Efficient fuels for future engines

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Efficient Fuels for Future Engines

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PhD dissertation

Efficient Fuels for Future Engines

C.A.J. Leermakers

efficient [ih-fish-uhnt] - adjective

• performing or functioning in the best possible manner with the least waste of time and effort; having and using requisite knowledge, skill, and industry; competent; capable: a reliable, efficient assistant.

• utilizing a particular commodity or product with the least waste of resources or effort (usually used in combination): a fuel-efficient engine.

Late 14c., “making,” from Latin efficientem (nom. efficiens), prp. of efficere “work out, accomplish”
1 – Background
Internal combustion engines are crucial for the transport of both people and goods, and as such an essential part of today’s society. However, some obstacles will have to be overcome to keep the use of engines possible for the decades to come. - page 6

2 – Thermodynamic test setup
For the thermodynamic engine tests described in this dissertation an advanced single-cylinder engine concept is used. This engine (CYCLOPS), the procedures followed, and definitions used have been described many times by the author and his colleagues. This chapter is a combination of these descriptions. - page 14

3 – Impact of operating conditions on PCCI combustion
Combustion in an engine is affected by a large number of parameters, many of which can be controlled by a test bed operator. Operation of a test engine is much like controlling the engines of the Queen Elisabeth 2, the operating room of which is shown in this picture. - page 20

4 – Using diesel-like fuels for PCCI
In a short term scenario, application of any new combustion concept would be the easiest if readily available fuels can be used. Therefore in this chapter the performance of different types of diesel fuels are compared. - page 30

5 – Using low reactive diesels for PCCI
The usage of fuels other than regular diesel or gasoline, enables a choice of reactivity, and therewith allows to phase combustion as desired. A low-reactive aromatic solvent is added to diesel to tune its reactivity. - page 38

6 – Direct injection of butane-diesel blends
Apart from using alternative combustion concepts to achieve high efficiency and low emissions, CO2- and cost-effective fuels can also be used. In this chapter the direct injection of butane-diesel blends is investigated. - page 42

7 – Initial tests with RCCI
Combining the properties of two conventional fuels can yield the chemical and physical properties desired for advanced compression ignition engines. Using two fuel systems allows to adjust these fuel properties in real time. - page 48
8 – Testing the controllability of RCCI
Using two fuel systems opens up an extra degree of freedom to control combustion phasing. In this chapter the control space is explored using four different injection strategies. - page 56

9 – Commercial Naphtha blends for PPC
Naphtha streams, from a refinery such as the Pernis one of this image could provide easily applicable fuels for Partially- Premixed Combustion - page 66

10 – Butanol for PPC
The use of diesel blended with a promising second-generation bio-fuel can provide a viable approach for PPC. In this chapter n-butanol is used, which can be produced from switch grass. - page 76

11 – Fuel composition effects on PPC
Given an optimum reactivity, effects of the chemical composition of fuels on Partially-Premixed Combustion are explored, with the focus on load range capacity. - page 86

12 – Cinematographic imaging of methylidene radicals using LIF
A laser diagnostic technique, imaging the CH radical, is developed which may help in providing further understanding of processes in Low-Temperature Combustion. - page 100

13 – Cinematographic imaging of hydroxyl radicals in an optically accessible engine
Because high-speed CH-LIF was shown to have a very limited applicability under engine conditions, the same setup was used for more feasible imaging of the OH radical. - page 110

14 – Laser diagnostics of early soot formation (PAH)
A third laser diagnostic technique to study early stages of soot formation is developed. This technique uses simultaneous laser-induced incandescence of soot and fluorescence of poly-cyclic aromatic hydrocarbons (PAH). - page 120

15 – Summarizing discussion and conclusion
In this thesis the fuel effects on new combustion concepts have been investigated. Furthermore, laser diagnostic techniques have been developed to gain further understanding of the underlying processes. To conclude, in this last chapter the results are summarized and discussed. - page 136

Appendices
List of publications - page 140
From the author - page 142
Dissertation summary - page 143
Author’s Curriculum Vitae - page 144
1 – Background

Internal combustion engines are crucial for the transport of both people and goods, and as such an essential part of today’s society. However, some obstacles will have to be overcome to keep the use of engines possible for the decades to come.

Photo courtesy of Kevin Dooley under Creative Commons license
Combustion engines: their past and future

Worldwide, people rely on the use of motorized transport. Over the last century, both individual and mass transport systems have made the world a lot smaller or bigger, depending on how you look at it. People have been increasingly more able to travel from one village to another, but also around the world. Not only people transport has evolved significantly, a very important place in today's society is held by the transport of goods around the world. Heavy-duty road transport as well as sea freight take an indispensable role in keeping our modern-day world go round. This can be illustrated by the fact that energy consumption by the transport sector has more than doubled from 1973 through 2010 [1].

The internal combustion engine has, after the invention of the wheel some thousands of years ago, been the major breakthrough in facilitating such transport. Several main reasons for the success of combustion engines can be identified.

First of all, the availability of fuels that can readily be used in the engine, albeit after distillation, is a big enabler. It may seem a coincidence that the first commercial oil well (E.L. Drake, 1859, Pennsylvania) and the first combustion engine being produced in numbers (J.J.E. Lenoir, 1860, Paris) occurred in quick succession. Actually, one could say it is more accurate they owe their success to each other.

Second, fuels being easily and abundantly available, with only marginal energy needed for extraction and processing, makes that they are relatively cheap. Currently, about 90% of crude oil is processed to be used as fuels [2]. The chemical components found in crude oil and the processed fuels are generally of high energy density. This allows the engines that use these fuels to provide power for a significant time period using only a limited amount of fuel.

Lastly, the combustion engine itself in principle mostly involves relatively low cost materials and production methods. This makes that combustion engines are cheap to produce, use, and maintain, so that they have been widely deployed in a large range of appliances.

But, alas, every rose has its thorn. For the combustion engine two major complications, emerged from its success, became evident during the second half of the twentieth century. In late 1970 the United States oil production peaked and could not keep up with further growing demand in the years after that [3]. As with similar markets, this imbalance increases the product prices up to a level where the balance is restored.

It has been shown that the demand is only marginally influenced by price levels. However, the production rates are influenced as increasingly difficult and expensive methods can be employed to extract the oil, such as from oil sands and shales nowadays. Herewith, the trade-off between demand and production will be restored, as long as technology can keep up and users can afford the associated price.

By the mid of the last century, a second disadvantage of combustion engines became evident. Local emissions, like Nitrogen Oxides (NOx) and Particulate Matter (PM) have been shown to be particularly harmful for ground-level air quality and the environment in general. Nitrogen oxides may in the air convert to nitric acid which has been implicated in acid rain. Furthermore, NOx participates in ozone layer depletion and the formation of smog [4]. Particulate matter has been associated with climate effects, impact on vegetation, and most importantly with adverse health effects for humans and animals. Inhalation of particulate matter has up to now been shown to increase the risk of asthma, lung cancer, cardiovascular and respiratory diseases, birth defects, and premature death [5]. It is for these reasons that the European Union has introduced emission limits for different types of road transport vehicles (Figure 1–1).

Apart from the problems regarding such local emissions, combustion engines using conventional fuels emit carbon dioxide (CO2), which is generally thought to have a global impact as a greenhouse gas [6]. Although the discussions on these issues have not yet settled [7], automotive
Background

From those from an ideal gas, limited control of the speed of combustion and combustion phasing limited by NOx emission, knock, the maximum in-cylinder pressure, or pressure rise rate.

In addition to this, the combustion regime that is used can have a big impact on emissions so that no trade-off has to be chosen between fuel consumption (or CO\textsubscript{2}) and PM/NOx emissions.

Fuels also impact local emissions and again, a fuel contributing to lower PM or NOx emissions can save fuel and CO\textsubscript{2} emissions, by avoiding the formerly mentioned trade-off. Reduction of CO\textsubscript{2} emissions furthermore depends on the CO\textsubscript{2} footprint of the fuel, which in its turn depends mainly on two factors.

Primarily, the footprint is determined by the energy used in producing and refining the fuel.

Bio-fuels can reduce the impact significantly, although this varies a lot between different production methods. Even for crude-based fuels CO\textsubscript{2} can be reduced, if less energy is needed for processing or upgrading these fuels. Also the atomic Hydrogen/Carbon ratio directly influences the CO\textsubscript{2} emission per unit energy (e.g. Hydrogen engines [9]). As a second order effect, the fuel can act as an enabler for certain high efficiency combustion regimes. Conventional combustion concepts, as well as high efficiency regimes, are discussed in the next section.

Combustion engine concepts

Since the invention of the internal combustion, two traditional types of engines have been used, which will be shortly described next.

Spark Ignition engine

In the traditional spark ignition (SI), or Otto engine [10], fuel and air are mixed in the engine’s intake manifold, and later in the engine cylinder actively ignited by a spark, see Figure 1–2.

As the near-stoichiometric (ideal) mixture is compressed first, a fuel has to be used that is resistant to auto-ignition, such as gasoline. To further prevent auto-ignition and possibly...
**Compression Ignition engine**

In the compression ignition (CI), or diesel engine [10], only air is compressed in the engine’s cylinder (Figure 1–3). When the temperature is high, near top dead center, fuel is injected into the combustion chamber. A highly reactive fuel is used, to enable auto-ignition after a short ignition delay period.

After ignition, a lifted diffusion flame establishes. The rich fuel/air mixture at the foot initiates the formation of particulate matter. While most of this is oxidized at the edges of the diffusion flame, some is emitted as engine-out PM emissions.

Because of the high end-of-compression temperatures (necessary for auto-ignition), and locally stoichiometric mixtures in the diffusion flame, NOx is formed. Most strategies to decrease PM emissions by increasing soot oxidation, increase NOx emissions and vice-versa. This PM-NOx trade-off is also known as the Diesel Dilemma.

Over the past decades many technologies have been introduced to break with this trade-off. However, these mostly are expensive or come with a fuel consumption penalty. To further reduce emission levels to current legislation limits, after-treatment systems based generally on Selective Catalytic Reduction (SCR, [11]) and Diesel Particulate Filtration (DPF, [12]) technologies have to be used for the reduction of NOx and soot, respectively.

Breaching the maximum peak pressure, the compression ratio of SI engines has to be limited. Because of this, and the relatively slow flame propagation, the effective expansion ratio of the concept is limited. To control the power output, commonly a throttle valve is used which gives rise to gas exchange losses. Because of all of these factors, the fuel conversion efficiency is limited and as such, fuel consumption and CO₂ emissions are generally high.

As the fuel-air mixture is well-mixed (near homogeneous), no rich zones exist and as such, particulate emissions are negligible. However, after ignition a flame front passes through the combustion chamber which gives rise to high local temperatures. These high temperatures, in combination with the presence of oxygen and nitrogen, give rise to the formation of so-called thermal NOx.

Local cold spots in the combustion chamber cause flame quenching which together with crevice volumes results in incomplete combustion (unburned hydrocarbons (UHC) and carbon monoxide (CO) emission). Although (because of the near-stoichiometric operation) a relatively inexpensive three-way catalyst can be used to reduce these emissions, the incomplete combustion also limits fuel conversion efficiency.

![Figure 1–2: Spark Ignition engine schematic](image)
- Spark ignition
- Low reactive fuel
- Homogeneous mixture
- Port injection

![Figure 1–3: Compression Ignition engine schematic](image)
- Compression ignition
- High reactive fuel
- Spray
- Direct injection
Background

Not only bad news is associated with the compression ignition engine. The engine uses a high compression ratio, lean mixtures and operates unthrottled. Furthermore, contemporary diesel engines use improved heat release rates and do not suffer from incomplete combustion. As a result, the thermodynamic efficiency of the diesel engine is superior to that of the spark ignition engine.

The development of combustion technologies with intrinsically lower NOx and PM emissions can minimize the after-treatment system requirements and thus reduce the related costs. Such concepts should aim at reaching, or exceeding the fuel conversion efficiencies of contemporary diesel engines.

Low-Temperature Combustion

Concepts trying to achieve the aforementioned are generally classified under Low-Temperature Combustion (LTC). One thing these concepts have in common is that in all of them charge’s combustion temperature is lowered by changing the fuel specific heat capacity of the compressed mixture [13]. This heat capacity can be increased by taking in more air mass (i.e. run leaner), by changing the composition of the trapped mass (i.e. with Exhaust Gas Recirculation, EGR [10]), or a combination of the two.

The increased heat capacity can bring combustion temperatures below levels where thermal NO is formed on engine-relevant time-scales. Global temperatures should on the other hand be high enough to enable full oxidation of the fuel to carbon dioxide.

However, even when global temperatures are in the correct range, the high mixture stratification that is generally experienced in a diesel engine can still result in local temperatures high enough for NO formation.

It is therefore that Low-Temperature Combustion strategies aim at having a premixed-enough mixture prior to combustion. A relatively low stratification level, with limited deviations from the average mixture strength, will also limit local temperatures to the desired range.

Such a reduction in stratification is also beneficial for the reduction of Particulate Matter emissions as less rich spots will be present. Compared to the CI engine, stratification is reduced by promoting mixing of fuel and air before combustion starts.

The first concept that was introduced to apply such a premixed mixture in a high-efficient compression ignition engine was the HCCI concept, as will be described next.

Homogeneous-Charge Compression Ignition (HCCI)

The HCCI concept [14] (Figure 1–4) uses very early (port) fuel injection to have a homogeneous mixture by the end of the compression stroke, like in the SI engine. Unlike the SI engine, however, this mixture is not ignited by a spark but it is brought to auto-ignition by compression heat.

Auto-ignition is mainly governed by chemical kinetics. Therefore, the timing of this auto-ignition is highly dependent on in-cylinder conditions, see [15]. These in-cylinder conditions are characterized as the temperature - pressure - equivalence ratio history. Depending on the fuel used, the intake temperature and compression ratio have to be chosen such that auto-ignition happens near Top Dead Center.

Researchers were led to this concept from two sides, either with the goal of optimizing the efficiency of gasoline engines, or to clean up
After that, in most of the remaining chapters the impact of fuel composition is studied. In chapter 4, the effects of the composition of conventional diesel fuels are described for use of PCCI in the aforementioned short term scenario.

The high boiling range of current diesel fuels has the intrinsic risk of wall-wetting when injecting early [19][20][21] and such fuels are very prone to auto-ignition [22]. Kalghatgi and coworkers [23] showed that low reactive fuels such as gasoline increase the mixing time of fuel with air and can be used for PCCI combustion. A similar investigation on the tailoring of fuel reactivity to the demands of the combustion concept, which could be used in a longer term scenario, is described in chapter 5.

Even with these more advanced fuels, the operating range and controllability of PCCI are still limited. To gain more control of combustion, more control of reactivity and/or mixture stratification is necessary. This brings us to the two most advanced concepts, as described next.

**Premixed-Charge Compression Ignition (PCCI)**

Premixed-Charge Compression Ignition (PCCI) is a combustion concept that is characterized by low-temperature, partially-premixed combustion using early injections, large ignition delays and high percentages of Exhaust Gas Recirculation (EGR) [16][17], see Figure 1–5.

The injections are, however, not as early as in HCCI, to provide some stratification in the fuel-air mixture. The ignition delays are large enough to decouple injection and combustion. While this still limits the control of combustion phasing [18], the operating range is extended compared to HCCI.

Because the load range might still be limited, in a short-term scenario near standard components and conventional fuels should be used to enable the switch to conventional CI combustion at higher loads. This requires a smart choice of operating conditions, which is presented in chapter 3 of this dissertation.

**Reactivity-Controlled Compression Ignition (RCCI)**

Olsson [24] used two fuels to control the combustion onset in a HCCI engine. After that, Inagaki was the first to propose a dual-fuel concept to control the in-cylinder reactivity of the mixture [25], which over recent years has been further developed by Reitz and coworkers [26].

![Figure 1–5: PCCI engine schematic](image)
This latter group is now leading in the field of dual fuel PCCI with use of a port injection system for a low reactive fuel. This way, a large part of the fuel is well mixed and the desired level of both reactivity- and mixture stratification can be achieved by one or more early direct injections of a high reactive fuel.

The University of Wisconsin’s Reactivity Controlled Compression Ignition (RCCI, Figure 1–6) engine experiments [26][27] have demonstrated control and versatility of dual fuel PCCI combustion with the proper fuel blend and injection timings. Very low NOx and smoke emissions were shown, combined with extremely high efficiencies. This concept is evaluated in chapter 7.

For real-life use, this concept requires decent controllability. In chapter 8 of this dissertation, a description of the applicable control space for a number of parameters is presented.

The control over reactivity (stratification) enables shaping of the heat release profile such that thermal efficiency can be optimized. However, the very early injection of the low reactive fuel mixture may result in increased combustion losses. Therefore a second concept is investigated which attempts to shape the heat release rate using a single fuel. The latter concept uses advanced injection strategies to achieve the desired mixture stratification, as will be discussed next.

**Partially-Premixed Combustion (PPC)**

Partially-Premixed Combustion (Figure 1–7) is derived from the PCCI concept, but is closer to contemporary diesel engines [28]. It uses advanced injection strategies, with multiple injections to define the stratification level. It furthermore attempts to use cleaner-burning and mixing-enhancing fuels. [29]

Like in contemporary diesel engines low loads are more premixed and as load is increased combustion becomes more and more mixing-controlled. In PPC, the premixed range is broadened and specific fuel aspects are used to ensure that when at higher loads combustion becomes more mixing-controlled, emissions are still satisfactory [30].

As an example, commercially available naphtha blends can help to make the transition from fully mixing controlled combustion (as in a diesel engine) to more premixed regimes. The application of such naphtha blends is described in chapter 9. The application of certain bio-fuels (blended with regular diesel fuel) can enable the further use of aforementioned concepts. In chapter 10 of this dissertation, a number of n-butanol/diesel blends, used in Partially-Premixed Combustion mode, are presented.

Given an optimum reactivity for the PPC concept, a number of fuels has been blended both from refinery streams and from surrogate fuel components. The difference between these components is presented in chapter 11.
This dissertation

As discussed before, each of the prevalent combustion concepts has its own fuel appetite, which determines its load range capacity, efficiency and emission levels. This will be the main focus of this dissertation.

The concepts are mostly compared using experimental tests. The metal engine setup which was used for these experiments (CYCLOPS), is discussed in the following chapter 2. Some definitions (also regarding efficiencies) and processing standards which are used throughout the dissertation are also discussed in chapter 2.

These definitions are followed by experimental results from the metal test engine in chapters 3 through 11. As announced in the previous section, in these chapters the combustion concepts and their respective fuel appetites are explored, and the results of these experiments are presented in condensed article form. In most chapters, references are made to the full published version of the articles, to which the reader is referred for further in-depth information.

Further improvements of the combustion regimes described earlier rely on detailed knowledge and understanding of the underlying processes [31]. In chapters 12 and 13 the development of high speed- CH and OH Laser-Induced Fluorescence (LIF) techniques are described.

Given the limited applicability of these two techniques, a diagnostic method to study the formation of poly-cyclic aromatic hydrocarbons (PAH) and soot is described in chapter 14. This method is applied to both conventional and low-temperature combustion conditions to study phenomena witnessed earlier in the dissertation.

The body of this dissertation is concluded in chapter 15 by a general discussion of the results of the chapters and their respective conclusions.

References

For the thermodynamic engine tests described in this dissertation, an advanced single-cylinder engine concept is used. This engine (CYCLOPS), the procedures followed, and definitions used have been described many times by the author and his colleagues. This chapter is a combination of these descriptions.
Many of the results presented in this dissertation have been gathered on a thermodynamic test engine setup, referred to as CYCLOPS. This test setup, the procedures followed and definitions used for these thermodynamic tests will be discussed in this chapter.

**Thermodynamic test engine setup**

The CYCLOPS, as first described in [32] and [33], is a dedicated engine test rig, designed and built at the Eindhoven University of Technology (TU/e), based on a DAF XE 355 C engine, see Table 1. Cylinders 4 through 6 of this inline 6-cylinder HDDI engine operate under the stock DAF engine control unit; together with a water-cooled, eddy-current Schenck W450 dynamometer they are only used to control the crankshaft rotational speed of the test cylinder (i.e. cylinder 1).

**Table 2–1: CYCLOPS specifications**

<table>
<thead>
<tr>
<th>Base engine</th>
<th>6-cylinder HDDI diesel</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cylinders</td>
<td>1 isolated for combustion</td>
</tr>
<tr>
<td>Bore [mm]</td>
<td>130</td>
</tr>
<tr>
<td>Stroke [mm]</td>
<td>158</td>
</tr>
<tr>
<td>Compression ratio [-]</td>
<td>variable, original 17.0</td>
</tr>
<tr>
<td>Bowl shape</td>
<td>M-shaped</td>
</tr>
<tr>
<td>Bowl diameter [mm]</td>
<td>100</td>
</tr>
</tbody>
</table>

When data acquisition is idle, for instance during engine warm-up or in between measurement series, the CYCLOPS is only fired on the three propelling cylinders. Once warmed up and operating at the desired engine speed, combustion phenomena and emission formation can be studied in the test cylinder. Apart for the mutual cam- and crankshaft and the lubrication and coolant circuits, the test cylinder operates autonomously from the propelling cylinders. Stand alone air, EGR and fuel circuits have been designed for maximum flexibility as will be discussed next.

Fed by an Atlas Copco air compressor, the intake air pressure of the test cylinder can be boosted up to 5 bar. The pressure set point can be programmed from the engine control room and pressure is regulated by a pressure controller, which receives its input signal from a pressure sensor mounted in the intake manifold of the test cylinder. The fresh air mass flow is measured with a Micro Motion Coriolis mass flow meter, see [34]. Non-firing cylinders 2 and 3 function as EGR pump cylinders, see Figure 2–1, the purpose of which is to generate adequate EGR flow, even at 5 bar charge pressure and recirculation levels in excess of 70%. The EGR flow can be cooled both up- and downstream of the pump cylinders, down to ca. 30 °C, using a variable flow of process water as a coolant medium. EGR mass flow is both measured with a Coriolis mass flow meter, and estimated from the fresh air mass flow and computations regarding the volumetric efficiency. The EGR percentage in this dissertation is given as the weight percentage of EGR in the intake stream. For most investigations, this EGR stream is cooled, and as such dried. Several surge tanks, to dampen oscillations and ensure adequate mixing of fresh air and EGR flows, and pressure relief valves, to guard for excessive pressure in the circuit, have been included in the design.

