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# AMMONIA AS CARBON FREE FUEL FOR INTERNAL COMBUSTION ENGINE DRIVEN AGRICULTURAL VEHICLE

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Work Package 5  
Deliverable Report  
Karl Oskar P. Bjørgen (NTNU), Michal T. Lewandowski (NTNU),  
Shiwang Khare (NTNU)

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## Topic: D5.2

DEMONSTRATION OF PERFORMANCE OF ALTERNATIVE PILOT FUELS POSSIBLY  
USED IN THE FUTURE

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# 1 Introduction

This deliverable presents work performed on alternative pilot fuels for ammonia dual fuel operation. Previously in the ACTIVATE project, both biodiesel and diesel have been used as pilot fuel in ammonia engines. This has given the ACTIVATE team substantial experience with dual-fuel combustion. Previous experience has shown that the pilot injection must overlap well with the liquid ammonia injection both temporally and spatially. The ignition properties of the pilot fuel must, therefore, have the properties of typical diesel fuel, i.e. having a high reactivity and evaporating readily in a compression ignition engine thermodynamic environment. When using a fuel with low reactivity, for instance, a long ignition delay time and long flame lift-off length will likely complicate the optimization of the combustion process for dual fuel operation with ammonia. Therefore, in this report, an evaluation of an alternative fuel is performed in a controlled environment and compared to a reference diesel fuel. The combustion and emission characteristics are measured, analyzed and assessed along with a discussion on its applicability to dual fuel combustion with ammonia.

## 1.1 HTL fuels

The chosen fuel for assessment is a hydrothermal liquefaction (HTL) fuel produced from a biobased waste feedstock. The carbon present in the fuel originates from biological resources and the combustion products are therefore considered carbon-neutral. The production process of HTL fuels involves using water at sub-/supercritical conditions as a solvent [1]. The process breaks down the hydrocarbons in the feedstock, producing a high energy density crude oil (high H/C ratio) which can be upgraded to high-quality products downstream in the process. Additionally, the process also removes oxygen from the feedstock by dehydration and decarboxylation. The upgrading process could involve hydrotreatment of the crude oil or distillation, and depending on the degree of upgrading, high-quality diesel or gasoline-type fuel can be produced.

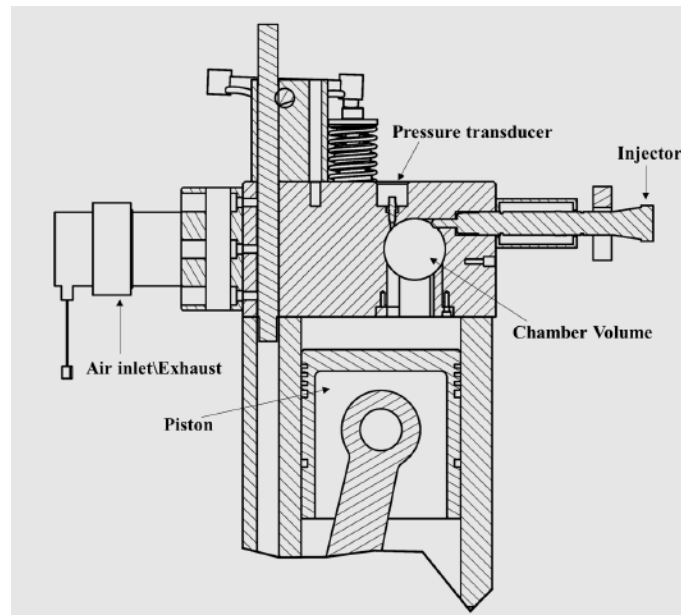
The major benefit of HTL fuels is that the feedstock could be anything containing hydrocarbons, for instance, woody residue, solid municipal waste or sewage sludge. The preparation of the feedstock before it is added to the HTL reactor does not require drying, which saves a significant amount of energy in the production process. As mentioned, the water is part of the process and is needed.

## 1.2 Objective

The objective of this work is to study the combustion properties of a novel biofuel with the aim of assessing its suitability as a pilot fuel for ammonia dual fuel operation. This will be investigated by performing experimental and numerical work on a novel biofuel which is intended for automotive purposes.

