laminar flame s_L is a key physical data for combustion processes and combustion models. It is a fundamental property of reactive fuel-oxidizer mixtures, varying with composition, pressure and initial temperature and therefore very important both for validation of reaction mechanisms and the specific design of combustion systems in general and engines for automotive industry in particular. The laminar burning velocity can be well measured with a heat flux burner which stabilises a flat and quasi-adiabatic flame by compensation of its heat losses. Due to this properties and a nearly unstretched flame shape, this type of burner is currently seen to be among the most accurate ways to determine s_L at atmospheric pressures. In this work, such a heat flux burner was used for the measurement of the adiabatic laminar burning velocity of OME blends in comparison with gaseous/liquid fuels within a range of equivalence ratios varying from 0.7 to 1.9 and initial temperatures of 298 K up to 363 K in atmospheric conditions.

OME is a dimethylether (DME) molecule that includes n numbers of the oxymethylene groups (-O-CH₂-). These oligomeric oxymethylene dimethylethers have different boiling points of 315K, 429K and 474K (for $n=1, 3, 4$) [2]. In this study the emissions of NO_x and soot particle numbers of CO and HC were shown for OME_{1a} and

compared to diesel mixtures. An environmental assessment was done by Deutz et al. [3] showing a dramatic increase of the exergy efficiency along with the reduction of NO_x and soot. These results were also proved by several authors [4, 5, 6]. Comparisons with diesel fuel in terms of freezing point was investigated [7]. Furthermore, it was tested in several test engines [8, 9, 10, 11]. Experimentally Dias et al investigated the effect of dimethoxymethane ($\text{C}_3\text{H}_8\text{O}_2$) or diethoxymethane ($\text{C}_5\text{H}_{12}\text{O}_2$) addition in ethylene flames and there soot formation [12]. Oestreich et al. investigated the reaction kinetic and the equilibrium parameter [13] whereas Sun et al. applied jet-stirred reactor experiments and used them to create a kinetic model [14].

2. Experimental Method

The used heat-flux burner was proposed by de Goey, van Maaren and Quax in 1993 [15] and is based on experimental work of Botha and Spalding in 1954 [16]. The advantage of this method for measuring the laminar burning velocity is the investigation of an unstretched flame under quasi-adiabatic conditions. The stabilization of a planar flame has been further proved by van Maaren et al [17] and could be achieved with a temperature controlled burner plate, which allows for compensation of heat losses from the flame by preheating the unburnt gases. The heat-flux burner setup used at the TU Bergakademie Freiberg (TUBAF) is shown in figure 1. The detailed design of the test rig is described elsewhere [18, 19] including the evaluation of uncertainties and data analysis process. In the following the experimental setup and method used in the present work is briefly outlined.

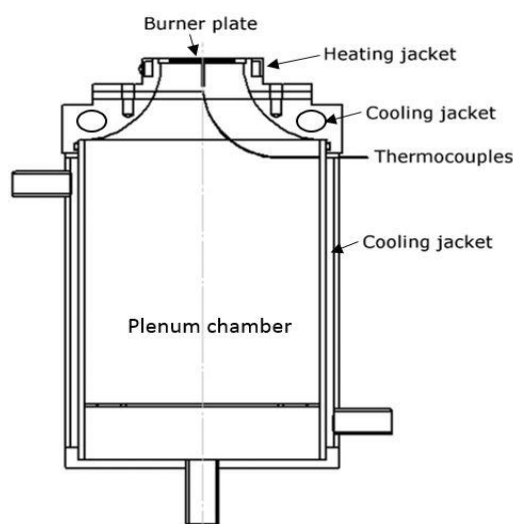


Figure 1 Schematic view of the utilized Heat-Flux burner

At the TU Bergakademie Freiberg the gas flow is controlled by 5 mass flow controllers (MFCs) from Bronkhorst. Before the experimental campaign, the MFC setup was calibrated with a system of type Definer 220, Bios Corp, which corrects the volumetric flow for temperature and pressure. The liquid fuel is stored in a stainless steel tank and pressurized with nitrogen to 5 bar (g). A mass flow controller based on the Coriolis effect (mini-CORI-Flow™, Bronkhorst B.V.), controls the flow of the liquid fuel. The pure liquid, without carrier gas, is vaporized in the direct evaporator. To create a homogenous mixture of the vaporized fuel and air, a specially designed mixing chamber is used. The heat-flux burner test rig was automated by a program based on LabVIEW™ and gives the possibility to control liquid and gas flows. Furthermore, it logs the ambient conditions as well as the signals from the thermocouples and executes the post processing and subsequent computation of the laminar burning velocities. For further details on experimental uncertainties related to gas flows and other possible sources of errors, we refer to Eckart et al. [19].