Direct injected fuel to cylinder 1 is provided by a double-acting air-driven Resato HPU200-625-2 pump, which can deliver a fuel pressure up to 4200 bar. An accumulator (~ 0.114 dm³) is placed near (~ 0.2 m) the fuel injector to mimic the volume of a typical common rail and dampen pressure fluctuations originating from the pump. The steady state fuel mass flow is measured with a Micro Motion mass flow meter.
Thermodynamic test setup

A prototype common rail injector is used which can inject the fuel with a pressure up to 3000 bar. The nozzle used for these experiments has similar characteristics to the nozzle used in [32], which gave the best performance in the late-DI PCCI regime. This nozzle has 8 holes of 0.151 mm diameter with a cone angle of 153 degrees, injecting into the M-shaped piston bowl.

For port fuel injection, a Vialle28 injector is mounted in the intake manifold with an angle of 120 degrees resulting in a spray positioned on the intake valve. Port fuel injection is started just after intake valve open and after exhaust valve close (i.e. 300 °CA bTDC) to spray directly into the cylinder and avoid possible blow-through of gasoline. The net fuel pressure of the port fuel injection system is set to ca. 3 bar by controlling the rotational speed of the fuel pump in the gasoline tank.

For measuring gaseous exhaust emissions, a Horiba Mexa 7100 DEGR emission measurement system is used. Exhaust smoke level (in Filter Smoke Number or FSN units) was measured using an AVL 415 smoke meter three times per operating point, of which the average is used. The engine is equipped with all common engine sensors, such as intake and exhaust pressures and temperatures, and oil and water temperature. These quasi steady-state engine data, together with air and fuel flows and emission levels are recorded at 20 Hz for a period of 40 seconds by means of an in house data acquisition system (TUeDACS), see [34]. The average of these measurements is taken as the value for the operating point under investigation.

Finally, a SMETEC Combi crank angle resolved data acquisition system is used to record and process cylinder pressure (measured with an AVL GU21C uncooled pressure transducer), intake pressure, fuel pressure and temperature and injector current. All of these channels are logged at 0.1 °CA increments for 50 consecutive cycles, which is common practice in combustion indication. From these data, the average and standard deviation of important combustion parameters, such as CA10, CA50 and the Indicated Mean Effective Pressure (IMEP) are calculated online by the SMETEC software. This is used to increase the ease of measurement. For the final analysis, the pressure data are post-processed with a custom Matlab script.

To limit end of compression temperature to avoid premature auto-ignition, the geometric compression ratio of the test cylinder is adapted, either by using different head gaskets, a low compression piston, or both. The method used for various investigations is described in the respective chapters, together with changes made to the standard configuration used for specific tests.

Procedure

Prior to a measurement series, the engine speed is set to a desired value and the engine is warmed up until lubrication oil and coolant fluid temperatures are 90 and 80 °C, respectively. All operating conditions are set to their desired values and the test cylinder is fired at a conventional timing to heat the combustion chamber and exhaust. Measurements are only started after the CO₂ content of the exhaust flow has stabilized.

All operating points should have acceptable combustion stability. Stable combustion is defined by the coefficient of variation of IMEP $\text{cov}_{\text{IMEP}} = \frac{\sigma_{\text{IMEP}}}{\mu_{\text{IMEP}}}$ (with $\sigma$ and $\mu$ being the standard deviation and the mean of the IMEP, respectively) being below 5%. Preferably, all operating points should also meet each of the following emission levels:

- CO emissions below 2000 ppm,
- UHC emissions below 1000 ppmC, with a target below 400 ppmC,
- NOx emissions below 200 ppm with a target below 50 ppm to reach EURO VI,
- FSN smoke number below 1 with a target below 0.2 to reach EURO VI.

As a consequence of the exotic operating conditions, hardware and setup limitations should be kept in mind.
• Originally, this engine has been designed for peak firing pressures of 225 bar. This limit has been lowered to 200 bar due to the highly asymmetric load on the crank shaft.

• Pressure rise rates (PRR) should not exceed a certain limit to prevent engine damage and excessive combustion noise. The setup has proven to work with pressure rise rates of 30 bar/°CA. Nevertheless, this limit is lowered somewhat (15 bar/°CA) to remain on the safe side.

• Wall wetting could lead to liner damage by means of oil dilution. Although most of this fuel goes to the crank case, a small fraction will be emitted in the exhaust gas. As an indicator for wall wetting, the HC emissions have been limited to 2000 ppmC.

During the experiments, many times start of actuation (SOA) of injection timing is varied. For every SOA, the engine is stabilized for at least 60 seconds and until the standard deviation of the IMEP is below 0.1 bar. Starting from conventional CI timings, SOA is advanced at 5 degree increments, skipping SOAs at which combustion is not acceptable. Acceptable combustion in this aspect is defined by both engine hardware limitations and combustion quality targets.

While varying the injection timing, for each fuel the injection duration is determined which is necessary for a certain target load in the conventional combustion regime. This injection duration is then kept constant, while varying start of actuation and other operating conditions.

For each fuel and actuation duration, the average fuel mass flow is used with the resulting IMEP to compute the Indicated Specific Fuel Consumption (ISFC) or thermal efficiency.

By doing this, ease of measurement is greatly increased compared to keeping IMEP exactly constant and varying the injected fuel mass accordingly.

Definitions

When comparing emission levels and fuel consumption for heavy duty engines, it is common practice to calculate these brake specific (i.e. with respect to the power output at the crankshaft). In this test setup, not just the test cylinder is connected to the engine brake, so this practice is not possible. Therefore in this case, the IMEP as calculated from the in-cylinder pressure signal is used. To be able to evaluate the combustion performance also at different intake pressures and varying exhaust back pressure, the gross IMEP (thus excluding the gas exchange stroke) has been used to calculate the indicated fuel consumption and emissions in all results presented.

Specific emissions are computed from their respective concentrations as measured by the Horiba 7100, using their molar masses. Only NOx is treated as NO2 in line with European legislation. Smoke emission is computed from the measured FSN, using the empirical correlation of Christian et al. [35].

Efficiencies

As detailed in the introduction (Ch. 1), the efficiency of energy conversion in an internal combustion engine consists of four components.

The efficiency of the conversion of chemical energy into heat, or the combustion efficiency, provides information about the completeness of combustion. To calculate this combustion efficiency all specific emissions (i.e. ISCO, ISHC,
Thermodynamic test setup

ISPM and ISH, should be known. However, soot (ISPM) is often considered to be negligible for combustion efficiency since the specific emissions are low and they do not contain a lot of energy. Equation (2–1) represents the way in which combustion efficiency is calculated, where the heating value of hydrocarbon emissions is assumed to be that of the fuel.

$$\eta_{\text{comb}} = 1 - \frac{\sum_{i=\text{CO, HC, BI}} IS_i \cdot LHV_i}{\text{ISFC} \cdot LHV_{\text{fuel}}}$$  \hspace{1cm} (2–1)

ISH, is calculated using the water-gas shift reaction and gross indicated ($\eta_{\text{ind}}$) efficiency is calculated according to

$$\eta_{\text{ind}} = \frac{P_{\text{ind}}}{m_{\text{fuel}} \cdot LHV_{\text{fuel}}}$$  \hspace{1cm} (2–2)

$P_{\text{ind}} = W_{\text{ind}} \cdot n$ is based on the work done $W_{\text{ind}}$ in the compression and expansion stroke and on the engine speed $n$ in rev/s. $LHV_{\text{fuel}}$ represents the lower heating value of the fuel and $m_{\text{fuel}}$ is the fuel flow rate. Once gross indicated efficiency (based on pressure trace) and combustion efficiency (based on both pressure trace and emission level) are known, one can calculate the thermal efficiency,

$$\eta_{\text{th}} = \frac{\eta_{\text{ind}}}{\eta_{\text{comb}}}$$  \hspace{1cm} (2–3)

This thermodynamic efficiency describes the efficiency in conversion of heat to work in the compression and expansion strokes.

The pumping work, or gas exchange efficiency of the engine depends, unless one believes in the “Turbo-Fairy”, on turbine and compressor efficiency, the use of short- or long-route EGR and the amount of dilution applied.

Lastly, the mechanical efficiency, from work on the piston to work at the crankshaft, could be influenced by the combustion regime, as the loading of the engine’s frictional components may change. However, the mechanical efficiency mostly depends on the engine hardware used.

Of these different efficiency components, both the thermodynamic and gas exchange efficiencies are to be targeted with new combustion regimes. The combustion efficiency, in its turn, should stay near the levels of contemporary combustion engines.

Heat release parameters

The apparent rate of heat release is calculated using an air-standard first-law analysis, with the ratio of specific heats dependant of temperature, but not of the gas composition.

Analysis of logged injector actuation current and injection pressure data furthermore shows a constant 4 °CA lag between start of actuation (SOA) and start of injection (SOI) at 1200 rpm. In most results, the calculated crank angle at which 10% of the cumulative apparent heat release (CA10) is used as main indicator for the start of combustion (SOC), because of its considerably higher stability compared to CA5.

With this, relevant combustion properties such as ignition delay, ignition dwell, combustion delay and combustion duration are defined. The burn duration is defined as the duration between SOC and the crank angle at which 90% of the fuel has been burnt (CA90). Moreover, the duration between the end of the main injection (EOI$_{\text{main}}$) and start of combustion is also evaluated. This so-called ignition dwell, represents the separation between injection and combustion events. Combustion Delay (CD=CA50 - SOI) is used to describe the average mixing time.

In summary, the following definitions are used:

- Start Of Injection (SOI) = SOA + 4.
- Start of Combustion (SOC) = CA10
- Ignition delay (ID) = SOC - SOI$_{\text{main}}$
- Burn duration (BD) = CA90 - CA10
- Ignition dwell (IDw) = SOC - EOI$_{\text{main}}$
- Combustion Delay (CD) = CA50 - SOI

CD is also used to characterize the transition between the conventional diesel combustion regime and the PCCI regime. As SOA is advanced from conventional timings, at first CD remains nearly constant. At even earlier timings, CD increases. These points, with increased CD, are defined as PCCI combustion.
Controllability

One of the challenges of (Partially) Premixed Combustion can be (a lack of) controllability. In [36] it was proposed to use the derivative of CA50 with respect to a change in injection timing, to quantify the controllability:

\[ s_{ID} = \frac{\delta CA50}{\delta SOI} \]  

(2–4)

The sensitivity of ignition delay \( s_{ID} \) can be extracted from a SOA sweep by using a first order regression fit on the measured points. At very early injection timings, where ignition is dominated by global parameters, the response to injection timing is very low (i.e. \( s_{ID} \ll 1 \)). On the other hand, with very low-reactive fuels and late injection timings, a small change in injection timing can lead to a big change in combustion phasing, or even misfiring. As such, \( s_{ID} \) can also be much larger than one. For good controllability a value near unity, as is experienced for conventional diesel combustion, is desired.

Premixed fraction

It has been postulated that Partially-Premixed Combustion can vary in the amount of premixed combustion. In some of the following chapters, this degree of premixing is quantified by comparing the integral of the premixed combustion phase with the total heat released. The premixed phase is defined using a method similar to the one used by Solaka and coworkers [37], where a Gaussian profile is fitted to the rising flank of the premixed peak, defined as

\[ G(x) = h \cdot e^{-\frac{(x-x_0)^2}{2\alpha^2}} \]  

(2–5)

where \( x_0 \) represents the central position of the peak, and \( h \) and \( \alpha \) the height and standard deviation (width) of the Gaussian profile, respectively. From Figure 2–2 it can be seen that the fit follows the premixed heat release closely. The Gaussian profile is merely a mathematical representation of the premixed reaction phase. However, it shows a robust measure of the premixed fraction for all operated cases.

Summary

In this chapter, the thermodynamic test engine setup was described and procedures and definitions used were given. For more information on these subjects the reader is referred to [38] and other papers the test setup was used for, which are referred to in their respective results chapters.

References


Acknowledgements

Many thanks go to the people who have initially built the CYCLOPS setup: Wout de Boer, Gerard van Hattum and Marc Willekens, and those technicians who have maintained it over time; Hans van Griensven, Theo de Groot, Gerard van Hout, Bart van Pinxten and Henry Vliegen.

The work of Peter Frijters and Michael Boot on this setup is very much acknowledged, as well as the help of all students who kept the engine in one piece, and helped to improve it over time: Bas van den Berge, Jos Reijnders, Kevin Wagemakers, Peter-Christian Bakker, Bas Nijssen and Jesus de Abreu.
3 – Impact of operating conditions on PCCI combustion

Combustion in an engine is affected by a large number of parameters, many of which can be controlled by a test bed operator. Operation of a test engine is much like controlling the engines of the Queen Elisabeth 2, the operating room of which is shown in this picture.

Photo courtesy of Bene Diaper

The experimental results presented in this chapter are part of the Master thesis work of the author and have, in an extended form, been published as Leermakers et al., IJVD 62(1):1-20, doi:10.1504/IJVD.2013.051611. For further information the reader is referred to the full article.
As discussed in the introduction, in a short-term scenario, using near-standard components and a conventional diesel fuel, PCCI combustion could be made possible by a smart choice of operating conditions, albeit for just a limited load range. In the following chapter the effects of these operating conditions on ignition delay, available mixing time, combustion phasing, and emissions are investigated.

**Measurement matrix**

All experiments described here are performed on the CYCLOPS test setup, as described in the previous chapter. For the short-term scenario a standard European diesel fuel is used. To limit end-of-compression temperature to avoid premature auto-ignition, the geometric compression ratio of the test cylinder has been lowered to a value of 12:1 by using the standard XE355C piston, two head gaskets and a spacer plate.

In this measurement series, the following operating conditions are varied, as they span the low-to-medium load range where PCCI might be applied.

- Four constant injector actuation durations: 850 - 1150 - 1550 - 2100 μs, using a single injection strategy, targeting net IMEPs of 6 - 7.5 - 10 - 12.5 bar;
- Four EGR levels: 0 - 15 - 40 - 60 wt%;
- Six intake pressure levels (Pin): 1.05 - 1.25 - 1.5 - 1.88 - 2.1 - 2.5 bar absolute;
- Intake temperature (Tin) using both heavily cooled EGR, resulting in 300 K maximum, and uncooled EGR, resulting in 370 K.

Except for intake temperature, which is only tested at two intake pressures and three loads, all possible combinations are tested, taking engine hardware limitations and combustion quality targets into account. Testing this full matrix enables the identification of feasible PCCI operating ranges. For every combination of operating conditions under investigation, a sweep of start of actuations (SOA) of the injector is performed.

All tests are done at 1200 rpm. Fuel injection pressure is set to 1500 bar and fuel temperature near the injector is 30 °C. Unless stated otherwise, the EGR flow is heavily cooled to approximately 300 K.

**Results**

The results of decoupling injection and combustion are illustrated for the PCCI concept, first for an initial timing sweep. Then for one parameter (i.e. the EGR level) the effects on combustion phasing, performance, pressure rise rate and emissions are discussed in detail, with a discussion on the respective origins of the effects. After that, for intake pressure and temperature respectively, all relevant results are shown one by one. The best points experienced for a number of loads are given in order to stress the practical relevance of the measurements presented. To conclude, a summary is given of the relevant effects of different parameters on PCCI combustion.

**Results: Injection timing**

Premixed-Charge Compression Ignition (PCCI) combustion is characterized by decoupling of combustion and injection, to enable premixing of fuel and air and to lower combustion temperature. From an initial timing sweep, see Figure 3–1, one can see that as SOA is advanced from late timings, at first combustion delay and ignition dwell remain near constant as
injection and combustion are coupled. However, as SOA is advanced beyond -20 °CA aTDC, CD and ignition dwell significantly increase.

For the operating conditions shown in Figure 3–1, with a low end of compression temperature and heavy EGR, for all SOA values the ignition dwell is seen to be positive and injection and combustion are thus separated. Apart from the operating conditions, this separation might be artificial, since CA10 is used as start of combustion, and not CA0. However, the choice for CA10 is still considered valid as this represents the start of a rate of heat release more significant than the marginal values experienced at CA0.

In this work, because of this choice not the absolute value of the ignition dwell is used to define PCCI combustion, but the change in dwell and combustion delay compared to its near constant value at conventional timings. SOAs where these parameters are significantly longer have an increased mixing time and are considered to represent PCCI combustion.

From Figure 3–2 the effects of this elongated mixing time can be seen. The decoupling at timings before -20 °CA aTDC results in significantly lower NOx levels, and smoke emissions approaching zero. Fuel consumption is seen to be the lowest at a timing of -25 °CA aTDC, which is already defined as PCCI combustion.

As timing is further advanced and ignition dwell is large, both wall wetting [39], overmixing and overleaning [40] give rise to higher HC and CO emissions. The combustion quality target concerning HC emissions (i.e. max. 2000 ppmC to prevent excessive wall wetting) is met here, and as such the results are considered valid. However, fuel consumption significantly increases. At even earlier timings (<-45 °CA aTDC) presumed wall wetting, or incomplete combustion of the soot formed earlier in the stroke, results in smoke emissions increasing again.

Results: EGR level

Adding EGR is the classic way to reduce NOx emissions from conventional diesel combustion, through charge dilution and thereby lowering combustion temperatures. In the following subsections, the effects of EGR on combustion phasing, performance and emissions are shown in detail for PCCI combustion.
Impact of operating conditions on PCCI combustion

Combustion phasing and performance

From Figure 3–3, where timing sweeps are shown for different EGR levels, the effect of EGR on combustion timing can be seen. As can be expected, a higher EGR level gives a longer ignition delay and slower combustion, resulting in a significantly later CA50.

Not for all timings and EGR levels results are plotted; lacking are those combinations at which unacceptable combustion occurs, in this case because of too high pressure rise rates.

For a constant fuelling rate, as in the results under investigation, IMEP characterizes performance and efficiency. In Figure 3–4, one can see a distinction between two regimes. The nearly horizontal lines, at about 5 bar IMEP, represent conventional diesel combustion (CDC). For this regime, EGR only affects combustion phasing, and for a constant CA50, EGR is not observed to have a significant effect on efficiency.

Figure 3–4: Impact of EGR on IMEP, plotted vs. CA50. 5 bar target IMEP, 1.25 bar Pin.

HC and CO emissions

In the CDC combustion regime, HC and CO emissions are insignificant due to high localized temperatures during the combustion and the proximity of oxygen enabling their oxidation [41], even at low loads. As discussed in chapter 1, EGR allows the combustion process to be controlled by reducing the local temperature and/or by decreasing the oxygen partial pressure in the cylinder. While NOx emissions can be lowered this way, complete post-oxidation of HC and CO can become more difficult to achieve.

As discussed by Heywood [42], and summarized by Kashdan et al. [43] and Colban et al. [44], there are a number of possible sources of engine-out HC emissions. For gasoline SI engines, trapping of fuel in crevice volumes is one of the major sources of HC emissions. For CI engines, this source is particularly of importance when early-direct-injection strategies are adopted, since in-cylinder pressures are relatively low and there is significant time available for fuel spray dispersion towards these crevices.

Another potential mechanism for HC emissions formation is through flame quenching. Quenching of oxidation reactions may occur due to excessively low-temperature zones caused by heat transfer to combustion-chamber walls, or by natural thermal inhomogeneities as a result of mixing in the bulk gases. Overmixing, to
local equivalence ratios below the lean combustion limit of the mixture, can also lead to regions that do not permit complete combustion on relevant engine time scales. This is mainly thought to occur at low loads, particularly for conditions where ignition delay is long, which allows for a long mixing time.

Finally, wall wetting can be a source of HC emissions in direct injection engines. Depending on combustion chamber geometry and injection timing, spray impingement on cylinder walls results in the formation of liquid films, which gives incomplete evaporation and oxidation of the fuel. Any remaining unburned hydrocarbons within the combustion chamber can subsequently be emitted into the exhaust.

Kook et al. [40] also discuss a number of possible causes of CO emissions.

While HC emissions can consist of both uncombusted and partially oxidized fuel, CO emissions are always a result of incomplete combustion. This suggests that these CO emissions also may result from the extended ignition delay encountered in low-temperature systems. This increased mixing time results in over-mixed conditions, where combustion temperatures are too low for full oxidation of CO to be completed on engine time scales.

Considering the above, for both HC [43] and CO emissions [40], maximum cycle temperature is found to be a dominant and first order parameter.

For the points under investigation here, EGR both increases the available mixing time and lowers the combustion temperature, through changing the heat capacity of the charge. For earlier injection timings, while entering the PCCI regime, the latter effect has a predominant effect on HC and CO emissions. Both show a clear correlation with CD, which is shown for CO emissions in Figure 3–6. HC emissions follow the same trend (not shown here) which indicates that for these low loads in the PCCI regime, HC and CO emissions are predominantly caused by more and larger cold zones which cause flame quenching.

**NOx emissions**

As with other LTC concepts, EGR is used to lower the adiabatic flame temperature of the combustion. In the CDC regime, NOx levels (Figure 3–7) are seen to be effectively reduced by adding EGR, as expected. In CDC, every fuel parcel becomes stoichiometric at some time, while traveling through the diffusion flame. As such, it will feel the flame temperature belonging to the (diluted) stoichiometric mixture.

For longer ignition delays, in the PCCI regime, the fuel parcels will not experience stoichiometry and local combustion temperatures will largely depend on local equivalence ratios. The effect of EGR becomes smaller and combustion temperatures are predominantly lowered by the leaner local mixture composition.
Smoke emissions

For particulate emissions, in conventional diesel combustion, an increased EGR level lowers the air excess ratio and therefore more soot is emitted, see zoomed plot in Figure 3–8.

As start of actuation is advanced into the PCCI regime, and mixing time is increased, no direct effect of EGR can be seen. Here, smoke emission is predominantly caused by the longer mixing time and the lower combustion temperatures and soot oxidation rates associated therewith. When injection timing is even further advanced (<-45 °CA aTDC), some wall wetting is believed to occur and smoke emission increases to unacceptable values. For all other points under investigation the absolute smoke levels are quite low, because of the relatively low loads and the injection pressure and equipment used.

Results: Air intake pressure

Combustion phasing and performance

A lower air intake pressure significantly retards combustion phasing, resulting in a longer combustion delay (CD) (Figure 3–9). This is necessary to phase combustion correctly at early timings, because when CA50 is advanced to before TDC, pressure rise rates become unacceptable.

Considering that all comparisons are based on the gross IMEP and that the fuel mass is kept constant, intake pressure in itself does not give a big difference in IMEP, as the gas exchange strokes are excluded. CA50, however, is the dominant parameter. Like was seen with EGR, for longer combustion delays, IMEP again correlates with this CD (not shown here).

