Combustion Behavior of Carbon-Free Fuels for Large Engines

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Introduction

Global warming is on a pathway of about +3 °C compared to preindustrial times, if the current measures to counteract are considered [1]. This would lead to the collapse of ecosystems, a further loss in biodiversity, an increase in extreme weather events, and an overshooting of irreversible climate tipping points, which leads to further global warming [2]. Thus, near-term measures to reduce humankind's greenhouse gas emissions to net zero have to be implemented on a political, societal, and technical level. Focusing on the technical level, the energy demand for mobility and transportation is a main driver of CO_2 emissions. Since the energy demand for this sector is projected to rise in the foreseeable future, there is a strong need for new energy carriers with reduced global warming potential. Regarding the large engines sector, the IPCC is recommending ammonia and hydrogen from renewable sources as promising fuels for shipping in their latest report on the mitigation of climate mitigation [3]. Ammonia can serve as a hydrogen carrier with a higher volumetric energy density than hydrogen combined with a low carbon intensity. Still, its properties to be used as a fuel are challenging and have to be explored thoroughly.

The present PhD project investigates the combustion behavior of alternative fuels for large engines. For this, the aforementioned fuels ammonia and hydrogen are considered due to their carbon-free nature and their applicability in large engines. Experimental studies are performed to investigate the combustion behavior of the fuels under fundamental and engine-relevant conditions. The experimental results serve as a base for the validation of simulation models, which capture the particular characteristics of the new fuels. An experimental-numerical methodology is being developed to predict the combustion behavior of the new fuels and thereby reduce the required experimental efforts. This helps reduce the time to implement the new fuels into the fleet, and thereby speed up the mitigation of greenhouse gases from all sectors using large engines.

Methodology

To investigate the combustion behavior of new fuels, characteristic parameters have to be determined in fundamental experiments. The laminar burning velocity (LBV) is an intrinsic property of fuels, governing the combustion efficiency and stability. Therefore, it is also a main input parameter for flame propagation modeling. To experimentally determine the LBV of different fuel mixtures, optical investigations of spherically propagating flames under quasi-isobaric conditions have been performed on a constant volume combustion chamber [4], see Figure 1a). Applying Schlieren imaging, the flame propagation is captured with a high-speed camera. The LBV is derived by extrapolating the gathered flame propagation to an unstretched

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flame and calculating the flame speed of the unburnt gas from the burnt gas by applying mass continuity.

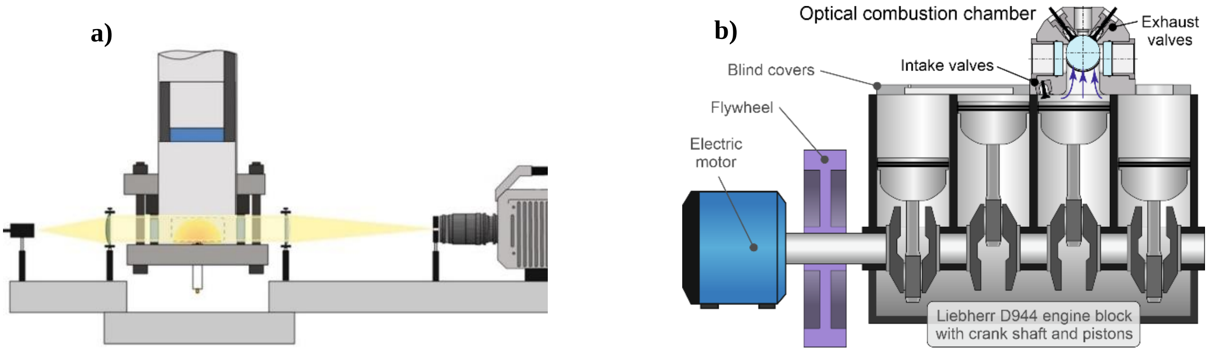

Figure 1: Experimental setup of test rigs used with optical access a) Rapid compression machine as constant volume combustion chamber [4] b) Optical test rig Flex-OeCoS [5]