Educt analysis was performed using a 6-fold determination of an Agilent GC/MS (7890B GC, 5977B MSD) equipped with an Agilent HP-5ms (30 m x 0,25 mm x 0,25 μm) column. The GC oven was remained at 35 °C for 5 min and then heated to 195 °C at a rate of 20 K/min. Helium was the carrier gas (1 ml/min). The compounds were identified comparing their mass spectra and retention time with the NIST library. Therefore, it was found that the OME_{1b} additive consists of 96.26 Vol.% OME₁, 1.67 Vol.% Hexylenglykol and 2.07 Vol.% Methanol. The density of the mixture was 873.4 kg/m³ at T=288K compared to 835kg/m³ for diesel B7 [5].

3. Results and discussion

In contrast to the literature data compiled in the introduction, only few experimental measurements of the laminar burning velocity for OME were done. Sun et al. published results for OME (n=3) for equivalence ratios from 0.7 to 1.6 at atmospheric conditions and T=403K using an electrically-heated constant-volume cylindrical combustion

vessel [20]. They found the maximum point of the laminar burning velocity at about 75cm/s for an equivalence ratio of 1.2.

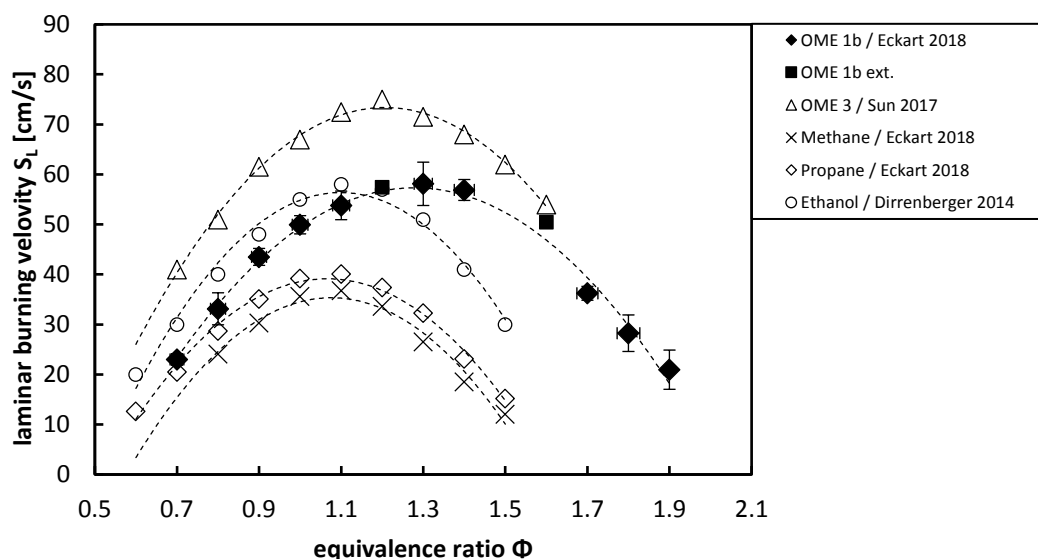


Figure 2 Comparison of the experimental laminar burning velocity for methane and propane ($T_{\text{gas}} = 298$ K), OME_{1b} ($T_{\text{gas}} = 363$ K, squares show extrapolated data points for direct comparison), ethanol [21] ($T_{\text{gas}} = 358$ K), and OME₃ ($T_{\text{gas}} = 403$ K) measurements [20] at atmospheric conditions.

The laminar burning velocities presented in Figure 2 were measured at atmospheric conditions in the temperature range of 298 K to 403 K and are compared with the work of Dirrenberger [21] and Sun [20]. The dashed lines are second order polynomial fits and show the overall trend of the measurements. Data of the burning velocity for propane, ethanol and air are not as numerous in the literature as for methane. The cross and diamond data points are for C₁ (methane) and C₃ (propane) hydrocarbons without oxygen in the molecular structure. For these fuels the maximum points are located around $\phi \leq 1.1$ and $s_L = 36$ cm/s for methane and $s_L = 40$ cm/s for propane. The circle data points show the result for ethanol with one oxygen atom in the general molecular structure and are measured at nearly the same temperature as the filled data points for OME_{1b} with two oxygen in the general molecular structure. From these curves, a clear shift of the maximum laminar burning velocity to higher equivalence ratios (less air) with increasing oxygen content is obvious. In the results of Dirrenberger the maximum point of the burning velocity of ethanol is already located around $\phi = 1.15$ and $s_L = 58$ cm/s [21] and further shifts to $\phi = 1.2$ in the case of OME₃ (Sun et al.) [20]. Moreover, the presented data for OME_{1b} settles the maximum laminar burning velocity at about $\phi = 1.3$ and again an absolute value of $s_L = 58$ cm/s (like ethanol). This trend could be due to the best C + H / O ratio of OME₁. Amongst these five compounds, OME₃ is the one with the highest velocities, while methane and propane are those with the lowest. In addition, these measurements were done for the highest preheating temperature.