HC and CO emissions

Figure 3–10 shows that at elongated mixing times, HC emissions again show a nearly perfectly linear correlation with CD. The higher intake pressure here only shows a direct influence on this CD. This CO/HC trend with CD was also seen with EGR and was attributed to less complete combustion due to lower local temperature as a result of a more premixed charge.
Impact of operating conditions on PCCI combustion

If the hydrocarbon emissions were to a large extent a result of wall wetting, an increase of intake pressure should have made much more of a difference. An increase of intake pressure (and therewith in-cylinder density) reduces the penetration length of the liquid spray, and thus wall wetting. This shows that wall wetting might be present, but is insignificant compared to the over-mixing and over-leaning effects as seen before for EGR.

NOx and smoke emissions

As ignition delay is increased into the PCCI regime, even when only slightly, NOx levels are greatly decreased, because of a more premixed charge (see Figure 3–11).

Only small differences can be seen between the different pressure levels, attributed to their respective oxygen concentrations. Air excess ratios were 1.2, 1.4, 1.7 and 2.1 for intake pressures 1.5, 1.88, 2.1 and 2.5 bar, respectively.

Smoke emissions, for both CDC and slightly premixed CI, from Figure 3–12 can be seen to depend on the intake pressure and thus the global equivalence ratio.

One can clearly see that premixing greatly reduces smoke emissions levels, and at a CD of 30 °CA, smoke emissions even approach zero, for all pressure levels.

As CD is further increased, even lower combustion temperatures and resulting lower soot oxidation and possibly wall wetting, result in considerable smoke levels.

It is therefore desirable to have the CD not excessively long, while still achieving the desired NOx and smoke levels.
Results: Air intake temperature

With high levels of premixing, more homogeneous conditions are achieved and at such conditions, control of intake temperature is essential.

For the selected fuel and compression ratio, an intake temperature of 300 K can be seen to be about right to phase CA50 just after TDC for the earlier injection timings, see Figure 3–13. The higher 355 K temperature can be seen to advance combustion significantly, resulting in CA50 even before TDC, which results in unacceptably high pressure rise rates.

At the latest injection timings, in the conventional diesel combustion regime, less effect of intake temperature can be seen, as in this regime combustion phasing is more directly coupled to the injection timing and temperature has less of an effect. When long mixing times are used, particular attention has to be given to intake temperature control. Load and fuel consumption, parameterized by IMEP and ISFC, are not directly affected through the higher intake temperature. However, indirectly they are affected in two ways. First, as the higher temperature advances combustion to early timings, this results in higher fuel consumption. For the same CA50, however, the higher temperature level has a lower fuel consumption, caused by the shorter CD and more complete combustion associated with that. For compactness, graphs have not been included here, as they show exactly the same trends as presented for intake pressure.

The principal motivation for elevating intake temperature has been to reduce wall wetting. From the results, however, it can clearly be seen that CA50 is advanced by the higher starting temperature, and CD is thus shortened. HC and CO emissions benefit from the much shorter mixing time and higher combustion temperatures, see Figure 3–14 for HC emissions (CO emission trend not shown here). For the points under investigation, no clear indication of (a reduction of) wall wetting can be seen and most CO and HC emission are thought to be formed by cold zones in the combustion chamber. If wall wetting would be present, one could expect a sharp rise in UHC emissions disproportional to CO emissions.

The shorter CD, although even slightly, together with a higher starting temperature increases the NOx emission significantly (not shown here), even at the high EGR rates used. It is therefore of great importance that the EGR gases that are used are cooled. For very short CDs, in the CDC regime, no significant effect of the higher temperature on particulate emissions can be seen.
Impact of operating conditions on PCCI combustion

Best points

For the purpose of comparison, best points are defined in three ways:

- **Best conventional diesel combustion (CDC) point**: where the gross ISFC is lowest, without any emission levels imposed.

- **Best point with After Treatment**: Assuming SCR efficiency to be minimum 90%, maximum NOx levels may be 4 g/kWh to meet Euro VI levels post SCR. Furthermore, smoke emission may be 0.1 g/kWh if a passively regenerated DPF is used to further reduce smoke to Euro VI levels post DPF. The point with lowest ISFC, while still meeting these two targets, is taken as the best point for this case.

- **Best direct Euro VI point**: This case is thought to be of importance during cold starts for instance, where after treatment systems are not effective. The point where Euro VI levels (0.4 g/kWh for NOx and 0.01 g/kWh for smoke) are ISFC is lowest is taken to be the best point.

Note that even when NOx and smoke limits are met for the best points, an oxidation catalyst may have to be used to meet Euro VI limits on ISCO and ISHC.

In Table 3–1 the best points are given for the 5 and 10 bar IMEP cases. For all points under investigation, smoke is not the limiting factor in meeting Euro VI levels, but NOx is. Furthermore, best ISFC is experienced when CA50 is slightly after TDC. For the points where EGR is used, these gases are cooled to ambient conditions.

At this compression ratio, very high pressure rise rates are experienced for the CDC best points. Furthermore one can note that best ISFC is experienced when no EGR is used. Therefore this is really conventional diesel combustion, although the ignition dwell for the 5 bar point is positive. This is attributed to the short injection duration for this load. For the 10 bar IMEP case, because of the longer injection duration, ignition dwell is negative and thus a large overlap between injection and combustion exists.

### Table 3–1: Diesel best points. Red values beyond hardware limits.

<table>
<thead>
<tr>
<th>Conditions</th>
<th>5 bar IMEP</th>
<th>10 bar IMEP</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>SOI [°CA aTDC]</strong></td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td><strong>Pin [bar]</strong></td>
<td>1.24</td>
<td>1.27</td>
</tr>
<tr>
<td><strong>Tin [K]</strong></td>
<td>298</td>
<td>303</td>
</tr>
<tr>
<td><strong>EGR [wt %]</strong></td>
<td>no EGR</td>
<td>40%</td>
</tr>
<tr>
<td><strong>CA50 [°CA aTDC]</strong></td>
<td>3.42</td>
<td>5.45</td>
</tr>
<tr>
<td><strong>Ign dwell [°CA]</strong></td>
<td>2.46</td>
<td>4.79</td>
</tr>
<tr>
<td><strong>CD [°CA]</strong></td>
<td>9.42</td>
<td>11.45</td>
</tr>
<tr>
<td><strong>MPRR [bar/°CA]</strong></td>
<td><strong>43.9</strong></td>
<td>26.1</td>
</tr>
<tr>
<td><strong>Performance</strong></td>
<td>185.8</td>
<td>188.1</td>
</tr>
<tr>
<td><strong>Emissions</strong></td>
<td>3.83</td>
<td>2.44</td>
</tr>
<tr>
<td><strong>ISPM [g/kWh]</strong></td>
<td>0.0001</td>
<td>0.0003</td>
</tr>
<tr>
<td><strong>ISCO [g/kWh]</strong></td>
<td>3.76</td>
<td>5.50</td>
</tr>
<tr>
<td><strong>ISHC [g/kWh]</strong></td>
<td>0.72</td>
<td>1.46</td>
</tr>
<tr>
<td><strong>ISNOx [g/kWh]</strong></td>
<td>16.42</td>
<td>2.61</td>
</tr>
</tbody>
</table>
If after-treatment systems are to be used to meet Euro VI legislation limits, a medium EGR level of 40% is seen to give best ISFC. This classic route to low-temperature combustion uses the same injection timing and suffers of a 1.2% penalty in fuel consumption, as compared to the best point where no NOx limits have to be met.

As engine-out NOx levels have to be further reduced to directly meet Euro VI, even more EGR is used and injection is somewhat advanced, for the 10 bar best point to an unconventional early-injection timing combustion delay is then long enough to meet the targets. Also MPRR is effectively lowered by the EGR. Somewhat higher ISCO and ISHC notwithstanding (accounting for about 60% of the ISFC penalty compared to the CDC best point), fuel consumption is nearly the same as with the higher NOx limit.

This fuel consumption trade-off will tip towards the Euro VI best points if one also considers additional costs related to the higher NOx levels (e.g. SCR fluid, investment costs, etc.).

Conclusion

In the PCCI regime, NOx and smoke have been shown to be efficiently reduced with this elongated mixing time. The lower combustion temperatures associated with a better mixed charge, though reducing NOx, result in lower combustion efficiency, which can be seen in higher CO and HC emissions and fuel consumption. For viable PCCI combustion, one thus would require a CD which is long enough to bring both NOx and smoke levels down to acceptable values. However, for the completeness of combustion, the resulting HC and CO emissions and therewith associated fuel consumption, mixing time should be as short as possible.

For most parameters, a strong correlation with the combustion delay exists, independent of how this CD is achieved. The mixing time can be increased by increasing the EGR level, lowering intake pressure and/or temperature and by advancing injection timing. While injection timing and intake pressure are easy to set in a modern heavy duty engine, in-vehicle-use issues are associated with lowering intake temperature, especially at high levels of EGR, because of the large coolers that are necessary. While the desired CD may be relatively easy to achieve by different parameters, to meet the maximum pressure rise rates and to have as low as possible fuel consumption, combustion phasing has to be optimized.

Even when using a low compression ratio, while using a fuel as reactive as current EN590 diesel not every CD can be chosen, especially at higher loads. Even at low loads, very high EGR levels and a low intake pressure and temperature are necessary to allow combustion to be phased correctly. The best points have shown that it is possible to achieve Euro VI NOx and smoke levels with a fuel penalty of less than 3% compared to the best conventional diesel point at the same compression ratio. The combustion efficiency associated with these Euro VI points is only slightly worse, but at higher loads the pressure rise rate reaches the limit.

References


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4 – Using diesel-like fuels for PCCI

In a short term scenario, application of any new combustion concept would be the easiest if readily available fuels can be used. Therefore in this chapter the performance of different types of diesel fuels are compared.
As discussed in the introduction, in a short-term scenario, using near-standard components, conventional diesel fuel should be used for PCCI combustion. However, with conventional Heavy Duty Direct Injection (HDDI) hardware and such diesel fuels a number of challenges are present for PCCI. The high boiling range of current diesel fuels has the intrinsic risk of wall-wetting when injected early [46][48][49], and these fuels have Cetane Numbers ranging between 40 and 60 and are thus very prone to auto-ignition [50]. In the following chapter the effects of using such different diesel-like fuels are investigated.

**Diesel-like fuels selection**

For the short term scenario, fuels are selected that both reflect short term changes in diesel fuel composition and are expected to be compatible with current conventional CI diesel engines (see Table 4–1). The European diesel fuel selected (EN590) reflects the current trend in Europe towards lower density, low-sulphur, low poly-aromatic diesel fuels with relatively high Cetane Numbers and a lower final boiling point temperature. In the United States (US), until now, diesel fuels are characterized by a significantly lower Cetane Number. Testing such a fuel can give an idea of the effects of a lower CN and might show whether such a cheap, readily available distillate fuel makes a good PCCI fuel.

Table 4–1: Pure fuel specifications. Note: RME is used as a 30 vol% blend with EN590, called B30

<table>
<thead>
<tr>
<th></th>
<th>EN590</th>
<th>US</th>
<th>RME</th>
<th>n-C7</th>
</tr>
</thead>
<tbody>
<tr>
<td>T10 [°C]</td>
<td>210</td>
<td>215</td>
<td></td>
<td></td>
</tr>
<tr>
<td>T50 [°C]</td>
<td>268.5</td>
<td>269</td>
<td>BP=300</td>
<td>BP=98</td>
</tr>
<tr>
<td>T90 [°C]</td>
<td>333.3</td>
<td>323</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DCN [-]</td>
<td>55.9</td>
<td>41</td>
<td>≈ 53</td>
<td>≈ 53</td>
</tr>
<tr>
<td>Aroms [m%]</td>
<td>30.7</td>
<td>35</td>
<td>none</td>
<td>none</td>
</tr>
<tr>
<td>Density [kg/m³]</td>
<td>≈ 825</td>
<td>848.1</td>
<td>875-900</td>
<td>684</td>
</tr>
<tr>
<td>LHV [MJ/kg]</td>
<td>41.54</td>
<td>42.78</td>
<td>≈ 37.2</td>
<td>44.56</td>
</tr>
</tbody>
</table>

In 2009 the European Commission has decided in Directive 2009/28/EC that the share of energy from renewable sources in the transport sector must amount to at least 10% of final energy consumption in the sector by 2020. For diesel, the most likely scenario is therefore the increased blending of biodiesel with petroleum-derived distillate diesel. Given that the base fuel already has about 5% RME, a test blend of the reference diesel with an added RME content of 30% is used to accentuate possible effects.

With current diesel fuels, having high upper boiling point temperature, injection of fuel early in the compression stroke might result in wall-wetting, because vaporization is slower or even incomplete due to the lower gas temperature and density at these timings. A comparison of the HC emissions from pure n-heptane (n-C7) with those from regular diesel should give an indication of the potential gains that could result from lowering the boiling point range of current diesel, since their Cetane Numbers are similar. As n-heptane is often used as a single component substitute fuel for diesel spray and combustion modeling, comparing these two fuels can tell if n-heptane is also a valid surrogate fuel for PCCI combustion.

**Measurement matrix**

All experiments described here are performed on the CYCLOPS test setup, see chapter 2.

All tests were done at 1200 rpm. Fuel injection pressure is set to 1500 bar and fuel temperature near the injector is 30 °C. The EGR flow is cooled to a temperature of ca. 300 K.

To limit end-of-compression temperature in order to avoid premature auto-ignition, the geometric compression ratio of the test cylinder has been set to 12:1 by using the standard XE355C piston, two head gaskets and a spacer plate.

Auto-ignition chemistry is mainly governed by chemical kinetics. Therefore, control of the combustion phasing does not only depend on fuel type but also on in-cylinder conditions, see [47]. These in-cylinder conditions are in-
fluenced using different levels of the following parameters: Fuelling rate / EGR level / Intake pressure, see Table 4–2.

Table 4–2: Operating conditions

<table>
<thead>
<tr>
<th>Intake pressure</th>
<th>1.25 bar - 1.5 bar</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aim load (IMEP)</td>
<td>5 bar - 7.5 bar - 10 bar</td>
</tr>
<tr>
<td>EGR level [wt%]</td>
<td>No EGR - 15 - 40 - 50 - 60</td>
</tr>
</tbody>
</table>

All possible combinations are tested, taking the hardware safety limitations and combustion quality targets mentioned on page 16 into account.

In all experiments a single injection per cycle is used. For every combination of operating conditions under investigation, a sweep of start of actuation (SOA) of the injector will be performed.

Results and discussion

In view of the large quantity of results acquired, only a selection of the operating points tested is presented here. The results that are presented correspond to an actuation duration of 850 microseconds (6.12 °CA), except for n-heptane, where because of its significantly lower volumetric energy density, the injector was actuated for 900 microseconds to achieve the 5 bar target IMEP.

Combustion phasing

The differences between the fuels with respect to combustion phasing, as shown in Figure 4–1, can be divided into two parts.

For all injection timings the US diesel fuel, which has a Cetane Number of about 15 points lower than that of a European diesel fuel, shows an increase in CA50 of 3-5 degrees for all injection timings. This is in accordance with expectations and although the difference may seem small, especially near TDC this difference can have a large impact on efficiency.

The other three fuels have similar reactivity as expressed in the cetane number. Any differences between these fuels are thought to origi-
**Performance**

The performance of different fuels is characterized by the indicated specific fuel consumption (ISFC), where the fuelling rate is normalized for a constant load and thus the differences in density are taken into account. Because of different combustion delays, in Figure 4–3 the ISFC is shown against CA50, thereby enabling comparison at similar combustion phasing. The sequences in this figure represent SOA sweeps, with the rightmost points starting at late timings, and CA50 earlier for earlier SOA timings. For even earlier injection timings CA50 stabilizes while fuel consumption gets worse, as will be shown next.

![Figure 4–3: Performance: ISFC vs. CA50](image)

While all the fuels have nearly the same IMEP, fuel consumption shows some differences. Clearly, the EU diesel is the best performing fuel, followed by the US diesel and n-heptane. Worst performing is the biodiesel blend, obviously due to a significantly lower energy density. While comparing the ISFC for a fixed CA50 gives an idea of the energy density and thermal efficiency for each fuel, the ISFC is also plotted against CD for all operating points (Figure 4–4).

The trend of increasing fuel consumption with larger combustion delays will be explained by a reduced combustion efficiency, as will be shown in the next section.

![Figure 4–4: Performance: ISFC vs. CD](image)

To take the differences in lower heating values into account, approximate values as given in Table 4–1 are used for the energy densities of the fuels to compute the thermal efficiency, as shown in Figure 4–5.

The EN590 diesel has the highest efficiency for a certain CA50. All other fuels perform slightly worse. After the experimental investigation, some suspicions arose on the validity of the lower heating value for EN590, but no fuel was available for a retest. Assuming a higher value of 43 MJ/kg for the LHV of diesel (which is more in line with commonly reported values) would put the thermal efficiency in line with that of the other fuels. Figure 4–5 furthermore confirms that describing performance of the biodiesel blend with the ISFC, as in Figure 4–3, is a bad

![Figure 4–5: Performance: Indicated efficiency vs. CA50](image)
Using diesel-like fuels for PCCI

measure, as its differences can be fully attributed to its lower energy density. Thermal efficiencies are all quite low, but this is as expected for the compression ratio of 12 and the low load.

**HC and CO emissions**

Lowering the boiling range of a conventional diesel fuel might be a solution to reduce presumed wall wetting. When comparing ISHC emissions at a constant SOA, see Figure 4–6, a clear distinction between the fuels is visible. From these results, the North American diesel fuel clearly performs worst. The biodiesel blend and n-heptane perform best, with the reference EN590 diesel fuel in between. Also the trend with high levels both at late and early timings, with much lower levels in between, is clearly visible. The same trends occur for CO emissions (not shown).

These findings are largely attributable to the mixing time associated with the different fuels. When looking at a constant CD, certainly when only taking points from the PCCI regime (with a longer CD than for diesel-like combustion) into account, this effect becomes clearly visible. First, in Figure 4–7 the effects of fuel composition on the HC emissions are shown, only for the PCCI regime. Here the trend is that HC emissions increase for longer CDs. While for the European and North American diesel fuels this correlation is nearly the same, for the biodiesel blend the trend is somewhat lower.

This effect can be explained by three reasons. First, local temperatures can be higher with biodiesel blends than for regular diesels, see [51]. There it is proposed that local combustion temperatures can be higher due to reactions occurring in mixtures that are closer to stoichiometric, due to the oxygen content of biodiesel. For the same initial conditions (p, T) full oxidation of the fuel is then somewhat more likely. Most of this difference, however, should be attributed to the fact that the boiling range of the biodiesel used is towards the upper end of that of regular diesel. For the same mixing time, this heavier fuel is expected to be less prone to overleaning. If premixed burn occurs in a too lean mixture, local combustion temperatures remain low, with too slow burning for full CO \rightarrow CO_2 conversion on engine-relevant time scales. As shown in [52] and [53] lower injection pressure can help in this matter. As in the PCCI regime injection pressure is generally not required to be very high, lowering fuel pressure can be an efficient strategy to prevent overleaning. Together with the better intrinsic oxidation associated with the oxygen-containing biofuel, these effects are thought to result in low HC and CO levels for every CD.
Because n-heptane has a much lower boiling point than the other fuels, overleaning is more likely to occur for this fuel. Looking at HC emissions, indeed this assumption seems valid. For every CD longer than 18 °CA, HC emissions are significantly higher than those of regular diesels. While for a constant SOA these HC emissions are low, this is entirely due to the shorter CD. For the same CD, the higher volatility even worsens HC emissions, so wall wetting is certainly not the driving mechanism. For CO (Figure 4–8) however, the assumed volatility effect is not visible when using n-heptane. Between the two diesel fuels, no significant differences can be seen for CO emissions. Overall, although small differences are visible between the fuels, the CD, or mixing time, is still the dominant parameter.

![Figure 4–8: CO emissions: ISCO vs. CD (PCCI only). 5 bar aim IMEP, 1.5 bar, 60% EGR](image)

**Smoke emissions**

Smoke emissions have proven to be very difficult to compare among the different fuels. As in these experiments advanced fuel injection equipment, low loads, a nozzle with small holes and an already relatively high injection pressure are used, the absolute smoke emission levels are under the Euro VI level of 0.01 g/kWh for almost all points. In an attempt to show differences originating from fuel composition, results are presented for the highest load, with the highest in-cylinder equivalence ratio. Though not all SOA can be used for all fuels, at these conditions it is the best comparison possible from the investigated points.

For all operating conditions and loads under investigation, n-heptane did not produce any significant smoke levels, see Figure 4–9. This phenomenon is directly related to its paraffinic structure, as compared to the aromaticity of normal diesel fuels and to faster mixing because of a lower boiling point.

![Figure 4–9: Smoke emissions: ISPM vs. CD 8 bar aim IMEP, 1.5 bar, 60% EGR](image)

Although smoke levels are low, the EN590 diesel clearly benefits from an increased CD. An only slightly elongated mixing time already reduces smoke levels to near zero. For all SOA the US diesel has much lower, near zero smoke levels. It is clear, however, that this largely comes from the longer CD associated with its low Cetane Number. This also shows that, at least for smoke emissions, the trend of ever increasing CN is not desired. Unfortunately, since the polyaromatic content is not known for the US diesel, no conclusions can be drawn about the effect of these polyaromatics. Finally, although the biodiesel blend mixes slightly worse because of its lower volatility, its oxygenation makes that smoke levels are significantly lower than those experienced with conventional diesel fuels.
**Using diesel-like fuels for PCCI**

**NOx emissions**

To compare NOx emission levels for different fuels, an operating point using 30% EGR is chosen. This relatively low EGR percentage obviously gives higher NOx levels than the 60% EGR point discussed up till now, making the comparison of different fuels more significant. In the conventional diesel combustion regime, at relatively late injection timings, the common NOx–SOA trend is experienced: NOx emissions increase as combustion is advanced towards the most efficient phasing. On the difference between the fuels, however, no clear trend can be seen. As SOA is advanced, resulting in slightly elongated CDs, from a CD of ca 20 °CA one can clearly see the trend of decreasing NOx levels with CD, see Figure 4–10.

![Figure 4–10: NOx emissions: ISNOx vs CD](image)

From this combustion delay, the equivalence ratio span of the mixture is thought to become so lean, that even local equivalence ratios become leaner than stoichiometric. This results in lower local combustion temperatures and accordingly in reduced NOx levels.