While knowledge of the laminar flame behavior of new fuels is the fundament of their characterization, investigating the behavior under turbulent conditions is of the highest importance for the application of those fuels in internal combustion engines. Special attention has to be brought to the flame-turbulence interaction for hydrogen and ammonia-hydrogen mixtures because of the strong differential diffusion of those fuel mixtures. This particular characteristic causes an increase in the response of the flame speed to turbulence intensity and has to be appropriately captured by flame models. To this end, optical investigations of turbulent flame propagation under application-relevant conditions have been performed on the optical research engine test rig "Flex-OeCoS" [5], see Figure 1b). Similar to the laminar investigations, the flame propagation has been captured with a high-speed Schlieren imaging setup. The apparent flame propagation speed is based on the projected flame area growth over time. The thermodynamic conditions in the combustion chamber are characterized by fine wire thermocouple measurements and in-cylinder pressure measurements [6] as well as heat release rate calculations [7, 8]. The flow and turbulence conditions are characterized by high-speed particle image velocimetry (PIV) measurements [5].

Discussion

<u>Laminar flame propagation</u>

The results of the laminar flame propagation have been published and presented in [4, 9]. The investigated fuel is a gas mixture representing partially dissociated (or "cracked") ammonia, which contains ammonia itself, hydrogen, and nitrogen. The hydrogen serves as a combustion promoter to improve the poor combustion behavior of ammonia. In engine applications, a part of the ammonia can be dissociated into hydrogen and nitrogen upstream of the engine. The measurements are conducted for cracking ratios of $\gamma = [10\% - 40\%]$, equivalence ratios of $\varphi = [0.7 - 1.3]$, and initial conditions of

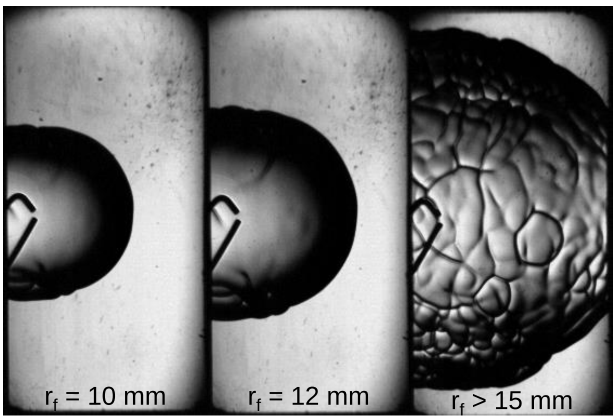

Figure 2: Schlieren image sequence of flame propagation of $NH_3/H_2/N_2$/air mixture; γ = 40%, φ = 0.9, T_0 = 298 K, p_0 = 5 bar; onset of instabilities visible for flame radii > 15 mm [4]

p_0 = [1 – 10 bar] and T_0 = 298 K. The results are compared to the results of methane, which serve as a baseline.

The outwardly spherical propagation of a lean $NH_3/H_2/N_2$/air flame with a cracking ratio of γ = 40% and p_0 = 5 bar is depicted in Figure 2. Within the evaluation range of r_f < 12 mm, the flame surface is assumed to be unwrinkled and thereby evaluable for the LBV. For larger flame radii, the onset of instabilities is visible by the strong wrinkling. These instabilities are caused by differential diffusion of the fuel mixture and mainly the contained hydrogen. This is represented by an effective Lewis number of the mixture below unity. For cases with a higher cracking ratio, a leaner fuel/air mixture, or a higher pressure, the LBV cannot be evaluated due to the onset of instabilities within the evaluation range.

Figure 3 a) shows the results of the LBV of $NH_3/H_2/N_2$/air flames for an equivalence ratio and pressure variation at T_0 = 298 K and a cracking ratio γ = 40 %. The LBV is peaking in the stoichiometric to slightly rich area and is decreasing over increasing pressure, as expected. In comparison to the literature results of Mei et al [10], an overestimation of the LBV can be observed in the lean area. Consulting the experimental Markstein Length, an underestimation of the stretch sensitivity of the flame front can be found as the source of the deviation, which is caused by a low and narrow evaluation range of the present test rig (6 mm < r_f < 12 mm). To compare the LBV of cracked NH_3 flames to CH_4 flames, CH_4 flame results have been gained performing reaction kinetic calculations in Cantera using the GRI 3.0 mechanism [11, 12]. While the equivalence ratio effect is similar for both fuels in the lean area, it is less pronounced for cracked NH_3 in the rich area. This is caused by the peak LBV of the admixed H_2 in the rich area (ϕ = 1.6 – 1.8).