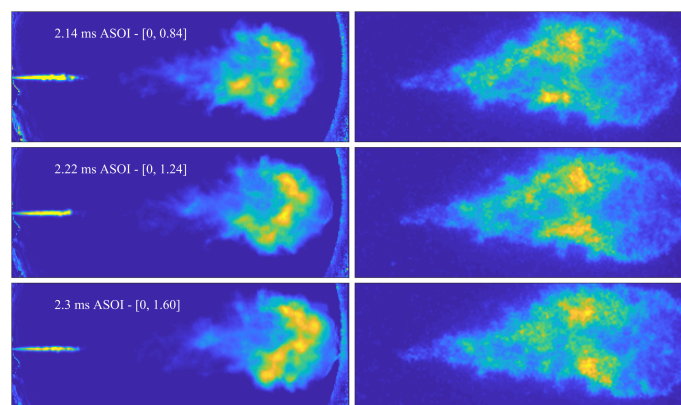
# 2 Experimental setup

The experimental work was performed in the Optical Accessible Compression Ignition Chamber (OACIC) at NTNU Department of Science and Technology. A more detailed description of the test bench, including the measurement techniques, is provided in Milestone Report M5.4. A brief summary of the equipment is given below.



**Figure 2.1:** Cross-section drawing of the OACIC.

The OACIC is a single-cylinder engine with a modified head allowing for optical access to the combustion chamber; see illustration in Figure 2.1. The rig enables direct measurement of the diesel flame using various optical techniques and has previously been used for studying biofuels for compression ignition engines. In this study, the optical techniques of direct measurement of the flame broadband light emission (natural luminosity) and ultraviolet (UV) light emission are performed using high-speed cameras. The natural luminosity (NL) is a proxy for in-flame soot mass, while UV light indicates where OH radicals are present in the flame, indicating high-temperature combustion. The in-cylinder pressure is measured using a piezoelectric sensor from Kistler, providing information on the heat release from the injected fuel. The injector used is of the type Bosch common rail with a single hole, producing a single flame in the field of view of the engine head optical access. Figure 2.2 shows a sample of a temporal measurement conducted in the OACIC, showing soot and OH\* chemiluminescence.



**Figure 2.2:** Optical measurements in the OACIC.

## 2.1 Operating points

The OACIC was operated at a constant speed of 500 rpm and two different operating points. The operating points are based on the thermodynamic conditions at top dead center (TDC). These conditions were obtained by varying the intake air conditions via the air compressor and the air heater. The aim of having different operating points was to investigate the effect of changing the ambient gas temperature at TDC while keeping the density fixed. The ambient gas temperature is known from the literature to influence the combustion significantly, where a low temperature leads to long ignition delay and long flame lift-off lengths (FLOL), while a high temperature leads to the opposite. These processes affect the initial location of fuel ignition, which can influence the subsequent premixed combustion phase significantly. The FLOL determines the degree of oxygen being mixed in with fuel vapour from the spray, which determines the equivalence ratio under which the flame is combusting, which in turn influences the production of soot and other pollutants. The ambient gas density was held at  $16.5 \text{ kg/m}^3$ , while obtaining ambient gas temperatures of 876.1 K and 924.7 for conditions 1 and 2, respectively.

## 2.2 Fuels tested

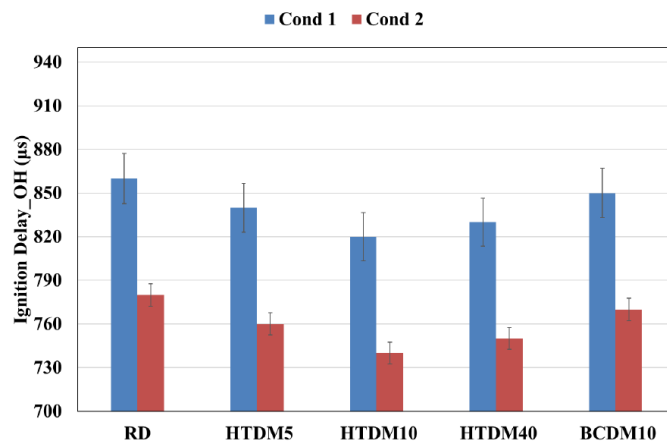
The fuels tested were a reference diesel and four blends of HTL fuel and reference diesel. The hydrotreated and distilled mixture (HTDM) was blended with diesel at 5, 10 and 40 w%, while the biocrude distilled mixture (BCDM) was blended with diesel at 10 w%. Comparing HTDM and BCDM, it is possible to compare the two upgrading processes of HTL fuel to each other. The gradual increase in HTL fuel ratio for the HTDM is investigated by comparing HTDM5, HTDM10 and HTDM40.