Differences between the fuels could originate from different volatility or flame temperatures. As no significant differences can be seen between the fuels, both effects are either counterbalancing or insignificant compared to the effect of the mixing time. For this moderate EGR level, the current Euro V NOx legislation limit of 2 g/kWh is already approached at a moderate CD of 30 °CA. The upcoming Euro VI limit of 0.4 g/kWh is achieved at a longer CD of 45 degrees. Using more EGR, NOx levels can be decreased below current legislation limits, already at much lower CDs, which is beneficial with respect to the increasing effect of CD on HC and CO emissions.

**Maximum pressure rise rate**

Because the composition and the Cetane Number of the fuel were found to influence the combustion phasing significantly, it is expected that these will also affect maximum pressure rise rate. As can be seen from Figure 4–11 indeed the US diesel, having both the latest CA50 and the longest mixing time and thus the most homogeneous, lean mixture, has the lowest maximum pressure rise rate. n-Heptane, which was seen to have the earliest CA50 and shortest CD, has the highest pressure rise rates.

![Figure 4–11: Maximum pressure rise rate vs. CA50](image)

Certainly when injection is advanced into a more and more premixed combustion regime, a significant level of homogeneity is achieved for all fuels. CA50 then stabilizes and is decoupled from SOA. As the mixture gets more time to premix, all local equivalence ratios become leaner than the value at which minimum burn duration is experienced. From this point...
onwards, both the ignition delay and the burn duration are reduced as mixing time is increased and local equivalence ratios become even leaner. This effect has been illustrated in Figure 2.1 of [54]. Accordingly, maximum pressure rise rates are reduced significantly at these highest mixing times.

Summary and conclusions

At the relatively low compression ratio under investigation, the US diesel, having a somewhat lower Cetane Number than European diesels, was shown to effectively increase Combustion Delay (CD = CA50 - SOI). While this helps to phase combustion correctly, the increased mixing time reduces NOx and smoke levels significantly. CO and HC emissions are, however, seen to increase with mixing time, and the resulting poor combustion efficiency has a negative effect on fuel consumption.

When comparing fuels of different composition in the PCCI regime, the CD is seen to be the dominant parameter. While other differences between fuels, for instance in volatility and reactivity, have their own effects on emissions and performance, the major impact is related to the combustion phasing and the resulting available mixing time. A longer mixing time for all fuels has a negative effect on combustion efficiency, CO and HC emissions and the associated fuel consumption. NOx and smoke levels, as well as the maximum pressure rise rate are effectively reduced, for the latter also because this allows combustion to be phased more after TDC. Because of their composition, the biodiesel blend and n-heptane also produced very low smoke levels, as expected from literature.

n-Heptane was also investigated to verify its validity as a single component surrogate fuel for diesel modeling. This validity has proven to be limited under the PCCI regime, since for these conditions, combustion phasing for n-heptane is proven to be significantly different from that of diesel. Because the combustion phasing is earlier for n-heptane and the resulting CD is shorter, all parameters associated with those are different, as compared to regular diesel fuel. This means that when using n-heptane for modeling, CO and HC are generally underestimated, while NOx levels will be overestimated. A better surrogate fuel would need to have the same auto-ignition characteristics for the conditions under investigation. A suggestion for such a fuel, consisting of n-decane, methylcyclohexane and toluene has been proposed in [55].

In this chapter, indicated efficiency was shown to be maximum 45%, partly attributed to the low compression ratio of 12:1. In the following chapter, a higher compression ratio is used, which enables a higher efficiency. However, a less reactive fuel is required to delay auto-ignition and phase combustion correctly. Such a low reactive fuel can also have additional emission benefits.

References


Acknowledgements

Funding for this project was provided by NCM (Dutch committee on engine fuels and lubricants) and SMO (Dutch foundation on engine education). This funding and the analysis of fuels by Shell Global Solutions UK are gratefully acknowledged.
5 – Using low reactive diesels for PCCI

The usage of fuels other than regular diesel or gasoline, enables a choice of reactivity, and therewith allows to phase combustion as desired. A low-reactive aromatic solvent is added to diesel to tune its reactivity.

Photo courtesy of Simon Santerre, 2009. Taken in Montreal, QC.

The experiments presented in this chapter have been performed by Bas van den Berge, under supervision of the author, and have, in an extended form, been published as Leermakers et al. (2011), SAE Technical Paper 2011-01-1351, doi:10.4271/2011-01-1351.

After publication of this paper, an error was found in the calibration of the cylinder pressure sensor. This has been corrected for the present chapter.
In a longer term scenario, both engine hardware and fuels can be adapted to overcome intrinsic PCCI challenges. The compression ratio of the CYCLOPS test setup is set to 15:1 by using the standard XE355C piston and a double head gasket. The higher compression ratio (as compared to the previous chapter) enables a higher efficiency, but increases end-of-compression temperature. Consequently, a less reactive fuel is likely to be required to delay auto-ignition and phase combustion correctly. To evaluate the effect of lowering diesel fuel reactivity, the reference diesel is blended with Shellsol A100, which is an aromatic solvent with diesel-like properties except for a much lower reactivity and a somewhat higher volatility, compare Table 5–1 to Table 4–1 on page 31.

Table 5–1: Shell demonstrates A100 volatility characteristics

<table>
<thead>
<tr>
<th>IBP</th>
<th>T10 [°C]</th>
<th>T50 [°C]</th>
<th>T90 [°C]</th>
<th>FBP</th>
</tr>
</thead>
<tbody>
<tr>
<td>162.8</td>
<td>163.8</td>
<td>164.9</td>
<td>168.5</td>
<td>180</td>
</tr>
</tbody>
</table>

Both the reference diesel fuel and two initial test blends have been tested in an ignition quality tester (IQT, [56]) to determine their derived Cetane Numbers. The blends given in Table 5–2 have been made using the results of these IQT tests, assuming linear blending rules. In all results, the assumed CN is used to denote these blends.

Table 5–2: Derived CN of low-reactivity blends

<table>
<thead>
<tr>
<th>DCN [-]</th>
<th>55.9</th>
<th>40</th>
<th>30</th>
<th>25</th>
<th>20</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diesel [%]</td>
<td>100</td>
<td>73.7</td>
<td>53.6</td>
<td>42.2</td>
<td>29.8</td>
</tr>
<tr>
<td>A100 [%]</td>
<td>0</td>
<td>26.3</td>
<td>46.4</td>
<td>57.8</td>
<td>70.2</td>
</tr>
</tbody>
</table>

All tests were done at 1200 rpm. Fuel injection pressure is set to 1500 bar and fuel temperature near the injector is 30 °C. The EGR flow is cooled to a temperature of ca. 300 K.

A broad range of operating conditions was tested, with load varying from 5 to 15 bar gross IMEP, varying intake pressure, and with and without EGR. In this chapter, only the 5 bar aim IMEP, 2 bar intake pressure points are discussed, without using any EGR. These points have proven to give the most clear trends in initial tests with more combinations.

In all experiments a single injection per cycle is used and for every combination of operating conditions under investigation, a sweep of start of actuation (SOA) of the injector will be performed.

**Results and discussion**

It should be noted that the conditions that are presented are chosen to illustrate the effect of the different fuels on phasing and emissions and do not necessarily give the best achievable results for the emission levels.

*Combustion phasing*

The Cetane Number represents a fuel’s ignition delay under specified conditions. In Figure 5–1 it is shown that this trend also holds for the operating conditions under investigation here. Some points are missing from this graph, as at these SOA hardware limits or combustion targets were breached. The differences between diesel and the CN40 blend are not significant, because of the compression ratio used. For the other blends the trend of increasing ignition delay with decreasing (derived) Cetane Number is clearly visible, both in the conventional combustion regime and for PCCI combustion.

![Figure 5–1: Ignition delay vs. start of actuation. 5 bar aim IMEP, 2 bar, no EGR](image-url)
For emissions and performance in the PCCI regime, Combustion Delay has been shown to be the most important parameter. From Figure 5–2 it is noteworthy that for conventional operating points no clear difference in CD can be seen between the different fuels. This implies that the difference in ignition delay is offset by a higher combustion speed. For the PCCI regime, this does not seem to hold. In this regime, the lower reactivity clearly accounts for a higher combustion delay. Also from this graph the clear distinction between conventional and PCCI combustion can be seen from the change from a near constant combustion delay to a changing one for timings earlier than -20 °CA aTDC.

With the higher reactivity fuels a number of points cannot be measured because of excessively high pressure rise rates. The low reactivity fuels suffer less from this issue. These low reactivity blends, however, achieve high combustion delays and relatively late timings. At even earlier timings combustion delay becomes too large, which causes the charge to become too premixed and locally too lean to ignite. As such the CN20 blend was not usable for the operating conditions under investigation. The long ignition delays at this low load point create too lean mixtures, which fail to ignite under these conditions.

In Figure 5–3, the measured ISFC is plotted against CA50 of the four SOA sweeps. For a fixed CA50, fuel consumption worsens with lower fuel reactivity. This is, however, largely attributable to the lower energy density of the additive compared to the diesel base fuel. At earlier timings, the combustion delay is longer for the low reactivity blends, which leads to a lower combustion efficiency, as will be shown in the following section.

ShellSol A100, being a 98% C9/C10 Aromatic hydrocarbon solvent, has a somewhat lower LHV than the more aliphatic regular diesel fuel. As the blends consist of up to 58% of this aromatic solvent, this slightly influences the specific fuel consumption. Because the exact lower heating values of neither the components nor the blends are known, it is not possible to exactly compensate for this.

**HC and CO emissions**

As shown in the previous chapter, a more premixed charge with local mixtures that have lean mixture composition is associated with lower combustion temperatures. This makes that combustion efficiency decreases with combustion delay. As for the diesel-like fuels, also with the low reactivity fuels under investigation here, HC- (Figure 5–4) and CO-emissions (not shown) largely correlate with combustion delay.
Using low reactive diesels for PCCI

Smoke emissions

All points under investigation have shown to be very low sooting, which does not make a fair comparison of smoke emissions between the fuels possible. The combination of a high injection pressure, low loads and very small nozzle holes makes that no conclusions on sooting tendency can be drawn. Earlier, however, it was shown that a longer CD reduces sooting efficiently. Therefore, it is safe to assume that for this set of fuels, at higher sooting conditions a lower CN fuel, with its associated longer CD, will also reduce soot significantly. As this also reduces NOx, this is a way to break the common NOx/soot trade off.

Summary and conclusion

For the low reactivity blends it was shown that the difference in Cetane Number has the desired effect of increasing combustion delay. Similar to the previous low compression ratio study (chapter 4), a longer mixing time for all fuels has a negative effect on combustion efficiency, CO and HC emissions and the associated fuel consumption. NOx and smoke levels, as well as the maximum pressure rise rate are effectively reduced, for the latter also because this allows combustion to be phased more after TDC.

To be able to choose the combustion delay according to the operating conditions, especially at this higher compression ratio, a low reactivity blend is necessary. The blend with an estimated CN of 25 was found to be the most flexible in being able to choose the optimum CD for the conditions and load used. This high flexibility enables the possibility for a CD to be chosen which meets NOx and smoke targets simultaneously, without suffering from too high a loss of combustion efficiency.

References


Acknowledgements

Funding for this project was provided by NCM (Dutch Committee on engine Fuels and lubricants) and SMO (Dutch Foundation on Engine Education). This funding and the supply and analysis of fuels by Shell Global Solutions UK are gratefully acknowledged.
LPG (Liquefied Petroleum Gas) has for long been used as an automotive fuel in light vehicles like private cars and taxis. LPG is a by-product of the refining process of conventional gasoline and diesel fuels, resulting in a low fuel price [57]. LPG consists of butane and propane, and depending on fuel grade and region of the world, LPG ranges from nearly pure propane (95%) to nearly all butane (>80%). In the Netherlands, LPG is widely available and due to tax benefits it is attractively priced compared to, for example, diesel.

LPG can be used in heavy-duty diesel engines, combining port fuel injection of LPG and a direct injection of diesel. Dual fuel engines equipped with a port fuel injection (PFI) system can offer operational cost savings, but typically suffer from the problems of poor brake thermal efficiency and high HC emissions, particularly at low loads [58].

The goal of this research is to explore whether the use of a premixed fuel can neutralize the emission penalty of PFI LPG, while maintaining the operational cost savings. This might be extended to a further reduction of fuel costs combined with a simultaneous emission benefit.

A diesel-butane blend contains less energy per volume, resulting in higher fuel consumption in terms of L/km [57][59]. With the right blend composition this fuel consumption increase might be compensated by lower fuel costs.
Experimental apparatus

The fuel system of the CYCLOPS test setup was adjusted to inject pre-mixed diesel-butane blends directly into cylinder 1 (Figure 6–1). A standard LPG tank with a built-in low pressure fuel pump provides the blend at 5 bar over the vapor pressure to the high pressure pump. Fuel density is monitored to be confident that the fuel blends do not partially or fully separate within the fuel system.

The fuel pressure is set to 1500 bar. The injector leak flow is captured in a surge tank. This tank will reach a pressure of 10 bar maximum, because this is the highest vapor pressure of the blends at 90°C, which is the temperature of the cylinder head at the leak flow of the injector.

To test direct injection back to back with port fuel injected butane, the setup is also equipped with a port fuel injection (PFI) system. In this case, the low pressure pump in the LPG tank is directly coupled to this liquid fuel PFI injector.

Fuels and operating conditions

To test the viability of direct injection of a diesel mixed with LPG, a standard EN590 diesel fuel is compared to three butane-diesel blends, see Table 6–1. These blends are called But14, But33, But50, after their respective mass percentages of butane in the blend. Butane is used instead of LPG, both to be more certain of the blend composition and to limit blend vapor pressures for hardware safety reasons. Injector stability is guaranteed up to 10 bar back pressure, therefore the return pressure should not exceed this value. The blends have been chosen accordingly.

To calculate blend properties, data from Younglove [61] and the DIPPR database [62] are used. Kalghatgi has given a relation in [63] to calculate the estimated Cetane number (ECN), based on the octane number of a low reactive fuel, such as LPG. Furthermore, Kalghatgi states that the Cetane number scales linearly with the molar fractions of the two fuels in the blend. The more butane is added to the fuel the less reactive the blend becomes. Note that the energy density per unit volume also decreases when the butane content is increased. The maximum vapor pressure of the blends in the fuel line is calculated using Raoult’s law [64]. In this case the vapor pressure of diesel can be neglected.

Besides testing diesel and three diesel-butane blends, as a reference also port fuel injected pure butane is investigated, combined with direct injected diesel. In these cases, the same mass percentages of butane of the total injected fuel are used.

An engine speed of 1200 rpm and two loads of 8 and 12 bar gross IMEP have been tested. Loads are maintained constant by a longer actuation duration when more butane is added to the blend. Intake pressure is chosen such that lambda is kept constant at approximately 1.3 to see significant differences in smoke emissions between the blends. No EGR is used here.

### Table 6–1: Fuel properties of diesel-butane blends

<table>
<thead>
<tr>
<th></th>
<th>Diesel</th>
<th>But14</th>
<th>But33</th>
<th>But50</th>
<th>Butane</th>
</tr>
</thead>
<tbody>
<tr>
<td>wt % Butane</td>
<td>0</td>
<td>14</td>
<td>33</td>
<td>50</td>
<td>100</td>
</tr>
<tr>
<td>vol % Butane</td>
<td>0</td>
<td>20</td>
<td>43</td>
<td>60</td>
<td>100</td>
</tr>
<tr>
<td>LHV [MJ/kg]</td>
<td>43.00</td>
<td>43.39</td>
<td>43.92</td>
<td>44.38</td>
<td>45.75</td>
</tr>
<tr>
<td>LHV [MJ/L]</td>
<td>37.30</td>
<td>35.27</td>
<td>32.96</td>
<td>31.23</td>
<td>27.70</td>
</tr>
<tr>
<td>density [kg/m³]</td>
<td>830</td>
<td>790</td>
<td>757</td>
<td>690</td>
<td>550</td>
</tr>
<tr>
<td>ECN [-]</td>
<td>55.90</td>
<td>41.90</td>
<td>31.40</td>
<td>25.50</td>
<td>16.38</td>
</tr>
<tr>
<td>p_sat [bar]@365 K</td>
<td>negl.</td>
<td>4.50</td>
<td>7.98</td>
<td>9.88</td>
<td>12.9</td>
</tr>
</tbody>
</table>
Three Starts of Actuation (SOAs) are used for each operating point. These are chosen in a way that they result in a CA50 of 5, 7.5 and 10 degrees aTDC for the Diesel case (8 bar IMEP: SOA= -12, -9, -6 °CA ATDC; 12 bar IMEP: SOA= -14, -12, -9 °CA ATDC). The injection timing is kept constant for all blends, to reveal differences in combustion phasing between the blends, which would be representative for aftermarket in-vehicle application.

Mainly results for the lower (8 bar) load point are given. Where applicable, results for the 12 bar load point are also presented. The comparison to port fuel injected butane is made only for the most interesting quantities (i.e. HC and NOx emissions).

**Results and discussion: Combustion Phasing**

The fuels under investigation are characterized by their ignition delay due to the lower reactivity of butane. With a longer ignition delay the time to premix is elongated and with the help of local leaner mixtures, emissions can be reduced. For a fixed start of actuation (SOA), the ignition delay is extended with increasing butane content, meaning a retarded start of combustion, see Figure 6–2. The difference between diesel and But14 is negligible, and for But33 less than 1 °CA vs. diesel, but for But50 one can see that the lower reactivity influences the ignition delay with an extension of more than 2 °CA compared to diesel.

Although combustion starts later, end of combustion is still closer to TDC when more butane is added. This also means that due to the shorter burn duration, CA50 is placed slightly closer to TDC, resulting in higher peak temperatures, see the Emissions section which follows. With a shorter BD the timing of combustion can be controlled more easily, benefitting the efficiency. The downside of the shorter BD may be a higher pressure rise rate which can result in engine hardware damage and exceeding of the engine’s noise limits. It is therefore suggested to use a maximum mass percentage of 33% butane, if injection timing is not adjusted. In this case, pressure rise rates are comparable to the diesel-only case (not shown). The heat release shape shows a transition from diesel-like to a PPC-like single Gauss when 50% of the fuel is DI Butane.

At higher loads the difference in combustion phasing between the blends can be neglected. At these loads, ignition delay is mainly determined by the high temperature, minimizing the difference due to fuel composition [60][65]. For that reason, no figures of these measurements are shown here.

When using port injected butane, the increase in ignition delay seems to be more linearly proportional to the amount of butane, see Figure 6–3. Also, the heat release shape remains diesel-like, even when 50% of the fuel is port-injected butane.
Unburned hydrocarbon emissions

The main objective of testing direct injection of butane has been to compare its unburned hydrocarbon emissions with those of port-fueled butane. Figure 6–4 shows the hydrocarbon emissions for the 12 bar load point. For the PFI measurements, the HC emissions are nearly proportional to the amount of port injected fuel. This is clearly related to the amount of fuel trapped in the crevices. The crevice volume does not allow for combustion to complete and therefore any (premixed) fuel trapped in this volume results in unburned hydrocarbons.

For direct injected butane, hydrocarbon emissions are an order of magnitude lower than with PFI and little differences are seen compared to diesel-only. Apart from a possible improvement in fuel efficiency and therefore cost savings, the lower emissions levels open the door for aftermarket certification and large-scale OEM use of LPG in heavy duty applications.

Carbon monoxide emissions

As discussed before, the operating points are chosen in a way that significant differences should be observable for smoke emissions. The drawback of this relatively rich charge is that carbon monoxide emissions are quite high, see Figure 6–5. However, the differences between the blends are insignificant and comparable to that of diesel at these higher loads; the butane content does not seem to have a big influence on CO emissions.

Nitrogen oxide emissions

Since for these experiments no EGR was used, at higher load points all nitrogen oxide emissions levels are relatively high (Figure 6–6). For the port fueled butane points, NOx levels increase with the amount of injected butane. As such, the premixed butane may contribute in larger volumes of near-stoichiometric combustion. This will result in more high temperature regions and therefore more thermal NOx formation.
Direct injection of butane-diesel blends

For the low butane content DI points, from the heat release patterns combustion was still seen to be diesel-like, with diffusion flamelets surrounding a hot fuel jet. Consequently, the differences in NOx levels between the various DI blends are small, much smaller than between the PFI points. Also, the DI points show lower NOx emissions than the PFI points.

At the low load of 8 bar IMEP (graph not shown here), 33 wt% of DI butane is allowed without a significant increase in NOx emissions, and at the 12 bar load this is even 50 wt%.

Smoke emissions

Even though relatively rich operating points have been used, absolute smoke levels are still reasonably low, likely because of the short injection duration. Figure 6–7 shows that smoke emissions are even further reduced by adding butane to the blend. 33 wt% gives a 50 percent smoke reduction and 50 wt% butane reduces smoke levels to zero. This can be explained by four reasons. First, it can be related to the rapidly vaporizing fuel, creating locally leaner mixtures. Another way butane can reduce local rich spots, and probably the most dominant reason for lower smoke emissions, is by its lower reactivity. Due to its lower cetane number, ignition delay is increased, allowing more time for the fuel to mix with air.

Third, the butane in the blend will give rise to pressure gradients in the spray field. This will enhance gas perturbation and promote diesel atomization and enhance mixing with in-cylinder air to reduce the soot formation in the diesel-fuel spray [57][59]. Next to the higher vapor pressure, another important aspect of butane is the molecular structure. Aliphatics, like butane, are known to be less soot forming fuels, compared to aromatics present in diesel fuel. Furthermore, from flame studies it is known that short alkanes such as butane are less likely to form soot precursors than long alkanes as present in diesel.

Efficiency and fuel consumption

In the previous sections, it was shown that certain percentages of butane can be directly injected into a diesel engine, without an emission penalty. The main incentive of using butane as an alternative fuel is its lower price. To benefit fully from this price advantage, fuel conversion efficiency should not be negatively affected.

The indicated fuel efficiency, relating power output to the total injected energy (graph not shown here), only displays negligible differences. Yet, as expected due to the lower energy density per unit volume, some differences are seen in fuel volume consumption. Although the indicated efficiency does not change significantly, the fuel penalty in liters amounts to an increase with 10 to 20 percent, see Figure 6–8. The blends’ densities are measured in the low pressure fuel circuit to calculate fuel volume consumption.

![Figure 6–7: Smoke emissions for diesel and DI diesel-butane blends, 8 bar gross IMEP](image1)

![Figure 6–8: Indicated fuel volume consumption for diesel and butane-diesel blends, 8 bar gross IMEP](image2)
Fuel costs

In the previous sections, it was demonstrated that up to 33 wt% of butane can be added to diesel without compromising emissions. However, fuel volume consumption is somewhat increased. Possible fuel cost savings are computed using the average Dutch suggested retail prices for both diesel and LPG. Here, the price of LPG is taken, because it includes applicable taxes. Prices for the blends are calculated using their respective volume fractions.