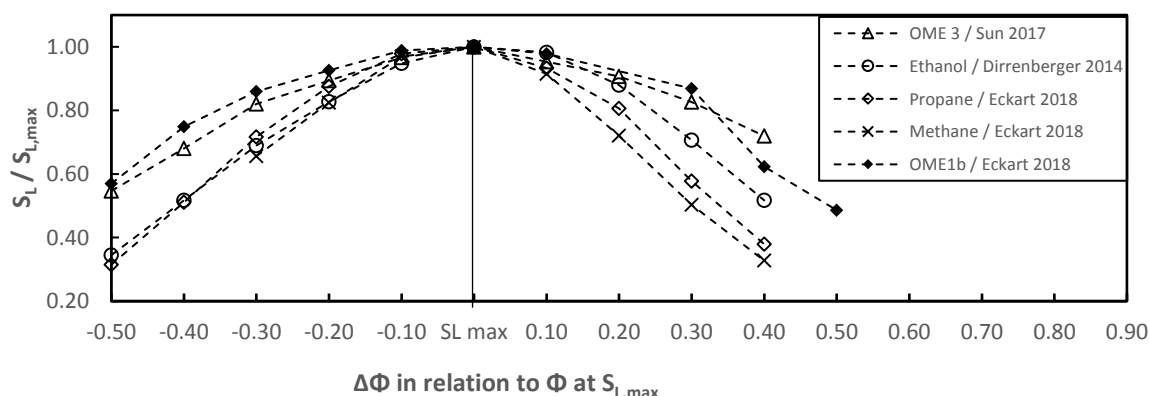


Figure 3 Comparison of normalised laminar burning velocities $s_L/s_{L,max}$ for $\Delta\phi$ in relation to ϕ at the position of the maximum laminar burning velocity $s_{L,max}$ for each chemical (methane and propane at $T_{\text{gas}} = 298$ K, OME_{1b} at $T_{\text{gas}} = 363$ K, ethanol at $T_{\text{gas}} = 358$ K [21] and OME₃ at $T_{\text{gas}} = 403$ K [20]) at atmospheric conditions.

In Figure 3 the mentioned curves were normalised to the individual maximum laminar burning velocity by $s_L/s_{L,max}$ and plotted against the deviation of the equivalence ratio $\Delta\phi$ in relation to the corresponding value at the position

of the maximum laminar burning velocity. It could be shown that the behaviour of $S_L/S_{L,max}$ for C_1 and C_3 hydrocarbons and ethanol on the fuel lean area is nearly constant but also very similar on the fuel rich side. In contrast, both measurements for OME show a less strong decrease of the laminar burning velocity on both sides of the maximum point. With the exception of OME₃, the burning velocities at $\Delta\phi = 0.4$ on the fuel rich side show lower values compared to $\Delta\phi = -0.4$. In the area of $\Delta\phi = -0.5$ to $\Delta\phi = 0.3$ OME_{1b} has the weakest dependence of all fuels. That means the burning velocity for this fuel will not change dramatically even for a large (spontaneous) variation in the equivalence ratio which can be an important advantage for technical combustion processes.

4. Conclusions

In the present study the laminar burning velocity of OME_{1b} fuels was investigated as one of the most important combustion properties for both technical designs and numerical reaction mechanisms. Oxygenated fuels like OME_n could be very important for the automotive industry in the nearby future in order to make combustion processes more efficient and to reduce the soot of engine combustion. OME_n can help to eliminate the conflict between low NO_x- and low particle emissions. The presented results of laminar burning velocities were compared to other C_3 fuels and one similar blend, namely OME₃. It could be shown that OME are in general more resistant to changes of the equivalence ratio than other fuels. Nevertheless, more experimental work is needed for extended ranges in temperature and pressure, using also different diagnostic methods such as gas chromatography. Along with theoretical studies this would open routes towards future controllable practical applications. Therefore, the experiments of the OME₁ fuel blends will be expanded to OME_n for $n > 1$ and further mixtures with other additives concerning the dependence on temperature and emission profile applied over HAB.