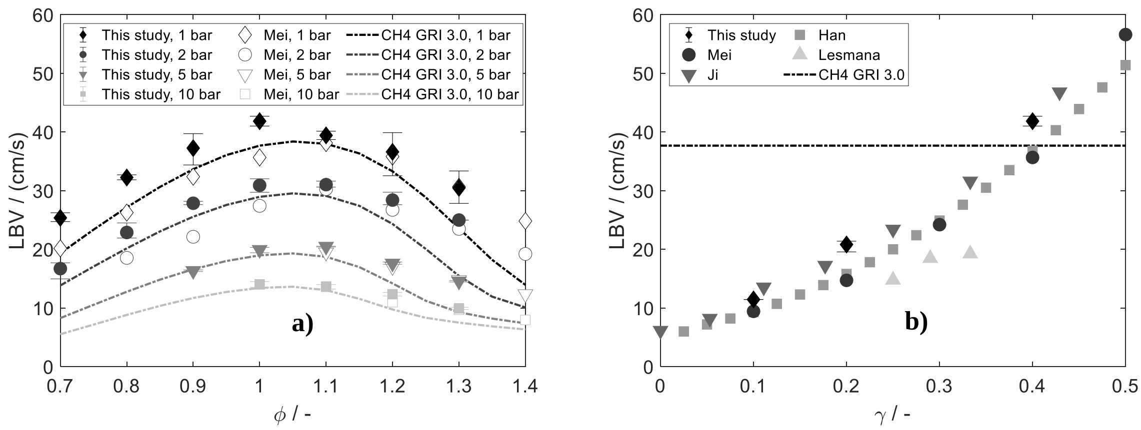

Figure 3: Laminar burning velocity of $NH_3/H_2/N_2$/air flames and CH_4/air flames at T_0 = 298 K [4] a) Equivalence ratio and pressure variation, γ = 40 %; Mei et al [10], GRI 3.0 [11] b) Cracking Ratio variation, p_0 = 1 bar, φ = 1.0; Mei et al. [10], Ji et al. [13], Han et al. [14], Lesmana et al. [15], GRI3.0 [11]

Figure 3 b) presents a comparison of the LBV results of the present study and literature results for a cracking ratio variation at T_0 = 298 K, p_0 = 1 bar, and φ = 1.0 [10, 13–15]. All results agree in a nonlinear increase of LBV for an increasing cracking ratio. This illustrates that the accelerating effect of additional hydrogen dominates over the decelerating effect of additional nitrogen in the fuel mixture. Considering the general large deviations in flame speed measurements of experimental results in the literature, a good agreement of the current results with the displayed literature results can be found, despite the limitations of the test rig. Compared to the reaction kinetic results for CH_4 flames under the same conditions, a cracking ratio of 35 - 40% is required to reach similar burning velocities, dependent on the considered source.

Turbulent flame propagation

The experiments of the turbulent flame propagation are currently being evaluated. The presented results are to be considered “work in progress” and will be published at a later time. The investigated fuel mixtures are NH_3 and cracked NH_3 and are compared to reference measurements of CH_4. The measurements are conducted for mixtures with cracking ratios of γ = [0%, 3%, 7%, 10%], equivalence ratios of φ = [0.60 – 1.20], and boundary conditions of p_c = [40, 70, 100 bar], n = [400, 600, 800, 1000 min^{-1}], ignition timing = -15°CA and T_{in} = 100°C for NH_3 and cracked NH_3 and T_{in} = 50°C for CH_4. The flame propagation for γ = 10%, ϕ = 1.00, n = 600 /min, p_c = 70 bar, and T_{in} = 100 °C is depicted in Figure 4, represented by an overlay of the Schlieren images and the detected flame area and contour. The flame shape is close to spherical in the given exemplary combustion cycle but can vary strongly from this shape due to the flow conditions in the combustion chamber. The flame-turbulence interaction is apparent by the small-scale winkled flame front.