Furthermore, for the But33 blend, the fuel costs are calculated for the most efficient point measured with 8 bar IMEP. From the normalized costs, see Table 6–2, one can see that a six percent cost advantage can be achieved with current fuel prices.

This best point has shown to simultaneously reduce smoke emissions by 50% without negatively affecting other emissions. For the higher 12 bar load point it was shown that 50 wt% of butane may be used, which can give even higher cost advantages (up to 10%). Obviously, cost savings will depend on pricing and taxation levels, which may greatly differ per country.

<table>
<thead>
<tr>
<th>Table 6–2: Fuel costs for diesel and the most promising blend, 20 July 2011, The Netherlands.</th>
</tr>
</thead>
<tbody>
<tr>
<td>€/L</td>
</tr>
<tr>
<td>L/kWh</td>
</tr>
<tr>
<td>€/kWh</td>
</tr>
<tr>
<td>€/kWh_blend/€/kWh_diesel</td>
</tr>
</tbody>
</table>

Outlook: LPG versus butane

In the experiments reported here butane was used. When LPG would be used, containing a certain amount of propane, it is believed that due to the even lower reactivity of propane, emissions might be reduced even more, though the maximum allowable fuel fraction in the blend may also be lower. Note that the energy density per volume of liquid propane is lower than that of liquid butane (-17% at room temperature), so it will further increase volumetric fuel consumption.

Conclusion

For direct injected butane, hydrocarbon emissions were found to be an order of magnitude lower than for port fuel injected butane. Furthermore, carbon monoxide and nitrogen oxides are not negatively affected compared to the diesel baseline. At a butane mass fraction of one-third and an 8 bar IMEP load point, smoke emissions decreased by 50%. Because a high combustion efficiency is retained, fuel cost savings can be significant, at more than 6 percent (at current Dutch price and tax levels). At higher loads (12 bar IMEP), even more butane can be added to the directly injected blend, without negatively affecting emissions, which enables even larger cost savings.

References


Acknowledgements

Joep Lammerts and Rob van Berkel from Vialle are acknowledged for their help in realizing the experiments.
Up to the time of this research the Reactivity-Controlled Compression Ignition (RCCI) concept has mainly been shown on Wisconsin’s SCOTe engine [66][67][68][69]. Another setup has been used in an independent-funded study [70], outside of the UW laboratory, though it was conducted in collaboration with UW staff. This study showed significantly lower efficiencies. In recent work, the concept was applied to a light-duty setup [71], in which high efficiencies were reproduced. The purpose of the current investigation is to extend the application of the dual-fuel RCCI concept outside the Wisconsin labs, and to try to reproduce their results in a completely different experimental environment, essentially for the first time.

The Wisconsin researchers have extended their work using multiple diesel injections [67], the use of alternative fuels [68] and strategies that rely on a single fuel, with and without ignition additive [72][73]. Although each of these extensions has offered advantages, in this first reproduction conventional diesel and gasoline are used, with one single injection for each of them. Various direct-injection timings are investigated, for three different port-injected gasoline (PIG) percentages. Besides this variation of injection timing and gasoline percentages, a dedicated set of experiments is used to investigate the sensitivity of combustion phasing to the injected quantities of diesel and gasoline. To conclude, the best points found for the RCCI concept are compared with conventional diesel combustion.
Measurement matrix and procedure

In the present investigations a strategy is explored to achieve RCCI combustion, using the fuels given in Table 7–1.

**Table 7–1:** General fuel properties of diesel and gasoline. LHV being the Lower Heating Value, and T10, T50 and T90 represent the 10, 50 and 90% distillation temperatures. Density given at 300K.

<table>
<thead>
<tr>
<th></th>
<th>Diesel EN590</th>
<th>Gasoline RON 95</th>
</tr>
</thead>
<tbody>
<tr>
<td>T10</td>
<td>210 °C</td>
<td>65 °C</td>
</tr>
<tr>
<td>T50</td>
<td>268.5 °C</td>
<td>115 °C</td>
</tr>
<tr>
<td>T90</td>
<td>333.3 °C</td>
<td>185 °C</td>
</tr>
<tr>
<td>DCN</td>
<td>55.9</td>
<td>14.7</td>
</tr>
<tr>
<td>Density</td>
<td>825 kg/m³</td>
<td>753 kg/m³</td>
</tr>
<tr>
<td>LHV</td>
<td>41.54 MJ/kg</td>
<td>43.2 MJ/kg</td>
</tr>
</tbody>
</table>

The compression ratio of the CYCLOPS test setup is set to 14.9:1 by using the standard XE355C pistons and a double head gasket. A Viale28 injector is mounted in the intake manifold for port gasoline injection. The injector is mounted with an angle of 120 degrees resulting in an injected spray directed at the intake valve.

To avoid high pressure rise rates (PRR), an EGR flow of 60 wt-% is used. The load is set to 11 bar IMEP. For injecting small amounts of diesel, an injection pressure of 1000 bar is used. Gasoline injection is started just after exhaust valve close (i.e. 300 °CA bTDC) to spray directly into the cylinder and avoid possible blow-through of gasoline. The net fuel pressure (relative to the intake pressure) of the port fuel injection system is set to ca. 3 bar by controlling the rotational speed of the fuel pump in the gasoline tank. For all measurements the following conditions, which are similar to those used by Reitz and coworkers, are used.

- 1200 rpm engine speed
- 11 bar gross IMEP load.
- 60 wt% cooled EGR @ 300K.
- Intake pressure level: 2.0 bar.
- Exhaust pressure level approximately 1.15 bar.

A single early direct diesel injection strategy is investigated, combined with port gasoline injection. Combustion phasing is controlled by varying the amounts of injected gasoline and diesel. To investigate the influence of both the early diesel injection timing, and the gasoline percentage, the following measurement matrix is used:

- Direct diesel injection start of actuation (SOA) sweep -40 to -90 °CA aTDC, with 10 degree increments.
- 3 gasoline mass percentages 70-80-90, with the remainder in one single diesel injection.

For calculating indicated efficiency the total injected fuel mass is used. Further efficiency definitions can be found in chapter 2.

**Combustion phasing**

When injecting diesel fuel early in the compression stroke, the mixing time is increased, creating a partially-premixed mixture of gasoline, diesel and air. When more time is available for the diesel fuel to mix with the premixed gasoline-air mixture, local lambda values become higher. Figure 7–1 shows injection timing sweeps of the diesel injection for three different gasoline percentages. As SOA is advanced, it is seen that start of combustion (CA5) is retarded. This indicates that local equivalence ratios are on the lean side of the equivalence ratio at which minimum ignition delay is experienced, as shown in Figure 2.1 of [74]. This results in monotonically increasing ignition delays with increasing mixing time and locally even leaner mixtures.

Furthermore, it was expected that when the gasoline percentage is increased for a constant diesel injection timing, start of combustion would also be retarded. From Figure 7–1 this appears to happen indeed. When the gasoline and diesel have enough time to mix, the local reactivity is dependent on the mixing ratio of the two components. In this case, the lower amount of diesel makes that the local reactivity is decreased and auto-ignition is delayed.
Initial tests with RCCI

This is generally accepted as a measure for the overall phasing of combustion, in the remainder of this chapter data are presented versus CA50. This enables comparison of the different gasoline percentages, at equal combustion timing. The highest gasoline percentage is shown to phase combustion correctly after TDC for all injection timings. The lower percentages, however, require a very early diesel injection. This is necessary to reduce diesel stratification and hence local reactivity to delay auto-ignition. At these long mixing times and lower gasoline percentages, combustion phasing appears to be very sensitive to even a small change in diesel injection timing.

Emissions

Longer mixing times create the possibility for partially-premixed air-fuel mixtures to combust at lean and low-temperature conditions. In the RCCI combustion concept, the majority of the injected fuel can be considered to be homogeneously mixed with the air and thus is able to combust under such conditions. The advantage of lean low-temperature combustion can be seen in Figure 7–4. As mixing time is increased, with earlier injection and the associated later CA50, NOx levels decrease dramatically. Note that all NOx emissions are below the Euro VI NOx emissions standard, which is 0.4 g/kWh.
Generally, when NOx and smoke emissions are decreased by lean low-temperature combustion, combustion becomes less complete, which comes with a penalty in HC and CO emissions, see Figure 7–6 and Figure 7–7. Two effects can be distinguished from Figure 7–6. First, as combustion is advanced for a fixed gasoline percentage, maximum cycle temperatures increase, leading to more complete combustion. Second, for a constant CA50, hydrocarbon emissions decrease with increasing gasoline percentage. This effect originates from the mixing time associated with these points. For the lower gasoline percentages, injection has to be advanced far into the compression stroke to achieve conditions lean enough for combustion to be phased after TDC. Locally, however, this gives rise to over-leaning.

As for NOx emissions, smoke emissions are also known to benefit from locally less rich conditions. With the highly premixed gasoline, and long mixing times for diesel, the smoke levels experienced are very low, see Figure 7–5. For the highest gasoline percentage of 90%, all smoke levels are well below the Euro VI norm of 0.01 g/kWh. This already shows one of the promising aspects of the RCCI concept. In conventional diesel combustion (CDC), a NOx-smoke trade-off is generally experienced, i.e. a measure to reduce NOx will lead to higher smoke emissions and vice versa. While the RCCI concept still partly shows this trade-off, unlike CDC it simultaneously shows EURO VI compliant engine-out soot and NOx emissions.

The same effects as discussed for hydrocarbon emissions can also be identified for CO emissions, see Figure 7–7. Again, for all gasoline percentages increasing CO emissions are found with retarding CA50. Also, for a constant CA50, lower carbon monoxide emissions are experienced at higher gasoline percentages. This shows that for combustion to be correctly phased after TDC, it is better to use higher gasoline percentages; an excessively long mixing time is not necessary then, which reduces the risk of over-leaning.
Initial tests with RCCI

In Figure 7-8, the indicated efficiency is presented. Commonly, the indicated efficiency increases when CA50 is advanced from late timings closer to TDC. However, unlike normally, for the measured points indicated efficiency even increases further when CA50 is advanced to before TDC. This is hypothesized to have its origin in an increasing combustion efficiency. As discussed before, for longer mixing times and late CA50 phasing, the charge is overleaned and combustion is too lean for complete combustion. As injection is retarded, combustion is advanced and because of the reduced mixing time CO and HC emissions decrease.

To verify this assumption, in Figure 7-9 the thermal efficiency is shown. Instead of using the injected fuel mass, as is done for the indicated efficiency, only the actual converted fuel quantity is used, as defined in chapter 2. The thermal efficiency is thus corrected for any combustion loss (i.e. HC and CO emissions). This shows efficiency to be significantly flatter at CA50 around TDC. Furthermore, the effects of increasing gasoline percentage are more clear. For the highest gasoline percentage, thermal efficiency is significantly higher compared to the lower gasoline percentages. These 90% gasoline points benefit from increased thermal efficiency compared to the lower gasoline fractions, even at constant combustion phasing. Therefore the origin of this increase must lie in a more thermodynamically favorable heat release pattern.

Maximum pressure rise rate

As discussed above, increasing the gasoline percentage results in higher rates of heat release. As can be expected, Figure 7-10 shows that for a constant CA50 this results in slightly higher maximum pressure rise rates. However, combustion phasing appears to be the limiting factor. The higher gasoline percentage allows for CA50 to be phased correctly after TDC, therewith reducing maximum pressure rise rates significantly. Therefore, also for the highest gasoline fraction, the maximum pressure rise rate is not expected to be an issue.
Initial tests with RCCI

Sensitivity to injected quantity

One of the most important possibilities of RCCI is the control of SOC by controlling the in-cylinder mixture reactivity. In conventional diesel combustion, start of injection is used as a control for start of combustion. In this case, when control is intended by changing the reactivity of the in-cylinder fuel, it is important to verify what the actual ignition trigger is. According to Reitz [71], global fuel reactivity can be controlled by adding diesel to the gasoline, creating a new in-cylinder fuel blend. However, the influence of adding diesel seems to have greater effect than the addition of gasoline. This indicates that local diesel stratification, dependent on injection timing and amount of fuel, might determine the timing of ignition. To assess the effect of the diesel injection on SOC, various gasoline fuel fractions are investigated. In Figure 7–11 one can schematically see the three experiments under investigation in this section. In the figures to follow, the baseline is indicated with a green diamond.

First, the amount of gasoline is increased (therewith also varying the load), indicated with a red square. It is found, see Figure 7–12, that when the gasoline fuel flow is increased, the change in SOC is far less significant than when the diesel fuel flow is increased, denoted with the purple triangles. As the diesel fuel’s reactivity differs more from the global reactivity, a change in diesel fuel quantity effects this reactivity more. Still, the global reactivity is only changed slightly. More importantly, the diesel spray will ensure a higher stratification and lower local lambda. It is also therefore, that this effect is less when injection timing is advanced, as this reduces stratification for all mixtures. From these results one can conclude that the diesel injection timing and quantity are the two most important parameters to control combustion phasing.

![Figure 7–10: Maximum pressure rise rate for different gasoline fractions and varying diesel injection timing](image)

![Figure 7–11: Diesel and gasoline fuel quantities for three different injection strategies. Global lambda indicated above bars and homogeneous background lambda indicated on the gasoline bar](image)

![Figure 7–12: Start of Combustion (CA5) for three different injection strategies.](image)
Initial tests with RCCI

Dual-fuel vs. Diesel-only

To discover the full potential of RCCI combustion, the concept is compared to diesel-only Conventional Diesel Combustion (CDC). The experiments done for this comparison are at equal loads: 11 bar gross IMEP. To create a similar experiment, 60 wt% of the total mass flow is EGR for both combustion concepts. However, such a large amount of EGR is generally not used at CDC. Therefore also experiments with 20 wt% EGR are included. For the RCCI concept 90 wt% gasoline was used, which showed to give the best results.

Figure 7–13: Nitrogen oxides emissions comparing three concepts, logarithmic scale

From Figure 7–13, one can see that the application of EGR is an effective method to reduce NOx emissions, independent of the concept used. However, the general drawback of the use of EGR is that the air/fuel ratio is reduced. For conventional diesel combustion, this results in high smoke production, as can be seen in Figure 7–14. Here lies the main advantage of partially-premixed combustion concepts; they allow for simultaneous reduction of both nitric oxides and smoke emissions.

Figure 7–14: Smoke emissions comparing three concepts, logarithmic scale

One of the drawbacks of the RCCI concept can be seen in Figure 7–15. The highly-premixed charge makes that hydrocarbons get trapped in crevices. Also, long mixing times and globally lean mixtures can lead to over-leaning. The resulting incomplete combustion gives rise to increased hydrocarbon emissions, which account for up to 2.5% of fuel consumption.

Even despite the higher combustion losses

Figure 7–15: Hydrocarbon emissions comparing three concepts

Figure 7–16: Fuel consumption comparing three concepts
for the RCCI concept, fuel consumption can be significantly reduced (≈-10%). The results in Figure 7–16 include the small effect (≈3%) of the higher heating value that gasoline-diesel mixture has compared to diesel. The latter, however, is small compared to the advantages the RCCI concept displays, i.e. short burn durations and low combustion temperatures.

One other possible issue associated with higher heat release rates can be an unacceptably high pressure rise rate. However, as is shown in Figure 7–17, pressure rise rates are acceptable and even lower than for conventional diesel combustion, using low EGR rates. This can be attributed to (a combination of) correct phasing of combustion after TDC and the increased heat capacity and dilution effect of the recirculated exhaust gas.

![Figure 7–17: Maximum pressure rise rate comparing three concepts](image)

**Conclusion**

Compared to more conventional combustion regimes, this dual-fuel concept can partly escape from the common NOx-smoke trade-off, reducing both to near-zero values, below EURO VI limits. Although hydrocarbon emissions are somewhat increased, indicated efficiencies are significantly increased. The absolute efficiencies are not as high as reported in other work, but the increase as such confirms the potential of the RCCI concept. The increase in indicated efficiency is shown to originate from higher thermal efficiency, because short burn durations at high gasoline fractions enable for CA50 to be phased closer to TDC, without combustion occurring too much before TDC. This, and lower heat losses through increased dilution enable a more efficient thermodynamic cycle.

Pressure rise rates are found to be as low as with conventional diesel combustion, for the same EGR percentage of 60 wt%. Although the dual fuel concept involves a much higher rate of heat release, this is phased better after TDC. A dedicated set of experiments has demonstrated that the late-cycle diesel injection is dominant for combustion phasing and that control has to be found in this single diesel injection.

In comparison to the RCCI results published by the University of Wisconsin’s Engine Research Center, under similar experimental conditions, similar results were found for NOx and smoke emissions. Also HC and CO emissions are similar. However, in absolute thermal efficiency some differences are found. In the best measurement series, Reitz and coworkers report a thermal efficiency of >55%, in contrast to the present measurements where a maximum of 49% thermal efficiency is achieved. Although absolute efficiencies are slightly lower, the relative increase in efficiency is comparable. As also the baseline efficiency is significantly lower, differences are expected to be found in the base engine.

**References**

Using two fuel systems opens up an extra degree of freedom to control combustion phasing. In this chapter the control space is explored using four different injection strategies.

The experiments presented in this chapter have been performed by Bas van den Berge, under supervision of the author, and have, in an extended form, been published as Leermakers et al. (2012), SAE Technical Paper 2012-01-1575, doi:10.4271/2012-01-1575.
To determine the possible viability of the RCCI concept for on-road application, controllability is of vital importance. The impact of control parameters can be highly load- and speed-dependent. However, in this chapter only one operating point has been chosen, for which a determination of the control space of a double injection strategy with respect to combustion phasing is presented. Furthermore, the effects of these parameters on emissions and efficiencies are also determined.

For the given speed/load point, three types of combustion phasing control can be distinguished: First, the balance between the high (DI) and low reactive fuels (PFI), i.e. gasoline and diesel respectively, is of vital importance. This first order effect has been extensively studied in [75] to enable viable single-cylinder tests of the concept.

Secondly, the timing of the DI doses, one early and one late, can be controlled. This gives some control on the level of stratification, both in mixture strength and reactivity. Especially the timing of the second injection can be used to phase combustion correctly. The timing of the first injection, however, also has a significant effect on this phasing.

Lastly, the ratio of the two diesel injections can be controlled. Again, this has its influence on the in-cylinder stratification of the charge. Also for this third type of control the sensitivity will be shown.

**Measurement matrix and procedure**

Like in the previous chapter the CYCLOPS test setup is used with a compression ratio of 14.9:1 equipped with two fuel injection systems.

Different injection strategies, using the fuels given in the previous chapter, are explored to determine their respective control effects on combustion phasing and emissions. A single target load of 11 bar gross IMEP is investigated. The fuel mass flow is kept constant, and small variations in load (originating from varying efficiencies) are allowed accordingly. The engine speed is set to 1200 rpm. An EGR flow of 60% weight percent is set, both to limit pressure rise rates, as found in [75] and to have nitrogen oxides emissions below Euro VI levels [76][77].

The latter two references have stated that a combustion temperature higher than 1500 K is necessary to promote the reactions from CO to CO$_2$, and that on the other hand it is important to be below 2000 K to avoid thermal NOx formation (Zeldovich’ mechanism). The combination of an EGR fraction of around 50 wt% and a global lambda value of approximately 1.5 has been shown to yield such temperatures. To achieve this desired air excess ratio, intake pressure is set to 2.0 bar absolute.

The recirculated exhaust gas is cooled to $\approx$300 K and exhaust pressure was constant at 1.15 bar absolute. While this value does not represent real-life conditions and has its effects on charge temperatures, EGR composition and the amount of internal EGR, a more realistic value, above the intake pressure, was not possible for the setup at the time of the experiments.

In [75] it was shown that unburned HC emissions can be limited by injecting a rich enough, well-timed gasoline mixture. Therefore 80 wt% of the injected mass is gasoline, of which the injection is started at 300 °CA bTDC to spray through the intake port, directly into the cylinder and avoid possible blow-through of gasoline. The net fuel pressure (relative to the intake pressure) of the PFI system is set to $\approx$3 bar by controlling the rotational speed of the fuel pump in the gasoline tank.

Summarized, for all measurements the following conditions are kept constant:

- 1200 rpm ($\sigma$ =0.44 rpm),
- 11 bar target gross IMEP by using a total fuel flow of 1.23 g/s ($\sigma$ =0.022 g/s),
- 2 bar absolute intake pressure ($\sigma$ <0.005 bar),
- 1.13 bar absolute exhaust pressure ($\sigma$ =0.014 bar),
- 62 wt% heavily cooled EGR ($\sigma$ =0.9 wt%),
- 306 K intake temperature ($\sigma$ =2.4 K),
- Port injected gasoline of 80% of injected mass, timed before IVC.
For these constant load, speed and ambient conditions, which result in a lambda value of 1.60 ($\sigma = 0.03$), four diesel injection strategies are investigated. All injection timings are referred to by their Start of Actuation (SOA).

First, as a benchmark, 20 wt% of injected mass is injected in a single diesel injection. For injecting such small amounts, a diesel injection of 1000 bar is used. This is the minimal pressure to have stable operation of the injector, using a 500 microsecond (=3.6 CAD) actuation duration. For this single diesel injection the start of injector actuation (SOA) is swept from -40 to -90 degrees aTDC, with 10 degree increments. The remaining 80% of the fuel is gasoline and port-injected.

In the second and third strategies, which are both graphically shown in Figure 8–1, the 20 wt% diesel is equally divided over two injections, one early (DI1) and one late (DI2). To increase injection duration for stable operation of the injector, for such low quantities the injection pressure has to be lowered to 500 bar. It will be shown that this pressure reduction in itself has major implications for e.g. emission levels, but unless another injector nozzle is used, this is the only way to achieve such small injections.

In the second strategy the late injection is fixed at -10 degrees aTDC, with an early injection variation from -40 to -90, with 10 degree increments. In the third strategy the early injection is fixed at -70 degrees aTDC, with a late injection variation from -25 to -5, with 5 degree increments.