# 3 Results

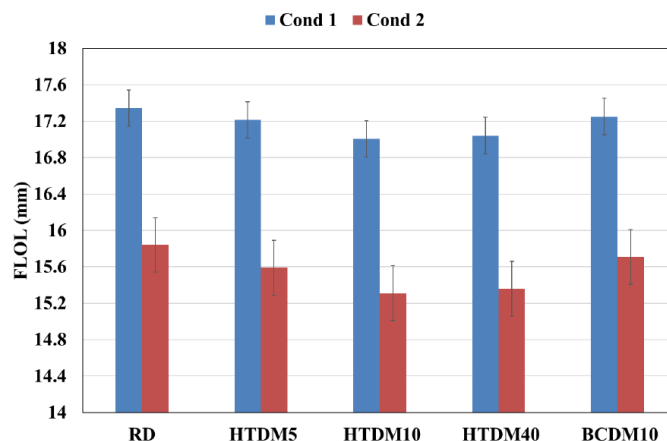
## 3.1 Combustion characteristics

The ignition delay time (IDT) is presented in Figure 3.1. The IDT is defined as the time between the start of energizing time and the first occurrence of OH\* chemiluminescence signal. The results show that all IDTs for the HTL fuel blends are shorter compared to diesel fuel. This indicates that the HTL makes the blend more reactive, leading to short IDTs. Comparing HTDM10 and BCDM10, where the HTL blend ratio is equal, the BCDM10 has a slightly longer IDT than the HTDM10. The HTDM is hydrotreated, meaning that oxygen is removed and the fuel is more paraffinic, i.e. obtaining more straight alkanes, which generally results in higher reactivity. Comparing condition 1 to condition 2, the IDT are all roughly  $90 \mu\text{s}$  shorter, but condition 2 still shows the same trend. The measured stabilized FLOL is shown in Figure 3.2. The trend follows the trends found for the IDT, this is previously reported in literature [2].

The in-cylinder pressure trace is shown in Figure 3.3. The combustion pressure shows that for all fuels, a similar shape of the pressure trace is seen, where the premixed combustion phase has a steep increase initially due to the premixing of fuel and air prior to ignition. The subsequent phase shows a slowly developing combustion, which is typical during the mixing-controlled phase, where the fuel burns as a diffusion flame. The difference in pressure between conditions 1 and 2 is due to