Acknowledgments

The authors gratefully acknowledge the financial support by the European Union and the state of Saxony in the ESF project (project number 040606100).

- [1] M. Haertl, P. Seidenspinner, E. Jacob und G. Wachtmeister, „Oxygenate screening on a heavy-duty diesel engine and emission characteristics of highly oxygenated oxymethylene ether fuel,“ *Fuel*, Bd. 153, pp. 328-335, 2015.
- [2] W. Maus, „Synthetic Fuels - OME1: A Potentially Sustainable Diesel Fuel,“ LVK_Wien, 2015. [Online]. Available: https://www.emitec.com/fileadmin/user_upload/Bibliothek/Vortraege/140217_Maus_Jacob_LVK_Wien_englisch.pdf. [Zugriff am 11 2018].
- [3] S. Deutz, „Cleaner production of cleaner fuels: wind-towheel environmental assessment of CO₂-based,“ *Energy & Environmental Science*, pp. 331-343, 2018.
- [4] A. Omari, *Fuel*, Bd. 209, pp. 232-237, 2017.
- [5] M. Haertl, *Fuel*, Bd. 153, p. 328–335, 2015.
- [6] I. Svensson, „SAE International,“ *SAE Technical Paper*, 2005.
- [7] C. Wang, „Polyoxymethylene dimethyl ethers as clean diesel additives: Fuel freezing and prediction,“ *Fuel*, Bd. 237, pp. 833-839, 2019.
- [8] S. X. Prabhakar, „Effect of Dimethoxy-Methane (C₃H₈O₂) on Combustion Characteristics of a Direct Injection Diesel Engine with Variable Compression Ratio Fuelled with Biodiesel Blends with Diesel (C_{10.8}H_{18.7}),“ *Oriental Journal of Chemistry*, Bd. 33, pp. 2937-2941, 2017.
- [9] M. B. Münz, „OME - Partikelbewertung unter Realfahrbedingungen,“ *MTZ - Motortechnische Zeitschrift*, pp. 16-21, 2018.
- [10] M. B. Münz, „OME in the Diesel engine – a concept for CO₂ neutrality and lowest pollutant emissions,“ *5. Internationaler Motorenkongress*, 2018.
- [11] L. Zhu, C. S. Cheung, W. G. Zhang und Z. Huang, *Fuel*, Bd. 90, pp. 1743-1750, 2011.
- [12] Dias, „Comparison of the effect of dimethoxymethane (C₃H₈O₂) or diethoxymethane (C₅H₁₂O₂) addition in a rich premixed ethylene flame,“ in *Thirty-third International Symposium on Combustion*, Beijing, 2010.
- [13] Oestreich, „Reaction kinetics and equilibrium parameters for the production of oxymethylene dimethyl ethers (OME) from methanol and formaldehyde,“ *Chemical Engineering Science*, Bd. 163, p. 92–104, 2017.
- [14] D. Sun, „Exploration of the oxidation chemistry of dimethoxymethane: Jet-stirred reactor experiments and kinetic modeling,“ *Combustion and Flame*, Bd. 193, pp. 491-501, 2018.
- [15] De Goeij LPH, Van Maaren A, Quax RM, „Stabilization of adiabatic premixed laminar flames on a flat flame burner,“ *Combust Sci Tech*, p. 92:201–7, 1993.
- [16] J. P. Botha, D. B. Spalding, „The Laminar Flame Speed of Propane/Air Mixtures with Heat Extraction from the Flame,“ *Proceedings of the royal Society / mathematical, physical and engineering sciences*, 1954.
- [17] Van Maaren A, „Laser doppler thermometry in flat flames,“ *Combust Sci tech*, pp. 99:105-18, 1994.
- [18] S. Eckart, „Renewable hydrogen in gas grids, Effects on laminar burning velocities,“ *International Journal of Energy Engineering*, Bd. 8, pp. 1-9, 2018.
- [19] H. S. Eckart, „Laminar burning velocities of low calorific and hydrogen containing fuel blends,“ *Energy Procedia*, Nr. 120, pp. 149-156, 2017.
- [20] Wenyu Sun, „Speciation and the laminar burning velocities of poly(oxymethylene) dimethyl ether 3 (POMDME 3) flames: An experimental and modeling study,“ *Proceedings of the Combustion Institute*, Bd. 36, pp. 1269-1278, 2017.
- [21] P. Dirrenberger, „Laminar burning velocity of gasolines with addition of ethanol,“ *Fuel*, Bd. 115, pp. 162-169, 2014.