The fourth strategy is derived from the third one, with the early injection fixed at -70 degrees aTDC, with a late injection variation from -25 to -5, with 5 degree decrements. Now, again with 500 bar injection pressure, the early-late balance is shifted to 70:30, to test the influence of this division. The four injection strategies are summarized in Table 8–1:

<table>
<thead>
<tr>
<th>Description</th>
<th>PFI</th>
<th>DI1</th>
<th>DI2</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Single early injection</td>
<td>80</td>
<td>20</td>
<td>00</td>
<td>DI1 timing variation, 1000 bar rail</td>
</tr>
<tr>
<td>50:50 SOI1 variation</td>
<td>80</td>
<td>10</td>
<td>10</td>
<td>DI1 timing variation, 500 bar rail</td>
</tr>
<tr>
<td>50:50 SOI2 variation</td>
<td>80</td>
<td>10</td>
<td>10</td>
<td>DI2 timing variation, 500 bar rail</td>
</tr>
<tr>
<td>70:30 SOI2 variation</td>
<td>80</td>
<td>14</td>
<td>06</td>
<td>DI2 timing variation, 500 bar rail</td>
</tr>
</tbody>
</table>

**Combustion phasing control**

The principal argument for testing the four injection strategies is to determine their respective control spaces with respect to combustion phasing. First, this effect is shown for the single injection strategy. Secondly, this is compared to an 50:50 early injection variation. After a comparison of the respective effects of the early and late injection in this 50:50 strategy, this late injection variation is also compared to a similar variation in a 70:30 strategy.

In Figure 8–2 the response of CA50 to injection timing is shown for all four injection strategies, which will be discussed next.
Testing the controllability of RCCI

59

shown later. At the injection timings of -50 and -40 a reduction of the negative slope can already be seen.

50:50: first injection variation

The second injection strategy under investigation consists of two equally divided diesel injections. The first is swept from -40 to -90, while the second is fixed at -10 degrees after TDC. From the cylinder pressure and heat release traces, as shown in Figure 8–3, the clear effect of advancing this first injection can be seen.

Single early injection

Looking at the blue diamonds in Figure 8–2, the response of CA50 can be seen for a single early injection. The first thing one can notice is that advancing this injection timing gives more time for the diesel to mix with both air and gasoline, resulting in a leaner and less reactive local mixture when approaching top dead center. Through this locally leaner and less reactive mixture, advancing injection timing results in retarded combustion.

A first order fit of the measured points gives a quantification of this negative slope. The combustion phasing response, defined as \( s_{ID} = \delta CA50/\delta SOI \) takes a value \( s_{ID} = -0.27 \). This negative and relatively low value means that the bandwidth of the control might be too low, as very large changes in injection timing will be necessary to have a significant impact on combustion phasing.

Furthermore, from the coefficient of determination (0.95) and the fit itself in Figure 8–2 can be seen that the behavior is not well approximated with a linear fit. For later injections, this is expected as the sign should change, as will be shown later. At the injection timings of -50 and -40 a reduction of the negative slope can already be seen.

50:50: first injection variation

The second injection strategy under investigation consists of two equally divided diesel injections. The first is swept from -40 to -90, while the second is fixed at -10 degrees after TDC. From the cylinder pressure and heat release traces, as shown in Figure 8–3, the clear effect of advancing this first injection can be seen.

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50:50: first injection variation

The second injection strategy under investigation consists of two equally divided diesel injections. The first is swept from -40 to -90, while the second is fixed at -10 degrees after TDC. From the cylinder pressure and heat release traces, as shown in Figure 8–3, the clear effect of advancing this first injection can be seen.
In Figure 8–2 (green triangles), the response of the 50:50 SOI1 strategy is compared to that of the single injection strategy. The coefficient of determination is comparable for the two strategies, and so is the fact that the slope is negative. However, as expected, because the mass in the early injection is halved, the slope is also significantly reduced; \( s_{ID} = -0.1 \). In fact it hardly shows any response to the timing of injection.

The required large change in DI timings to adapt combustion phasing, means that spray formation will be significantly affected through varying density, temperature and piston position. If these conditions change too much, the spray can not be optimized. As such, this strategy is undesirable to be used as a control parameter.

50:50 second injection variation

In the third injection strategy, the early diesel injection is fixed at -70 degrees after TDC and the second, late injection is varied to control combustion phasing. Again, in Figure 8–4 cylinder pressure and heat release traces are given, but now for the late injection timing variation. One can directly note that the injection timing response by CA50 is reversed, as will be further discussed below.

When the rate of heat release shapes are compared for the different late injection timings both the overall shape and the maximum values are similar, apart from a disappearing initial heat release stage when injection timing is retarded, similar to Figure 8–3.

For all timings, injection is finished before the corresponding heat release rate reaches a significant level. Even though the combustion event does not overlap with the injection event, this late injection timing variation offers a much higher level of controllability. The sensitivity now becomes larger (\( s_{ID} = 0.45 \)), as can be observed from the orange squares in Figure 8–2, and has changed sign with respect to the 50:50 SOI1 strategy where -0.1 is found. For such a small injection, and still without any overlap with the combustion event, it is fairly high. Nonetheless, is it not unity as one would find for a fully conventional injection strategy (CDC).

70:30 second injection variation

As a fourth, and last, injection strategy the amount of mass in first and second diesel injection is no longer kept equal. In this strategy again the late injection is varied to control combustion phasing. Again, in Figure 8–4 cylinder pressure and heat release traces are given, but now for the late injection timing variation. One can directly note that the injection timing response by CA50 is reversed, as will be further discussed below.

Summary

As discussed in the previous sections, a change in timing of single and early injections have an inverse effect on combustion phasing. Furthermore, in a double injection strategy the response of CA50 on a variation of the first injection is (very) weak.
The response to a variation in the late injection has a positive $s_{ID}$, which is nearly exactly linear and has a larger value compared to the early injection variation strategies. Furthermore, it was shown that the more fuel is admitted in the second injection, the larger $s_{ID}$ is. Therefore 50:50 SOI2 strategy was found to be most favorable with respect to combustion phasing response.

**UHC and CO emissions**

Not only do the respective injection strategies have their effects on the phasing on combustion, also emissions might differ significantly. In Figure 8–5 first the unburned hydrocarbon emissions are shown for the four strategies.

![Figure 8–5: Unburned hydrocarbon emissions vs. CA50 for injection timing variations in 4 different injection strategies.](image)

The single injection strategy differs most from the other three and shows an effect of the combustion phasing. Apparently, an early combustion phasing yields higher temperatures, high enough for combustion to be as complete as possible. But even at the earliest combustion phasing, with the highest maximum temperatures, unburned hydrocarbon emissions are still relatively high.

For this combustion concept, the unburned hydrocarbon emissions from the single injection strategy are generally thought to originate from the premixed charge trapped in crevice volumes. Remarkably the results for the double injection strategies are poorer (Figure 8–5 and Figure 8–7). For these double injections, the injection pressure had to be lowered to 500 bar, and together with the very short injection, this appears to be dramatic for the completeness of combustion. The length of the diesel jet penetration is too short to ignite all of the premixed gasoline-air mixture, or the injector may at this lower pressure suffer from bad vaporization or atomization, or even significant injector dribble.

NOx emissions, as will be shown later, indicate that maximum cylinder temperatures are comparable for all strategies that have the same CA50. Therefore, another reason for the high level of unburned hydrocarbons might be local richness. The late injection in the double injection strategy will make zones that are much richer than for the single early injection. This will hamper complete combustion of both the diesel fuel and the premixed charge.

The same observations as seen for unburned hydrocarbons also hold for carbon monoxide emissions, as shown in Figure 8–6. Again, for the single injection strategy the levels decrease with advancing combustion, but even at the earliest phasing remain high. The double injection strategies all give unacceptably high values, significantly reducing combustion efficiency.

![Figure 8–6: Carbon Monoxide emissions vs. CA50 for injection timing variations in 4 different injection strategies.](image)
Testing the controllability of RCCI

Both for CO and HC emissions, the different double injection strategies show very little differences. However, all of their values are nowhere near the upcoming, or even current, legislated limits. The exact origin and possible solutions for this issue should be further researched by looking at mixture fraction distributions in an optically accessible engine and/or using computational fluid dynamics to improve the spray targeting in such injection strategies.

The resulting combustion efficiency of the injection strategies is computed from the unburned hydrocarbons and carbon monoxide emissions, and shown in Figure 8–7. As most unburned hydrocarbons are thought to be gasoline, the heating value of the unburned hydrocarbons is assumed to be that of gasoline. As can be expected, the combustion efficiency shows the same trends as unburned hydrocarbons and CO.

Efficiency

As can be expected, the previously discussed trends for combustion efficiency have a significant effect on the gross indicated fuel efficiency, as shown in Figure 8–8.

For the single injection strategy, at early phasings a reasonable efficiency is achieved, while at later phasings the unburned hydrocarbon and carbon monoxide emissions take their toll and decrease efficiency. As such, the high efficiencies at early phasings are not caused by the thermodynamic process, but through more complete combustion. This is confirmed by taking the combustion efficiency into account to compute the thermal efficiency (Figure 8–9).
All double injection strategies have an indicated efficiency of about 10% lower than the single injection strategy. Tests by others, as referred to in the introduction, have shown that the dual-fuel concept, even with double injections, allows very high gross indicated efficiencies, up to 58%. However, because of the low completeness of combustion, this is not achieved in the present investigation. Furthermore, because of the even lower combustion efficiency, the double injection strategy adds up to 10% to fuel consumption compared to the single injection strategy.

**NOx and smoke emissions**

One of the most important reasons of developing a dual fuel concept is to reduce the engine-out nitrogen oxides and smoke emissions. In this way, expensive exhaust gas after treatment systems do not have to be used (as much), while upcoming legislation levels can still be met. In Figure 8–10, first the nitrogen oxides emissions are shown for the four injection strategies.

One can clearly see the effect of combustion phasing on nitrogen oxides emissions. With advancing combustion, peak temperatures rise considerably and when combustion is advanced before TDC, the charge remains at high temperature for a longer time. Because of the constant dilution level and oxygen concentration, this results in increased nitrogen oxides emissions. The inverse effect was seen earlier in a single injection strategy for the completeness of combustion, which benefits from the increased temperatures. However, because of the high dilution level applied in this concept, for most, or all, of the measured points NOx emissions are still well below the current and upcoming legislated emission levels.

The highly premixed nature of the dual-fuel combustion concept is known to reduce smoke emissions significantly compared to conventional diesel spray combustion. In Figure 8–11, the smoke emissions are compared for the four injection strategies.

Since all levels are low, for many of the measured points near or below upcoming legislated levels, no clear differences can be found between the strategies.

**Figure 8–10:** Nitrogen oxides emissions vs. CA50 for injection timing variations in 4 different injection strategies. Euro VI level depicted by purple line.

**Figure 8–11:** Smoke emissions (in Bosch Filter Smoke Number) vs. CA50 for injection timing variations in 4 different injection strategies.
Testing the controllability of RCCI

It is general practice to plot smoke emissions versus nitrogen oxides emissions to see how different strategies behave with respect to the common NOx-soot trade off. The latter is commonly experienced in conventional diesel combustion, where a measure to decrease one, leads to an increase in the other. From Figure 8–12 it can be seen that the early injection sweeps largely escape from this trade-off, while the late injection variations reduce the levels of the trade-off. For all strategies, this results in both smoke and NOx emissions below or near EURO VI emission levels.

For both smoke and NOx emissions, therefore the chosen injection strategy does not have a big impact. For smoke, also the combustion phasing has a minor effect, whereas for nitrogen oxides the emission levels increase with advancing combustion, but remain reasonably low.

Maximum pressure rise rate

The last parameter that is compared for the injection strategies is the maximum pressure rise rate. Largely premixed combustion can lead to unacceptably high pressure rise rates and the chosen injection strategy might have an effect on this. Figure 8–13 shows that the maximum pressure rise rate is largely independent from the chosen injection strategy, but mainly depends on the resulting combustion phasing.

For all strategies, pressure rise rates are comparable with conventional combustion strategies with the same combustion phasing. The pressure rise rates are efficiently suppressed by the high dilution rates used. To keep the pressure rise rate at an acceptable level, the chosen injection strategy is apparently not that important. However, CA50 is, so it is desired to have an injection strategy that offers a wide range of control. With such an injection strategy, combustion phasing can be shifted in a way that the maximum pressure rise rate always stays below acceptable levels.
Conclusions

Reactivity Controlled Compression Ignition through in-cylinder blending of gasoline and diesel to a desired reactivity has previously been shown to give low emission levels, combined with a simultaneous efficiency advantage. To determine the possible viability of the concept for on-road application, a determination of the control space of injection parameters with respect to combustion phasing has been presented. The four injection strategies under investigation can be described as:

1. Single diesel injection; early diesel injection timing variation
2. Two diesel injections divided 50:50, varying first injection
3. Two diesel injections divided 50:50, varying second injection
4. Two diesel injections divided 70:30, varying second injection

The following points were noted:

- A variation in the timing of the first or second diesel injection has an opposite effect on combustion phasing. The response is reasonably linear, but the sensitivity to the first injection is weak.
- The sensitivity of the late injections is positive and larger in absolute value compared to the early injections variation strategy. Furthermore, the sensitivity correlates with the amount injected in the second injection. As such, the 50:50 second injection variation is most favorable.
- For the single injection strategy, an early combustion phasing is necessary to have temperatures high enough for combustion to be as complete as possible. Even at the earliest combustion phasing, with the highest maximum temperatures, combustion efficiency is relatively low, caused by crevice volumes.
- All three double injection strategies give very poor combustion efficiency. For these double injections, injection pressure had to be lowered to 500 bar, and together with the very short injection this results in a low combustion efficiency. One hypothesis is that the length of the diesel spray penetration is too short to ignite all of the premixed gasoline-air mixture. A more plausible hypothesis is that the late injection in a double strategy results in zones too rich to combust completely.

- The dual-fuel concept, even with double injections, is known to be able to produce very high efficiencies. Because of the low combustion efficiency, this is not achieved in the present investigation.
- Because of the high dilution level and largely premixed mixture, all present injection strategies reduce the levels of the common soot-NOx trade-off significantly with both smoke and NOx emissions being near or below legislated levels for 2013.
- For all strategies, pressure rise rates are comparable with conventional combustion regimes with same combustion phasing. The pressure rise rates are efficiently suppressed by the high dilution rates used. The maximum pressure rise rate is largely independent from the chosen injection strategy, but mainly depends on the resulting combustion phasing. Therefore it is desired to have an injection strategy that offers a wide range of control, such as the single early injection or 50:50 late injection variations.

References
Commercial Naphtha blends for PPC

Naphtha streams, from a refinery such as the Pernis one of this image could provide easily applicable fuels for Partially-Premixed Combustion

Photo courtesy of Shell Photographic Services, Shell International Ltd

The experiments presented in this chapter have been performed by Peter-Christian Bakker, under supervision of the author, and have, in an extended form, been published as Leermakers et al. (2013), SAE Int. J. Fuels Lub. 6(1):199-216, doi:10.4271/2013-01-1681.
Fuels in the gasoline boiling range, with relative low-octane-number were shown to be very well suitable for Partially Premixed Combustion, showing the potential of low emissions of NOx and soot, with a simultaneous improvement in fuel efficiency [78]. The load range over which the concept can be applied was shown to depend on the reactivity, at best ranging from idle to full load, without major modifications to the engine setup.

Several refinery streams were used by Manente and coworkers [79] for this concept. As such refinery streams are not expected to be commercially available on the short term, for certain applications, the use of currently commercially-available naphtha blends of relatively high volatility could provide a practical solution. That is, if such a blend can give similar emission advantages as the earlier mentioned refinery streams, and has a suitable load range.

In this chapter a summary of the performance of three naphtha blends with respect to emissions and efficiency is presented. Besides the sensitivity to injection strategies, dilution levels and fuel pressure, emission performance is compared to upcoming legislated emissions levels. The effect of the blends’ chemical composition is shown over a broad load range and conventional diesel combustion benchmarks are used to show possible improvements in indicated efficiency.

**Experiment setup**

Prior to this investigation, the CYCLOPS test setup has been overhauled with new pistons and liners. The pistons are of a low-compression XE390C version, which together with the thickest head gasket available (1.45 mm), yield a compression ratio of 15.7.

**Fuels under investigation**

For certain applications the use of a currently commercially available naphtha blend of relatively high volatility could provide a practical solution as it might be produced by a refinery without additional investment.

Two commercially available naphtha blends have been selected, with different boiling range and aromatic content. These two naphtha blends (NB1 and 2, respectively, see Table 9–1), in principle are upstream precursors of pump gasoline and consequently, cheaper in production, which is confirmed by Kalghatgi and coworkers [78]. The main difference between NB1 and NB2 is their boiling range, which is substantially higher for NB2.

Additionally, a third blend (NB3) of 50 vol-% RON95 gasoline and 50 vol-% of the first naphtha blend was tested. The pump gasoline has been used to decrease reactivity since the naphtha blend 1 might still be slightly too reactive for PPC purposes. An additive is used with these low viscosity fuels to ensure sufficient lubricity for the components under high fuel pressure.

<table>
<thead>
<tr>
<th>EN590</th>
<th>RON95</th>
<th>NB 1</th>
<th>NB 2</th>
<th>NB 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>CN</td>
<td>52.4</td>
<td>14.7</td>
<td>45±5</td>
<td>50±10</td>
</tr>
<tr>
<td>LHV [MJ/kg]</td>
<td>42.7</td>
<td>41.8</td>
<td>43.48</td>
<td>43.31</td>
</tr>
<tr>
<td>Boiling range [°C]</td>
<td>170-360</td>
<td>65-185</td>
<td>94-140</td>
<td>142-200</td>
</tr>
</tbody>
</table>

The chemical composition of the two naphtha blends has been determined in a combined gas chromatography-mass spectrometer (GC-MS). Naphtha blend 1 has negligible aromatic content, an average carbon chain length of 7.88 ± 0.06 and an H/C ratio of 2.11 ± 0.01. Naphtha blend 2 has additional aromatic components, an average carbon length of 10.1 ± 0.6 and an H/C ratio of 2.02 ± 0.06.

Cetane numbers are estimated using a correlation of hydrocarbon type and carbon number to cetane number (see Figure 6 in ref [81]). Given that not all of the blend components could be resolved in the GC-MS, CN values are not available for all components, and the effects of blending multiple components are not certain,
an error interval is given for the estimated cetane number.

According to this method, both naphtha blends have a CN similar to diesel. The CN of RON95 has been estimated using the correlation of Kalghatgi [82]. Hence, the cetane number of NB3 is estimated to be 30 ± 10.

Conditions and procedure

Based on the results of Manente [83], the engine speed is set to 1250 rpm. An EGR flow of around 50 weight percent is used, both to limit pressure rise rates, as found in previous work [84], and to have nitrogen oxides emissions below Euro VI levels [85][86].

To ensure a combustion temperature higher than 1500 K to promote the reactions from CO to CO₂, and below 2000 K to avoid thermal NOx formation (Zeldovich’ mechanism), apart from an EGR weight percentage of around 50%, also a global lambda value of around 1.5 is used, as explained on page 57. To achieve such an air excess ratio, intake pressure is varied accordingly.

The recirculated exhaust gas is cooled to about 300 K and the exhaust back-pressure is regulated to 0.3 ± 0.2 bar higher than the intake pressure to mimic the presence of a contemporary turbocharger and enable the use of external EGR in practice.

Both single and advanced injection strategies will be tested at a load of 8 bar gross IMEP, by varying the start of injection (SOI) until the desired CA50 is reached within ± 1 °CA.

- Single injection - five SOIs aiming at CA50s of 2, 4, 6, 8, and 10 °CA aTDC.
- Influence of advanced injection on heat release patterns.

Furthermore, the following sensitivity analyses have been done:

- Air excess ratio of 1.5 versus 2.0.
- Effect of increased EGR with one fuel
- Fuel pressure variation at 8 bar IMEP

After these sensitivity analyses, the load range of each of the fuels will be shown, for which five loads have been selected. For each target load ± 0.5 bar, the fuel mass flow is kept constant, and small variations in load (originating for varying efficiencies) are allowed accordingly:

- Gross IMEPs of 8, 10, 12, 14 and 16 bar, corresponding to 32-64% of the engine’s rated torque, with CA50 fixed at 8±1 °CA.

Fuel pressure increases with load to keep injection duration roughly constant in crank angle domain and have similar spray formation over the load range. A moderate 1000 bar of fuel pressure at 8 bar load is taken as starting point and with every 2 bar of load increase, fuel pressure will be increased by 200 bar.

Results and discussion

The relevant results for all fuels will be discussed in four subsections to illustrate how viable the fuels are for usage in Partially Premixed Combustion.

First, a comparison of single and advanced injection strategies is made. After this, combustion phasing is varied. The effect of a slight increase in EGR is shown, as well as the results of varying fuel pressures. Finally, all fuels are compared over the investigated load range.

1 – Injection strategy variation

First, the possibility of running in PPC mode is investigated for the 8 bar IMEP case. The question is whether it is possible to achieve PPC-like conditions (sufficient ignition delay to separate injection and combustion to a large extent) through the fuels’ specific physical and chemical properties.

Naphtha blend 1

For Naphtha blend 1, when using a single injection, the heat release and ignition behavior are typical diesel-like, with a distinct premixed peak followed by some injection controlled combustion (see Figure 9–1). EGR helps to get a significant ignition delay, although a complete separation between injection and combustion is not obtained.
The even broader spread in Naphtha blend 2’s component reactivities (including e.g. n-decane and n-undecane) is expected to result in earlier and more low-temperature reactions, which could affect both efficiency (improper phasing) and emissions (soot production). Figure 9–2 clearly visualizes such undesired early combustion, when a double injection strategy at 1500 bar is used.

![Figure 9–1: Comparison of NB1 at 800 bar fuel pressure with single and multiple injections with pilots at -60 and -30 °CA aTDC. EOI of last injection and single are almost identical, vertical lines overlap.](image)

![Figure 9–2: Three phase compared to single phase heat release for double and single injection, respectively. NB2 @ 1500 bar fuel pressure and 50% of EGR. EOI are almost identical for the single and last injection, respectively.](image)

Table 9–3: Overview of engine parameters and results during NB2 combustion characterization

<table>
<thead>
<tr>
<th></th>
<th>Single</th>
<th>Double</th>
</tr>
</thead>
<tbody>
<tr>
<td>IMEP&lt;sub&gt;gross&lt;/sub&gt; [bar]</td>
<td>8.0</td>
<td>7.8</td>
</tr>
<tr>
<td>CA50 [°CA aTDC]</td>
<td>6.1</td>
<td>5.5</td>
</tr>
<tr>
<td>SOI [°CA aTDC]</td>
<td>-6.1/-61/-2.6</td>
<td></td>
</tr>
<tr>
<td>MPRR [bar/°CA]</td>
<td>7.4</td>
<td>4.8</td>
</tr>
<tr>
<td>η&lt;sub&gt;ind&lt;/sub&gt; [-]</td>
<td>0.496</td>
<td>0.481</td>
</tr>
<tr>
<td>η&lt;sub&gt;comb&lt;/sub&gt; [-]</td>
<td>0.994</td>
<td>0.966</td>
</tr>
<tr>
<td>ISNOx [g/kWh]</td>
<td>0.48</td>
<td>0.39</td>
</tr>
<tr>
<td>ISPM [g/kWh]</td>
<td>0.049</td>
<td>0.033</td>
</tr>
</tbody>
</table>

Apparantly, NB2 is not very suitable for early injections. Although the early injections help to reduce pressure rise rates, NOx- and PM emissions, again a significant reduction of combustion efficiency is noted (Table 9–3). This
results in an indicated efficiency that drops by more than 1.5% with respect to the single injection. This conclusion leads to the decision to use single injections as the starting point for comparing all fuels.