**Figure 3.1:** Ignition delay time based on OH\* chemiluminescence.

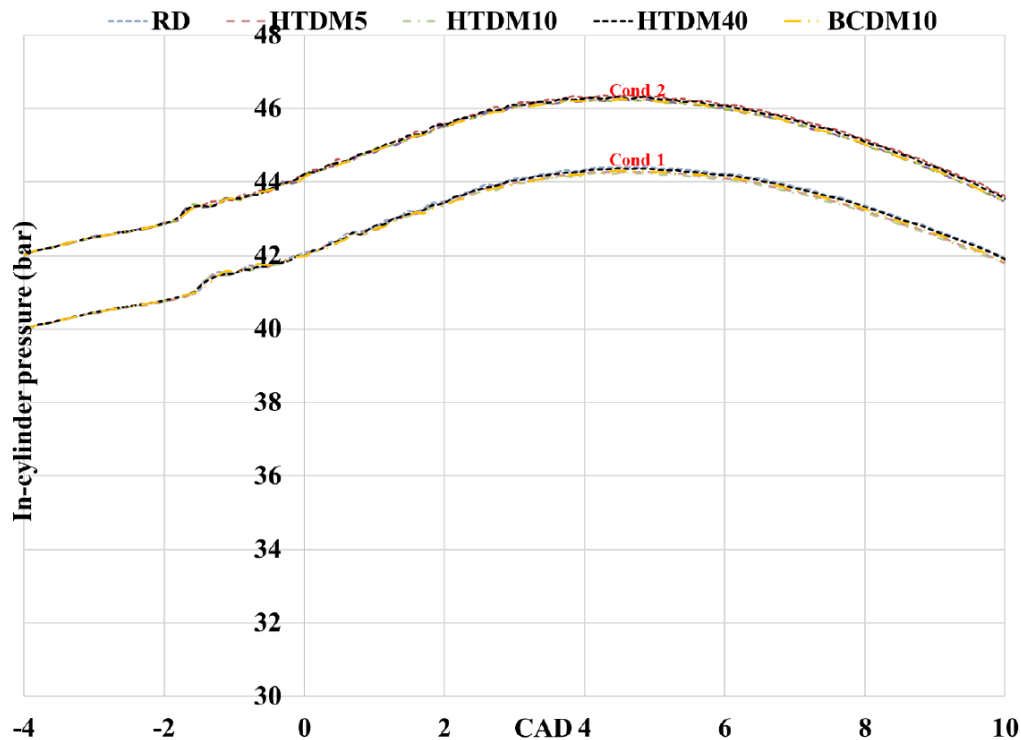


**Figure 3.2:** Flame lift-off length based on OH\* chemiluminescence.

the difference in intake air conditions for obtaining the constant air density at TDC and a varying ambient gas temperature.

### 3.2 Emissions characteristics

The sooting tendency of the spray flame is measured from the natural luminosity images. The NL measurement is a proxy of the soot mass in the flame, therefore the measurement only presents a qualitative quantity. Since the only parts of the flame is captured in these measurements, the absolute flame luminosity level of the flame is not directly indicative of sooting tendency, since different FLOLs results in different areas of the flame being visual. In order to avoid this issue, the spatial soot gradient (SSG) is calculated based on the NL measurement. This indicates the axial gradient of soot luminosity downstream of the FLOL. The result is shown in Figure 3.4. Blending in HTL fuel increases the sooting tendency of the flame, gradually increasing as more HTL is added. A higher soot tendency is observed for BCDM10 compared to HTDM10. This is due to the molecular composition of BCDM compared to HTDM, where HTDM contains mostly alkanes due to the hydrotreating process, and BCDM contains a significant amount of alkenes and cycloalkanes, known to increase

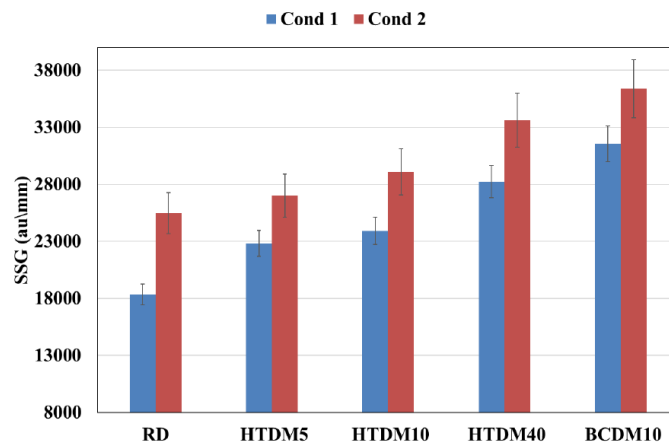


**Figure 3.3:** In-cylinder pressure trace of the two operating conditions for all fuels.

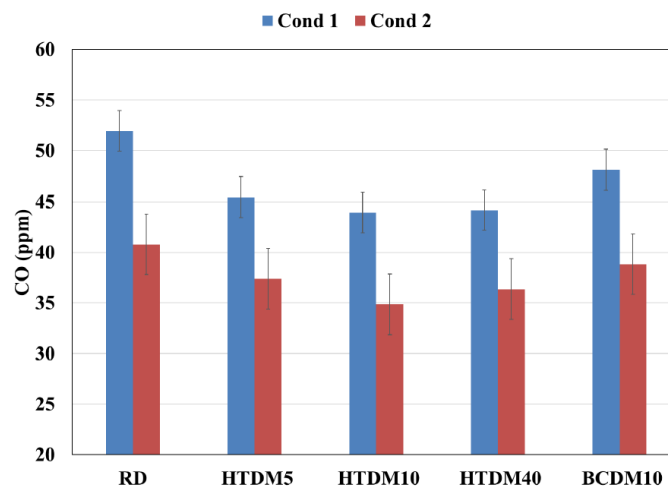
the sooting tendency of a fuel.