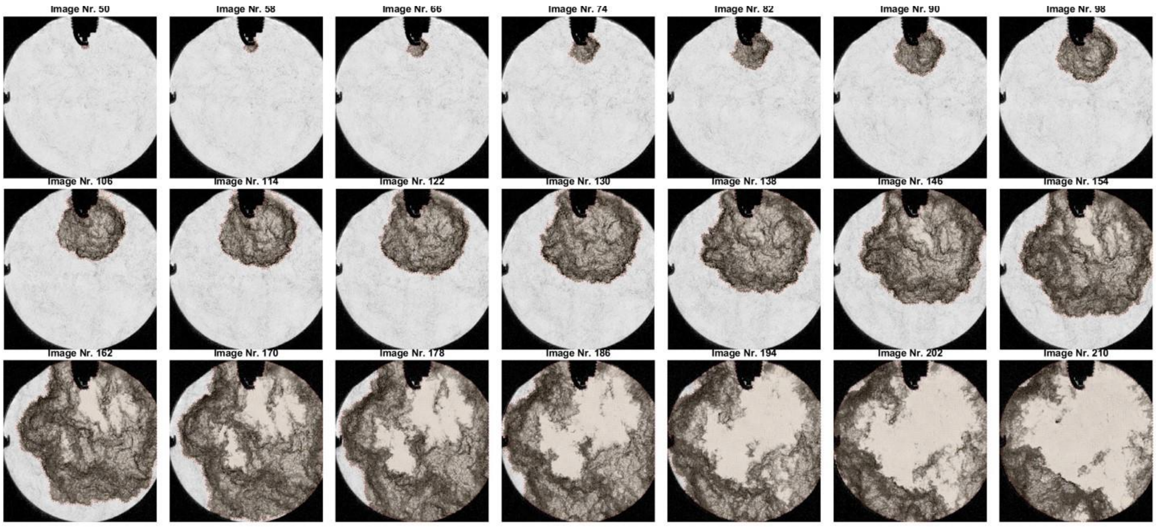

Figure 4: Overlay of Schlieren image sequence and detected area and contour of flame propagation of $NH_3/H_2/N_2$/air mixture; γ = 10 %; φ = 1.00, n = 600 min^{-1}, p_c = 70 bar, T_{in} = 100 °C

The preliminary results indicate an increase in flame propagation for increasing turbulence intensity for all fuel mixtures. The turbulence intensity is controlled by the engine speed and has been characterized in previous PIV measurements [5]. Pure NH_3 performs comparatively better under engine-relevant conditions than under laminar, quiescent conditions. The partial NH_3 cracking of up to γ = 10% effects a further significant increase in flame speed. The partially cracked NH_3 reaches similar flame speeds and combustion stability to CH_4. For lean cases, the effect of turbulence on NH_3 and cracked NH_3 flames is stronger compared to CH_4. This is caused by thermodiffusive instabilities accelerating the flame propagation, occurring for mixtures with effective Lewis numbers below unity.

Conclusions

Ammonia and hydrogen have great potential as fuels for large engines to reduce the greenhouse gas emissions of the transportation and energy sectors. While ammonia is an excellent carbon-free hydrogen carrier, its combustion behavior remains a challenge for implementation as a fuel. The combustion behavior of ammonia and cracked ammonia mixtures has been investigated experimentally under fundamental and engine-relevant conditions. The necessity of the performed experiments becomes apparent by observing the laminar and turbulent flame characteristics to differ strongly from conventional fuels. Because of the very low laminar burning velocity of ammonia, a cracking ratio of 35 - 40% - and thereby a significant addition of hydrogen - is required to reach the same LBV as methane under laminar conditions. Additionally, even with low amounts of hydrogen added, the flame surface is exposed to instabilities already at rather low pressures, speeding up the flame propagation.

In contrast, the investigations under turbulent, engine-relevant conditions expose a better performance of ammonia and cracked ammonia mixtures than expected from laminar results. With a comparatively low cracking ratio of $\gamma = 10\%$, the combustion gives satisfactory results regarding flame propagation and operation stability. This can be explained, inter alia, by the particular diffusion behavior of ammonia and especially hydrogen. The expectedly low required cracking ratios could be feasible for an on-board cracking process in maritime applications, possibly powered only by the waste heat of the combustion process.

Based on these experimental results, simulation models for laminar, turbulent, and application-oriented conditions will be reevaluated and adapted to reliably predict the combustion behavior of those new fuels. These simulation models enable a fast development process of large engines running on carbon-free fuels. Thereby, precious time can be saved on the track of net-zero greenhouse gas emissions, to prevent the crossing of the planetary boundaries at risk.

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