**Naphtha blend 3**

This blend was originally created to decrease reactivity. It should result in a larger separation between the injection event and combustion which could enable early injection PPC. Figure 9–3 shows that the increased resistance to auto-ignition for NB3 results in a distinctly different heat release pattern compared to NB1 and NB2.

Even for the double injections, ignition is postponed until TDC. For both single and double injections, heat release is seen to occur only in a premixed peak, without a distinct tail. Although NOx emissions and MPRR are reduced (see Table 9–4), it remains doubtful whether significant benefits will be obtained with such early pilot injections.

2 – Total dilution and combustion phasing variation

Even though the previous section has shown that multiple injections can have some advantages with respect to certain emissions, for the following section a single injection strategy is used at a moderate 1500 bar fuel pressure. Two target air excess ratios (i.e. 1.5 and 2.0) are studied and combustion phasing is varied.

**Emissions**

Hydrocarbon and CO emissions seem to correlate with the boiling range, as can be seen from Figure 9–4. Apparently, fast vaporization with the lower boiling fuels increases the amount of fuel present near the wall or in the crevices. That is also why a reduction of these emissions is observed with increased total dilution, i.e. a higher density reduces spray penetration and consequently inhibits fuel approaching the wall.

Confinement of the fuel closer to the center of the combustion chamber (i.e. richer conditions) will also increase the temperature locally and as such the NOx formation. This seems not to be counterbalanced by the near-proportional increase in heat capacity of the cylinder charge.

**Table 9–4:** Overview of engine parameters and results during NB3 combustion characterization

<table>
<thead>
<tr>
<th></th>
<th>Single</th>
<th>Double</th>
</tr>
</thead>
<tbody>
<tr>
<td>IMEPgross [bar]</td>
<td>7.7</td>
<td>7.6</td>
</tr>
<tr>
<td>CA50 [°CA aTDC]</td>
<td>6.1</td>
<td>6.2</td>
</tr>
<tr>
<td>SOI [°CA aTDC]</td>
<td>-8.9</td>
<td>-61/-4.5</td>
</tr>
<tr>
<td>MPRR [bar/°CA]</td>
<td>16.3</td>
<td>13.8</td>
</tr>
<tr>
<td>$\eta_{ind}$ [-]</td>
<td>0.476</td>
<td>0.457</td>
</tr>
<tr>
<td>$\eta_{comb}$ [-]</td>
<td>0.987</td>
<td>0.959</td>
</tr>
<tr>
<td>ISNOx [g/kWh]</td>
<td>0.85</td>
<td>0.52</td>
</tr>
<tr>
<td>ISPM [g/kWh]</td>
<td>0</td>
<td>0.0035</td>
</tr>
</tbody>
</table>

**Figure 9–3:** Both single and double injection yield a similar heat release for NB3 at 1500 fuel pressure and 50% EGR.

**Figure 9–4:** Overview of emissions for combustion phasing variation.
Furthermore, for all emissions clear trends with combustion phasing are visible. Earlier, hotter combustion results in more complete combustion but higher NOx emissions, and vice versa for retarded combustion.

Note that for the present conditions, all fuels are within PM EURO VI emissions levels, while neither meets EURO VI NOx levels. Since there is some margin with respect to PM emissions, a slight increase in EGR level might be possible. For Naphtha blend 3, an increase of the EGR level to 60 wt-% leads to NOx emissions below EURO VI levels yet the particulate emissions remain acceptable, as can be seen in Figure 9–5. Although the lower global temperatures give rise to a slightly reduced combustion efficiency, it is still acceptable.

Efficiency

Indicated efficiency is known to benefit from higher dilution because of reduced heat losses through the exhaust, as well as to the cylinder walls. This significant increase of approximately 2.5 percent points can be seen from Figure 9–6 for all fuels. However, the lower boiling range NB3 suffers from a slight efficiency loss because of the reduced combustion efficiency.

Lastly, one can note that for all fuels, a CA50 of around 4°CA aTDC is optimal with respect to efficiency, even though with a somewhat retarded combustion phasing (10°CA aTDC) the penalty in efficiency is limited.

3 – Fuel pressure variation

Alternative fuels with completely different characteristics (e.g. ignition behavior and structural effects) might be able to break with the trend of ever increasing fuel pressures, used to decrease particulate matter emissions.

Particulate emissions

When comparing all of the naphtha blends to EN590 diesel for reduced fuel pressures, one can see from Figure 9–7 that all blends outperform EN590 with respect to particulate matter emissions. While the diesel fuel already gives significant PM emissions at 1400 bar, each of the blends starts to give increased PM emissions, if
the injection pressure is low enough.

The naphtha blend 3, with the lowest reactivity clearly has the lowest amount of soot emissions, followed by the aliphatic (i.e. non-aromatic) blend 1. The latter’s soot emissions are quite constant at all pressures over 1100 bar. However, as fuel pressure drops to 1000 bar and below, one can see a steep rise in PM emissions. NB2 suffers from considerably higher smoke levels than the other two, but because of its higher volatility and chemical composition, it still outperforms diesel.

Heat release effects

The same ranking as is experienced for the particulate emissions (i.e. EN590, NB2, NB1, NB3) can be found in the heat release patterns. As an example, these heat release patterns are given in Figure 9–8 for 1000 bar fuel pressure. One should note that for all fuels, the load and CA50 are constant.

It is therefore, that only marginal smoke levels are present at that pressure. NB3 only shows a premixed peak, with no distinct tail and as such no PM emissions are experienced.

The ignition dwell, or the number of CA degrees injection and combustion are separated, is often said to correlate with the aforementioned soot emissions. However, Figure 9–9 shows only marginal differences of this dwell time with respect to fuel pressure.

Moreover, EN590, NB1 and NB2 do have similar dwell times. Apparently, the need for premixing to reduce soot is really fuel dependent, as ISPM emissions differs by 90% although injection dwell time is of the same order for these fuels. This reduction in PM emissions is therefore thought to originate in better premixing through the higher volatility and the chemical composition itself.

The diesel fuel clearly has the longest mixing-controlled tail, which is part of the origin of its higher particulate matter emissions. The diesel is followed by NB2, which at this fuel pressure has a significant heat release tail, as can also be seen in the smoke levels. NB1 on the other hand, still releases most of its heat in the premixed peak and shows only a small diffusive tail.

Figure 9–8: Heat release patterns at 1000 bar. 8bar IMEP CA50 = 4 °CA aTDC. Premixed fraction Gaussian fits shown with dashed lines, end of injection indicated on x-axis with vertical lines.

The effect of volatility on the amount of premixed charge is even more evident from Figure 9–10, where the premixed fraction of the heat release (as defined on page 19) is computed for all operating points. From this graph, it can be noted that even for the highest fuel pressure, both EN590 and NB2 already do not have a significant amount of premixing. Their premixed fraction is nearly constant, and as such they already combust in the mixing controlled phase. For the other two naphtha blends, a more distinct pattern is found, with the premixed fraction being reduced by lowering the
Commercial Naphtha blends for PPC

4 – Load variation

Given the results shown for one single load, all fuels have been investigated for a broader load range (i.e. 8-16 bar IMEP). This load range represents the range from about one-third to two-thirds of the engine’s rated torque output. The other conditions are given on page 68.

Heat release parameters

As shown in the previous section for a fuel pressure investigation, distinct heat release shapes were present for each of the fuels. These patterns, as described by the fraction of the fuel that burns in the premixed peak, were also shown to change when altering the fuel pressure. Also for a change in load these shapes are expected to change, as will be shown for the naphtha blends as well as for diesel.

Looking at the low load part in Figure 9–12 one can again see the distinction between the fuels. At these moderate loads, the low reactive NB3 has most of its combustion in the premixed regime, whereas the other naphtha blends are somewhat less premixed, but still more than diesel.

As load is increased, for the diesel fuel the premixed fraction hardly changes. For NB1 and NB2, though, the premixed fraction is slightly higher before it approaches the values of diesel. At these higher loads, the impact of volatility on the combustion behavior is reduced, and
chemical effects (i.e. ignition delay) are more dominant. For NB3, even though the premixed fraction decreases as load increases, even for the highest load it exhibits a significantly higher value than the other fuels.

For all of the fuels, the maximum pressure rise rate increases with load, as can be seen in Figure 9–13. However, the absolute levels remain acceptable because of the dilution level that is used for all experiments. Furthermore, independent of load a significant difference between the fuels remains visible. Here the high volatility fuels clearly have a drawback as they result in somewhat higher pressure rise rates.

Figure 9–14: Emission levels as a function of load for all naphtha blends and diesel.

With respect to combustion efficiency (i.e. unburned hydrocarbons and CO emissions) a trend with load can be observed. Given the constant dilution levels and air excess ratios, constant temperatures are expected. However, an increase in combustion efficiency can be noticed with load. The higher in-cylinder gas density at increased loads is expected to reduce the amount of fuel near the walls and in the crevices. For the low boiling fuel blends, still increased unburned hydrocarbon emissions can be observed for all loads, comparing to diesel. However, this increase is marginal and will not have a significant effect on indicated efficiencies.

Particulate emissions are seen to be largely fuel composition dependent. For the diesel fuel, some reduction of smoke levels is observed with load. However, they remain nearly an order larger than the EURO VI levels. Only for the lowest reactive NB3 blend, levels within EURO VI limits are approached or achieved for the whole load range.

Emissions

One of the promises of Partially Premixed Combustion, apart from high efficiency, is its superior NOx and PM emission performance. As shown before, the 50 wt-% EGR is not quite enough to reach Euro VI NOx levels engine-out, as can be seen from Figure 9–14. As was shown earlier, however, a slight increase to 60 wt-% was enough to bring NOx emissions below the legislated levels. Given the constant dilution levels and air excess ratio over the entire load range, no clear trends with respect to load can be seen for any of the fuels. Furthermore, no clear differences between the blends, or even comparing to diesel, can be observed with respect to NOx emissions.

Efficiency

Figure 9–15 depicts the efficiency trends for all fuels. A clear increase of gross indicated efficiency with load is visible for most blends. Lower (relative) heat losses through higher in-cylinder gas density and a lower heat loss coefficient are generally considered to be the origin of this effect.
Commercial Naphtha blends for PPC

were not achieved while using 50 wt-% EGR, a slight increase to 60 wt-% gave both EURO VI NOx and PM levels for the NB3 blend.

The analysis of the heat release pattern revealed a clear distinction between the sooting and non-sooting experiments. Even more, an interesting and strong correlation between the premixed fraction and the amount of soot produced was present irrespective of how this premixed fraction was realized. Specifically:

• Each of the fuels showed a decrease in premixed fraction as fuel pressure was lowered, and correspondingly an increase in the emission of particulates.

• When load is increased, all fuels, even the lowest reactive NB3, show a transition from more premixed to mainly mixing-controlled combustion. At that point even NB3 starts to show larger than EURO VI soot levels.

It should be noted that the premixed fraction was shown to correlate better with the increase in particulate emissions than the traditionally accepted measure of ignition dwell.

We have found that for the whole load range and all fuels, maximum pressure rise rates are efficiently suppressed by EGR. But more importantly for the low reactive Naphtha blend 3, over the whole load range EURO VI PM levels were approached or achieved, combined with a peak gross indicated efficiency of close to 50% clearly indicating the potential of this concept.

Conclusions

With respect to multiple or single injection strategies it was found that fuels of too high reactivity are not very well suited for strategies involving early injections. They suffer from a decrease in indicated efficiency because of significant amount of combustion in the compression stroke. NB3 is more suitable for such strategies; however, the benefits of an early pilot injection remained limited.

For the single injection strategy all fuels showed sufficient controllability with respect to injection timing, even the lowest reactive NB3. Also the shape of the heat release did not change significantly when combustion phasing is shifted. The emissions, however, show the expected trends with respect to combustion phasing and the resulting global temperatures. It should be noted that even though EURO VI NOx levels

Figure 9–15: Gross indicated efficiency as a function of load for all naphtha blends and diesel.

The low reactive Naphtha blend 3 was shown to have a much larger premixed fraction at low loads. This has helped to significantly reduce engine out emissions, especially of particulate matter. This higher grade of premixing was also shown to give somewhat lower combustion efficiency, however, this did not harm gross indicated efficiency for any load. Still, with NB3 a peak gross efficiency of close to 50% can be achieved. Also the other two naphtha blends have superior efficiency to diesel for the larger part of the load range.

References

In the previous chapter, commercially available naphtha blends were used for PPC. The low reactive Naphtha blend 3 approached or achieved Euro VI PM levels over the whole load range, combined with a peak gross indicated efficiency of 50%, clearly indicating the potential of this concept.

As an alternative to using such refinery streams, the use of conventional diesel blended with a promising second-generation biofuel of low-reactivity and relatively high-volatility could provide a viable approach. That is, if such a blend can give similar emission advantages as the earlier mentioned refinery streams, and has a suitable load range.

Furthermore, the bio-component could provide additional advantages, such as the soot-reducing effects of atomic oxygen and a further reduction in effective carbon dioxide emissions. For the present investigation, n-butanol (BuOH) has been selected as a blend component.

Butanol is thought to be an important future fuel component [87]. It has excellent properties for blending with gasoline (especially branched or t-butanol) [88]. Nevertheless, the more reactive isomer, n-butanol, could be suitable for PPC purposes. The high oxygen content of 21 wt-% is likely to contribute to low soot emissions and its relatively high heat of vaporization (~52.3 kJ/mole) is beneficial for lowering in-cylinder temperatures [89].

Moreover, butanol is of particular interest since it can be derived from biomass [90], like ethanol. Furthermore, butanol is favorable over ethanol for several reasons. It has a higher energy density, is less hygroscopic than ethanol (due to its structural shape with an elongated apolar chain [91]) and is less corrosive to several metals and polymers. Existing infrastructure could thus be used for transportation. Moreover, the lubric-
Bio-butanol can be directly used as gasoline fuel and the possibility to blend it with diesel in significant amounts (up to 40%) was shown in a recent publication by Valentino et al. [92]. Nevertheless, higher butanol content blends in a diesel engine have not been investigated yet.

In the present chapter, butanol fractions of 50 to 90% are used. The blends then have a reactivity range similar to the refinery streams which were mentioned before, so single-cylinder engine tests for their emission and efficiency performance can also be used to determine their applicable load range.

In this chapter a summary of the performance of the BuOH-diesel blends with respect to emissions and efficiency in the Partially-Pre-mixed Combustion regime is presented. Besides a presentation of the sensitivity to injection strategies, dilution levels and fuel pressure, emission performance is compared to upcoming legislated emission levels. The effect of the blending ratio on load ranges is shown and conventional diesel combustion benchmarks are used to show improvements in indicated efficiency.

**Experimental setup**

The CYCLOPS test setup is used with a low-compression XE390c piston, which together with the thickest head gasket available (1.45 mm) yield a compression ratio of 15.7.

**Fuel blends under investigation**

Table 10–1 gives an overview of the specifications of the fuels which are used in the blends.

<table>
<thead>
<tr>
<th>Fuels used for the blends</th>
</tr>
</thead>
<tbody>
<tr>
<td>n-butanol</td>
</tr>
<tr>
<td>CN [-]</td>
</tr>
<tr>
<td>AFR [m]</td>
</tr>
<tr>
<td>LHV [MJ/kg]</td>
</tr>
<tr>
<td>Boiling range [°C]</td>
</tr>
</tbody>
</table>

Five blends with relatively high butanol content (i.e. 90-80-70-60-50 vol-%) have been investigated for this research. No visual separation in the diesel-butanol blends was found over a period of several weeks. Apart from varying reactivity and volatility, using different blend contents also implies varying air fuel ratios and heating values due to the presence of oxygen in the butanol molecule.

For the reactivity of each of the blends, only a rough estimation using linear molar blending is given. The reference CN value for n-butanol, being 17, is taken from [94]. Some properties of the blends used, are given in Table 10–2.

**Table 10–2: Specific parameters for the tested blends**

<table>
<thead>
<tr>
<th></th>
<th>AFR m [-]</th>
<th>LHV [MJ/kg]</th>
<th>Estimated CN [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>BuOH90</td>
<td>11.48</td>
<td>33.99</td>
<td>20.5</td>
</tr>
<tr>
<td>BuOH80</td>
<td>11.82</td>
<td>34.96</td>
<td>24</td>
</tr>
<tr>
<td>BuOH70</td>
<td>12.17</td>
<td>35.92</td>
<td>27.6</td>
</tr>
<tr>
<td>BuOH60</td>
<td>12.52</td>
<td>36.89</td>
<td>31.1</td>
</tr>
<tr>
<td>BuOH50</td>
<td>12.87</td>
<td>37.86</td>
<td>34.7</td>
</tr>
</tbody>
</table>

**Conditions and procedure**

Like in the previous chapter 9, an engine speed of 1250 rpm, a cooled EGR flow of around 50 weight percent and a global lambda value of around 1.5 are used. Furthermore, the exhaust back pressure is set 0.3 ± 0.2 bar higher than the intake pressure.

At 8 bar gross IMEP, first the combustion behavior is tested for all blends, using a single injection strategy, with five SOIs aiming at CA50s of 2, 4, 6, 8, and 10 °CA aTDC. After that, a double injection strategy is compared to the more conventional single injection, by varying the start of injection (SOI) until the desired CA50 is reached within ± 1 °CA.

Furthermore, the sensitivity of combustion behavior with respect to the total dilution level will be analyzed, by increasing the intake pressure in 0.1 bar increments, while keeping EGR level and all other parameters constant. In fact, this procedure results in air excess ratios ranging...
Particulate emission levels from conventional diesel combustion are known to be sensitive to the fuel pressure used. Whether this is still the case when using butanol-diesel blends is tested using a fuel pressure sweep from 1400 bar down to 800 bar, with 100 bar decrements.

After these sensitivity analyses, the load range of each of the fuels will be shown, for which five loads have been selected. For each target load ± 0.5 bar, the fuel mass flow is kept constant and small variations in load (originating from varying efficiencies) are allowed accordingly.

For the gross IMEPs of 8, 10, 12, 14 and 16 bar, fuel pressure increases with load to keep injection duration roughly at a constant in crank angle domain, as was explained in the previous chapter. From 1000 bar at 8 bar load, with every 2 bar of load increase, fuel pressure will be increased with 200 bar. CA50 is fixed at 8±1 °CA over the whole load range.

**Results and discussion**

The results from the blends of butanol and diesel are presented in the following subsections. Where applicable these blends are also compared to pure diesel.

1 – Blending ratio and combustion phasing

Combustion characteristics (i.e. heat release patterns and emissions) will greatly depend on the content of the blend, through a different volatility and reactivity. Therefore, in the following subsections, heat release, controllability and emissions are investigated for one fixed target load (i.e. 8 bar gross IMEP).

**Heat release pattern**

Increasing the diesel content of the blend is expected to gradually smoothen the combustion. Therefore, a blending ratio sweep has been performed using a single injection and 50 wt-% EGR. For a fixed combustion phasing (CA50), Figure 10–1 reveals the expected decrease in maximum heat release rate with increasing diesel content.
Butanol for PPC

its, as may already be expected from the burn duration of only 3 °CA at 6 °CA aTDC. For the more reactive BuOH70 through BuOH50, timing can be advanced arbitrarily.

Controllability and stability

One of the challenges of (Partially) Premixed Combustion can be (a lack of) controllability. For good controllability a $s_{ID}$ value near unity, as experienced for conventional diesel combustion, is desired.

Figure 10–3 depicts the sensitivity for the butanol blends at 8 bar gross IMEP. As can be seen from this figure, BuOH50 and BuOH60 have such a near unity $s_{ID}$.

![Figure 10–3: Combustion phasing response varying the injection timing for four butanol-diesel blends.](image)

The BuOH80 blend, however, has a larger sensitivity and has proven to have significantly less stable combustion. This effect is experienced even more for pure butanol, for which combustion was too unstable to be included in these results, with high cycle-to-cycle variability and an associated compromised combustion efficiency.

Emissions

For the premixed combustion of pure n-butanol, low emission levels are expected. Especially with respect to particulate matter emissions, the atomic oxygen is expected to reduce this. However, this might only be a second order effect in the PPC regime. If it is not, adding diesel might give rise to only a small increase in soot levels proportional to the diesel content as long as the whole charge burns in more or less premixed mode.

The emissions for varying combustion phasing and diesel content are shown in Figure 10–4. First of all, nitrogen oxides levels seem to be mainly dominated by the ambient conditions (i.e. EGR levels, intake temperature, air excess ratio) and combustion phasing. An earlier combustion phasing leads to higher peak temperatures and longer residence times at such temperatures which both increase thermal NO formation.

Unburned hydrocarbon and CO emissions do show a trend with the diesel content of the blends. For a given CA50, higher diesel content blends have decreasing volatility and a later injection timing. This results in less significant crevice effects. Furthermore, higher local equivalence ratios and associated combustion temperatures result in faster and therefore more complete CO to CO$_2$ conversion. The latter relation can also be seen with respect to later combustion phasing and the associated reduced global combustion temperatures.

Regardless of the blending content, minimal to near-zero soot is formed for any combustion phasing. The atomic oxygen, as well as the highly premixed combustion mode as shown in Fig-
ure 10–1 contribute to near-zero smoke levels. Tests at higher loads might show which of these effects is more dominant.

2 – Multiple injections

Using diesel fuel, late cycle pilot injections are relatively hard to use, because the highly reactive fuel may start to burn before top dead center, which can be detrimental for efficiency. Butanol blends, because of the lower reactivity, are expected to be much more suitable for such late pilot injections, which are useful for decreasing local equivalence ratios and therewith peak temperatures. A decrease in nitrogen oxide emissions is expected without too much of a penalty in either HC or CO emissions as global temperatures remain at similar levels.