The concentration of CO in the exhaust stream is shown in Figure 3.5. The OACIC operates very lean due to the large displaced volume and the relatively low fuel mass injected via the single-hole injector. Therefore, pollutant emissions are not representative to normal engine mode but indicate a relative trend between the fuels and conditions tested. The CO emission is the highest for diesel fuel and is reduced by blending in HTDM fuel. However, at HTDM40, the CO concentration does not reduce further when increasing the blend ratio from 10 w%, and in fact, it increases slightly for the high-temperature case. The production of CO is generally related to poor hydrocarbon combustion, where CO does not have enough available O<sub>2</sub> to further convert into CO<sub>2</sub>. This could be due to poor mixing resulting from several parameters. A potential cause could be the viscosity. As we blend HTDM into diesel, the viscosity increases. Comparing HTDM10 and BCDM10, BCDM10 has a higher CO concentration in the exhaust, indicating the molecular composition of BCDM promotes poorer combustion or the higher viscosity of BCDM10 causes poorer fuel atomization and poorer mixing. BCDM is a "less" upgraded fuel, containing more unsaturated and branched compounds, requiring more energy during pyrolysis to break the hydrocarbons down into smaller and short-chained hydrocarbons, and therefore leading to poorer combustion.

Similarly, the measured concentrations of nitrogen oxides (NO+NO<sub>2</sub>=NO<sub>x</sub>) in the exhaust stream are presented in Figure 3.6. The results show a weakly increasing trend as HTDM is blended with diesel. NO<sub>x</sub> is generally produced as thermal NO<sub>x</sub> in hydrocarbon flames from atomic nitrogen present in the air subjected to high flame temperatures, explained by the Zeldovich mechanism. However, for fuels containing nitrogen, an additional pathway emerges, where the fuel-bound nitrogen reacts with oxygen in the air forming NO. The HTL fuels contain nitrogen, and if we assume that the



**Figure 3.4:** The spatial soot gradient based on the natural luminosity measurement.



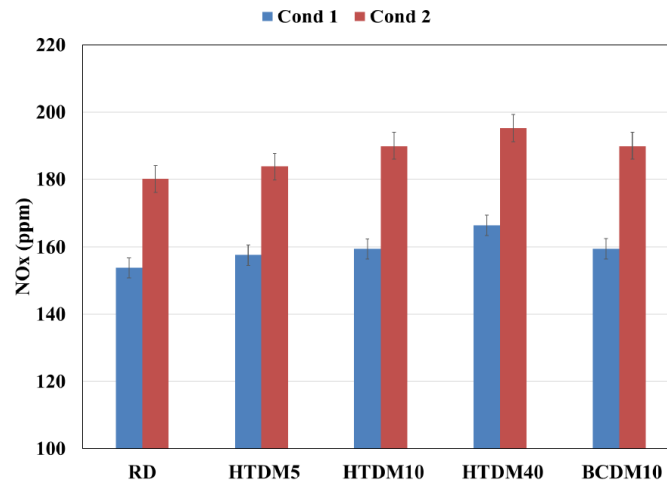
**Figure 3.5:** Concentration of carbon monoxide in the exhaust.

adiabatic flame temperature of the fuel blends is not significantly changed and the combustion mode is similar, then the observed increase in NO<sub>x</sub> as HTL fuel is added could be attributed to the fuel nitrogen pathway. When comparing the nitrogen content in the fuel blends tested, HTDM10 contains 2545 ppm by mass while BCDM10 contains 3920 ppm by mass. One might then expect that BCDM10 would have a higher concentration of NO<sub>x</sub> in the exhaust stream, however, the concentrations are almost identical for the two. A potential reason for this could be the way nitrogen is bound in the molecules of the two HTL fuels, causing the chemical kinetics to act in different ways.

## 4 Conclusions

This report presents the findings achieved from experimental work on HTL fuel as a potential pilot fuel for ammonia dual-fuel engines. The work consisted of performing combustion tests in an optical engine, where the ignition delay time, flame lift-off length, in-flame soot and exhaust gas emissions were measured. The results from the experimental campaign revealed that blending two types of upgraded HTL fuels up to 40 w% with diesel fuel did not alter the combustion and emissions





**Figure 3.6:** Concentration of nitrogen oxides in the exhaust.

characteristics significantly compared to reference diesel fuel. This is encouraging results with respect to using HTL fuel as pilot fuel since diesel fuel has, in previous work, been successful in igniting the liquid ammonia injection. There are several interesting aspects to consider further, such as the effect of fuel-bound nitrogen on the N<sub>2</sub>O formation in ammonia combustion.

## References

- [1] Saqib Sohail Toor, Lasse Rosendahl, and Andreas Rudolf. Hydrothermal liquefaction of biomass: A review of subcritical water technologies. *Energy*, 36(5):2328–2342, May 2011.
- [2] Dennis L. Siebers and Brian Higgins. Flame Lift-Off on Direct-Injection Diesel Sprays Under Quiescent Conditions. In *SAE Technical Paper Series*, March 2001.