Furthermore, these pilot injections can be useful for shaping the heat release to the desired pattern, and as such efficiency can benefit from this strategy. Most important, however, the pilot injections can be used to control excessive pressure rise rates, yielding noise reductions. This effect on the heat release rate is shown in Figure 10–5, where also the injector actuation signals are denoted.

From Table 10–3 also the other effects from this double injection strategy can be seen. Indeed, the maximum pressure rise rate and NOX levels are reduced, but there is a slight penalty in combustion efficiency. Additional fine-tuning and rate shaping of the multiple injections could improve the efficiency. Still a single injection with sufficient ignition delay is good enough for partially-premixed combustion at moderate to high loads.

Table 10–3: Engine parameters and results during BuOH60 injection strategy comparison

<table>
<thead>
<tr>
<th></th>
<th>Single</th>
<th>Double</th>
</tr>
</thead>
<tbody>
<tr>
<td>IMEP&lt;sub&gt;gross&lt;/sub&gt;</td>
<td>7.7</td>
<td>7.4</td>
</tr>
<tr>
<td>CA50&lt;sup&gt;[°CA aTDC]&lt;/sup&gt;</td>
<td>10.2</td>
<td>9.8</td>
</tr>
<tr>
<td>SOI&lt;sup&gt;[°CA aTDC]&lt;/sup&gt;</td>
<td>-7.9</td>
<td>-14.3/-3.4</td>
</tr>
<tr>
<td>MPRR&lt;sup&gt;[bar/°CA]&lt;/sup&gt;</td>
<td>11.5</td>
<td>7.9</td>
</tr>
<tr>
<td>η&lt;sub&gt;ind&lt;/sub&gt;</td>
<td>0.483</td>
<td>0.476</td>
</tr>
<tr>
<td>η&lt;sub&gt;comb&lt;/sub&gt;</td>
<td>0.989</td>
<td>0.981</td>
</tr>
<tr>
<td>ISNOx&lt;sup&gt;[g/kWh]&lt;/sup&gt;</td>
<td>0.57</td>
<td>0.37</td>
</tr>
<tr>
<td>ISPM&lt;sup&gt;[g/kWh]&lt;/sup&gt;</td>
<td>0.001</td>
<td>0.0002</td>
</tr>
</tbody>
</table>

3 – Total dilution effect

It is generally known that increasing the total dilution (i.e. the total amount of fresh air and EGR divided by the stoichiometric amount of air necessary for a certain amount of fuel) increases an engine’s efficiency. This fact occurs through a more ideal thermodynamic cycle, i.e. heat loss to the cylinder walls is lowered proportional to a cooler charge mass and the ratio of specific heats does not change as much between compression and expansion.

This observation implies that maximizing the total dilution will contribute to maximizing efficiency. However, it should be emphasized that for practical implementations, boost pressure cannot be increased infinitely. In particular high amounts of EGR can decrease the maximum boost pressure since using EGR reduces the available exhaust enthalpy that drives the exhaust turbine. Because of ever more efficient (multi-stage) turbo charger systems, still the effect of this total dilution will be investigated.

One total dilution sweep has been per-
formed with BuOH60. Limited by the setup’s maximum exhaust back pressure, the highest air excess ratio was around 2.5, while still using 50 wt-% of EGR and a pressure difference between intake and exhaust of -0.3 bar. The amount of injected fuel was kept at a constant 1.0 gram per second, whereas injection timing was adjusted to obtain a target CA50 of 7.5 ± 0.5 °CA aTDC.

Starting from an air excess ratio of 1.5, intake pressure was increased in 0.1 bar increments, while the EGR rate was adjusted to be near the 50 wt-% target. Figure 10–6 shows the gross indicated efficiencies for changing total dilution rates. This gross indicated efficiency increases by more than 10% (4% points) going from an air excess ratio of 1.5 to 2.5

Emissions levels, as shown in Figure 10–7, show the expected trends except for nitrogen oxides. NOx levels are expected to decrease with increasing total dilution due to the increased heat capacity. However, this is likely counterbalanced by a reduced spray penetration and increased local equivalence ratios, i.e. higher local temperatures increase NO formation. Both HC and CO emissions are hypothesized to decrease as a result of increased in-cylinder density at time of injection. This would affect spray penetration and results in less fuel near the cylinder wall. Finally, particulate matter emissions are close to zero caused by the mechanisms described before.

4 – Fuel pressure sensitivity

Conventional diesel fuel combustion is known to be sensitive to the fuel pressure used. As can be seen from Figure 10–8, where smoke emissions are shown as a function of the fuel pressure with all other parameters kept constant, for the EN590 diesel fuel the emission of particulate emissions significantly decreases as fuel pressure is increased.

Therefore, if low soot emissions are requested, the diesel injection pressure should be set to a high enough value, therewith increasing parasitic losses. For the BuOH60, however, at least for the load under investigation, no significant
increase in PM emissions is seen for decreasing fuel pressure. As far as smoke levels go, a reduction of fuel pressure is allowed.

The low sooting tendency of the BuOH60 can be explained using Figure 10–9, where the premixed fraction of combustion is computed for all fuel pressures and fuels. For BuOH60, independent of fuel pressure, the major part of the fuel combuts in the premixed heat release peak. For diesel, even at the highest fuel pressure the amount of premixed combustion is relatively low. The combined effect of mixing controlled combustion and the composition of diesel fuel results in high PM emissions.

This effect can be illustrated even more clearly if the particulate emissions are plotted as a function of this premixed fraction, as can be seen in Figure 10–10. In this graph, also three naphtha blends of medium reactivity are represented (Chapter 9), which helps to illustrate the clear trend of decreasing smoke levels with the premixed fraction.

5 – Load variation

Building on the sensitivity studies of the former sections, all fuels have been tested over the selected load range using a single injection and a target CA50 of $8 \pm 1 \text{°CA aTDC}$. Where applicable, the butanol-diesel blends are also compared to diesel, under the same conditions.

Heat release patterns

Figure 10–11 shows heat release patterns for five different butanol-diesel blends at 12 bar gross IMEP. At this load, differences between the blends are larger than was previously seen in Figure 10–1 for 8 bar IMEP.

The highest reactivity blends now (at 12 bar) show more mixing-controlled heat release patterns, similar to that of conventional diesel combustion (shown in black). Only the BuOH90 blend is still mainly premixed.

For one blend in particular, (i.e. the 60% n-butanol - diesel blend, shown in Figure 10–12),
a clear transition to mixing controlled combustion is observed when the load is increased from 8 to 16 bar gross IMEP.

To quantify the grade of premixing during this transition, again the premixed portion of the heat release is computed for every fuel-load combination (see Figure 10–13). As can be seen from this graph, for all blends the premixed fraction decreases with load.

For the lowest butanol contents (BuOH50 and 60), the premixed fraction saturates at roughly 25%. Above this load, no further decrease is observed due to a near constant ignition delay (not shown here). As the injection duration is kept roughly constant in the crank angle domain, the fraction of fuel injected during the constant ignition delay also remains constant.

Up to this saturation load, however, clear differences can be distinguished between the blends. For pure diesel this premixed saturation occurs already at much lower loads, and, over the load range under investigation, the premixed fraction is nearly constant.

Traditionally, instead of the premixed fraction of combustion, the separation between the injection and combustion events has been used as a measure for the grade of premixing of fuel and air. As soon as this so-called dwell time becomes negative, soot formation is expected to occur. From Figure 10–14, it can be seen that the dwell time becomes zero at roughly 10 bar gross IMEP for BuOH50 and at 14 bar for BuOH90.

At relatively low loads, significant differences in dwell time can be distinguished between the fuels. However, as load increases these differences become smaller and smaller, and for higher loads even for the lowest reactivity BuOH90 blend, dwell times become similar to those of diesel.

Furthermore, high butanol content blends, together with PPC-like conditions, might result in quite aggressive combustion. Burn durations, which can give an indication of the maximum pressure rise rates or noise, are shown in Figure 10–15.

This graph indicates that blending with a second fuel of low reactivity is necessary to slow
Butanol for PPC

Emissions

The major benefit of using the butanol-diesel blends is the soot reduction potential, as can be seen from Figure 10–16. For all the butanol blends, PM emissions are near or below the EURO VI legislated levels. Furthermore, they are up to two orders of magnitude lower than for the EN590 diesel fuel (for which levels have been divided by 10 for clarity). The blends with moderate amounts of butanol can reach the EURO VI levels, even with moderate fuel pressures (compared to currently available engines). This reduction in fuel pressure can help in increasing brake efficiency, as parasitic losses are reduced.

For nitrogen oxides emissions, no clear trends can be seen between the blends and diesel. NOx levels are in this case dominated by the ambient conditions, as the dilution level effectively suppresses the NOx emissions to near or below EURO VI levels. For butanol-diesel points not fully EURO VI compliant, a somewhat higher EGR percentage could be a solution and the penalty in PM might either be acceptable, or can be reduced with a slightly increased fuel pressure.

For carbon monoxide, all butanol blends perform just as well as diesel, with fully acceptable levels at increased loads. Unburned hydrocarbons, however, are somewhat increased when more butanol is used in the blends. Absolute levels of these UHC emissions are within acceptable limits.

Efficiency

Apart from the significant emission reduction, Partially-Premixed Combustion holds the promise of optimizing an engine’s efficiency, through shaping heat release to a thermodynamic optimum. The gross indicated efficiency for all blends is compared to that of regular diesel in Figure 10–17. As can be expected, for all fuels the relative percentage of heat loss reduces with increasing load, contributing to higher efficiency.
At higher loads, all blends show a transition to more mixing-controlled combustion and the load at which this transition occurs depends on reactivity. For the butanol blends, this transition comes without a significant soot penalty.

Given the conditions used, NOx levels were not all EURO VI compliant, but the EGR levels can be somewhat increased and the PM penalty is either acceptable or can be diminished with a slight increase in fuel pressure. These operational conditions also were shown to give very reasonable combustion efficiency (derived from HC and CO emissions) over the whole load range, similar to conventional diesel combustion.

Moderate blends were shown to give the best indicated efficiency over the whole load range; with BuOH50 having an average gross indicated efficiency of 50% over the whole load range. If possible with high efficiency turbochargers, by using a higher total dilution a pathway to even higher indicated efficiencies has been identified, with peak efficiency estimated at 55%.

Conclusions

From this chapter it can be concluded that moderate diesel-butanol blends (i.e. with 50, 60 or 70% butanol in diesel) are a viable approach to Partially-Premixed Combustion, with the added diesel increasing burn durations to acceptable values, and enabling stable operation.

All such butanol-diesel blends have shown an extremely high soot reduction potential compared to diesel-only, even at moderate fuel pressures easily achieving EURO VI PM levels.

References

11 – Fuel composition effects on PPC

Given an optimum reactivity, effects of the chemical composition of fuels on Partially-Premixed Combustion are explored, with the focus on load range capacity.

Photo courtesy of B. Johansson

Previous chapters have shown that conventional fuels, such as gasoline and diesel, have limited suitability for LTC concepts. Manente, however, has shown that when the reactivity is carefully chosen, a single fuel may be sufficient for operation over the full load range [96]. Using a fuel with a Research Octane Number (RON) of 70, stable Partially-Premixed Combustion (PPC) was shown for all load points.

Given this desired reactivity, further improvements on the load range capacity lie in the chemical composition of the fuel. For the purpose of this investigation seven fuels were blended, all with the same RON70, but different physical and chemical properties.

The load range capacity of these fuels is based on a number of criteria. First, at high load the mixing prior to combustion may be limited and depending on the performance of the fuel, excessive smoke formation could occur and/or hardware limits may be approached. At low loads, on the other hand, mixture stratification may not be optimal, as it has to remain ignitable. Differences between the fuels at these conditions will show up in combustion stability and efficiency. Lastly, in the mid load range PPC is known to produce high gross indicated efficiency, for which the fuels are also compared over the load range.

Experiment setup

For the experiments described in this chapter, the CYCLOPS test-setup is used at a compression ratio of 15.7:1, using XE390C pistons and a 1.45 mm thick head gasket.

Thermodynamic analysis and definitions

In addition to the definitions given in chapter 2 on page 17, in this chapter several additional definitions are used.

The experiments presented in this chapter have been performed by Bas Nijsen, under co-supervision of the author, and have, in an extended form, been submitted as Leermakers et al., “Low octane fuel composition effects on the load range capability of Partially Premixed Combustion” for publication in Fuel.
Thermal energy lost to the exhaust is computed by evaluating the enthalpy difference between the exhaust and the same mixture at ambient temperature. The remaining energy is assigned to residual heat losses in the cylinder (to coolant, oil and metal engine components).

To estimate the usable power at the crankshaft, two more losses have to be taken into account. Apart from the work used during the compression and expansion strokes of the engine for gas exchange, part is also lost to friction. Since no engine-specific information is available, this is estimated as a constant 1 bar Friction Mean Effective Pressure, as proposed by Reitz and coworkers [97]. This value is considered to be approximately correct for engine speeds from 600 to 1250 RPM. The losses in gas exchange and friction are independent of the fuel used, so all comparisons are based on the gross IMEP.

**Fuels**

Based on the practical applicability, the fuels can be divided into two groups (Table 11–1). The first four fuels are all blended from refinery streams, which make them practically applicable on the short term.

The first fuel (G) of this group has the composition of a typical gasoline base, mainly consisting of saturated hydrocarbons. Compared to regular pump gasoline, however, the fuel used is not upgraded to achieve a high octane number. Because of its composition, its boiling range is also comparable to that of gasoline.

The second fuel has a boiling range comparable to diesel and is therefore abbreviated as D. Refinery streams used for diesel blends typically have an octane number lower than the desired 70. Therefore such a traditional diesel stream is blended with 49% low-reactivity aromatic solvent of similar boiling range.

The third fuel is a paraffinic solvent in the lower part of the diesel boiling range, but with negligible aromatic content; hence the fuel is abbreviated as Diesel Low Aromatics (DLA). The solvent's reactivity is close to the target, with some components added to have exactly RON 70. The solvent is a narrow cut paraffinic stream, which is typically not used for fuel preparation. Testing two fuels in the diesel range, having different aromaticity however, can indicate the influence of the aromatic content.

Lastly, the fourth refinery fuel is a blend of the DLA solvent with an additional 30 vol-% of Rapeseed Methyl Esters (RME). Rapeseed oil is suitable as biodiesel or can be blended with petroleum distillates. RME contains long unsaturated hydrocarbons (typically C18-C20), which increase the boiling range of this fuel significantly compared to the other diesel based fuels [98]. Furthermore, RME contains molecularly bound oxygen, which results in 4.3% of oxygen mass in the blend. Due to the bio-derived content of this fuel, it is referred to as Diesel with Bio-Content or DBC.

The second group consists of three THEO research fuels, which are blends of Toluene, n-Heptane, Ethanol and iso-Octane. Although being costly and, hence, not practically applicable, these blends are well suited for research purposes. The limited number of components makes that the fuels can be handled in numerical simulations, and chemical and spectral purity makes that they are also suitable for use in optically accessible engines.

Blends of n-heptane and iso-octane are Primary Reference Fuels (PRF) for octane number Thermal energy lost to the exhaust is computed by evaluating the enthalpy difference between the exhaust and the same mixture at ambient temperature. The remaining energy is assigned to residual heat losses in the cylinder (to coolant, oil and metal engine components).

<table>
<thead>
<tr>
<th>Table 11–1: Properties of the fuel blends used.</th>
</tr>
</thead>
<tbody>
<tr>
<td>RON</td>
</tr>
<tr>
<td>------</td>
</tr>
<tr>
<td>G</td>
</tr>
<tr>
<td>D</td>
</tr>
<tr>
<td>DLA</td>
</tr>
<tr>
<td>DBC</td>
</tr>
<tr>
<td>PRF70</td>
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<tr>
<td>TRF70</td>
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<tr>
<td>ERF70</td>
</tr>
</tbody>
</table>
Fuel composition effects on PPC

tests [99]. Adding toluene or ethanol to the blend, a second variable (aromatic or oxygen content, respectively) can be set, while the balance between heptane and octane is changed to obtain the target octane number. The components have the additional advantage that their boiling points are comparable and as such the boiling range is similar for all THEO fuels. Therefore, they are suitable to study the effects of chemical composition in more detail.

A primary reference fuel of 70 vol-% isooctane and 30 vol-% n-heptane (PRF70) is used as the reference case for the other THEO fuels. The second THEO fuel is denoted TRF70 since it contains toluene (30 vol-% toluene, 30 vol-% iso-octane and 40 vol-% n-heptane). The toluene can give further information on the effects of aromaticity, with other parameters kept constant. The final fuel in this group is an Ethanol Reference Fuel (ERF70) with 20 vol-% ethanol, 37 vol-% iso-octane and 43 vol-% n-heptane. To study the effects of molecular bound oxygen, which is present in most bio-derived fuel components, ethanol is used, even though other oxygenates (e.g. esters) may behave differently.

Measurement matrix

The load range capacity of the fuels will be investigated at the following loads: 2, 4, 8, 12, 16 and 20 bar gross IMEP. The first load point is a test of both low load and low speed performance at 600 RPM, being a typical idling engine speed. At all other load points the engine speed is set to 1250 RPM, typical for a truck at highway cruising speed. For the two lowest load points 600 bar of fuel pressure is used. In the subsequent load points the fuel pressure will be set to 1000, 1400, 1800 and 2200 bar, respectively.

In the previous chapters it was shown that the injector-piston geometry combination is not well suited for early pilot injections. Therefore, in this investigation a single injection strategy is used. The injection duration of this single injection is fine-tuned for the load to be within ±0.5 bar of the target IMEP for one combustion phasing and subsequently kept constant for others. At every load point, injection timing is varied such that CA50 is positioned ± 1 °CA of 0, 2.5, 5, 7.5 and 10 °CA aTDC.

Like in the previous chapters, 50 (±5) wt-% of EGR is used, where combustion stability targets permit. Using this dilution strategy in the previous chapters it has been shown that NOx levels near the legislated EURO VI limit of 0.4 g/kWh can be approached. Apart from this dilution level, achieving this NOx level also requires an air excess ratio of 1.5. The air excess ratio is set to this value (±0.1) by regulating intake pressure. At the lower two load points, the intake air pressure is set to atmospheric, yielding higher air excess ratios. Exhaust pressure is controlled to be 0.3 (±0.2) bar above the intake pressure, to mimic a contemporary turbocharger.

Operation of the engine is limited by a number of hardware limitations and combustion quality targets, which are described in more detail on page 16 of chapter 2. For high load conditions, the maximum permissible cylinder pressure of 225 bar limits the use of early CA50. At 20 bar gross IMEP, the desired fuel pressure was not feasible because of high flow rates and due to the low viscosity of the fuels, which imposed high injector leakage. A defect in a seal of the fuel pump resulted in even more pressure loss for TRF70; the injection pressure is only half of the desired fuel pressure. For that reason, no results are presented for TRF70 at the highest load.

At the lower 4 bar gross IMEP load point, the air excess ratio and EGR fraction had to be adapted to meet the combustion stability requirements of $\text{cov}_{\text{IMEP}} < 3\%$. The exact operation conditions used can be seen from Figure 11–19 through Figure 11–23 in the appendix of this chapter.

Results and discussion

In the previous chapters, Partially-Premixed Combustion has been shown to be able of delivering high efficiency. For the mid- and high load ranges, where combustion phasing is retarded as
in the appendix of this chapter.

In Figure 11–1 the gross indicated efficiency is shown for the refinery fuels, with all fuels achieving or approaching 50% gross indicated efficiency for the higher loads, and over 45% for most of the other points.

Some differences can be observed between the fuels, but for all of them, an increase in efficiency up to 16 bar gross IMEP is visible. The origin of this trend can be explained by considering the energy budgets of the load range variation for fuel DLA. From Figure 11–2 one can see that from 16 to 20 bar, the relative importance of thermal exhaust losses and residual losses increase. As mentioned earlier, for 20 bar IMEP combustion was retarded because of hardware limitations. Secondly, the lower fuel pressure causes longer injection durations and as such it extends burn duration. Both of these effects are thermodynamically unfavorable and result in lower gross indicated efficiency.

Specific results describing the low load, low speed performance are presented subsequently, with the main focus the combustion stability and efficiency of the studied fuels. The results section is concluded with a discussion before moving on to the conclusions of the chapter.

Efficiency refinery fuels

For every fuel and load point, combustion phasing (CA50) was varied to obtain the highest possible gross indicated efficiency. The resulting optimum CA50 was shown to vary significantly between the fuels, with efficiency not very sensitive to combustion phasing for the present conditions. Therefore, the fuel-averaged best timing (5 °CA aTDC) is taken for the comparison of the fuels. Only at the two highest loads the CA50 used is retarded to comply with the maximum cylinder pressure limit, see Figure 11–19.
Fuel composition effects on PPC

Because CA50 is near constant for all fuels, clear trends can be seen with respect to the Ignition Delay for all fuels, as shown in Figure 11–3. RON is the same for all of them, but for the conditions under investigation here, significant differences are found between the fuels. For all loads, the fuel with the gasoline boiling range and the diesel without aromatics show similar ignition delays. The fuel in the diesel boiling range, however, shows a significantly higher ignition delay, whereas this is shorter for the fuel with the bio-content.

For all fuels, the ignition delay (ID) decreases up to 12 bar, after which it approaches a constant value. This behavior is also observed for the ignition dwell (IDw) in Figure 11–4 albeit a bit less pronounced. The Ignition Dwell decreases monotonically over the whole load range, becoming negative for all fuels between 10 and 15 bar. In fact the difference between ID and IDw is (by definition ID-IDw=EOI-SOI) an indication of the fact that the injection duration could not be kept constant for the higher loads.

One of the challenges associated with (partially-) premixed combustion is that burn durations may become very short. While this enables a highly efficient thermodynamic cycle, especially for all loads, the fuel with the gasoline boiling range and the diesel without aromatics show similar ignition delays. The fuel in the diesel boiling range, however, shows a significantly higher ignition delay, whereas this is shorter for the fuel with the bio-content.

Figure 11–3: Ignition delay as a function of load for the refinery fuels.

A possible hypothesis is that the MON number is better suitable for describing the chemical ignition phenomena under PPC conditions. It could also be that the conditions used here lie outside of the RON-MON range and that the ignition behavior is best described by extrapolating RON and MON using their sensitivity S [95]. One should note, however, that both the Research and Motor method exploit fully premixed conditions before ignition (without stratification), which is definitely not the case in PPC mode. As such, these numbers do not account for differences in the physical part of the ignition delay through different mixture distributions originating from physical properties such as the boiling range or viscosity (spray behavior).

Figure 11–4: Ignition Dwell as a function of load for the refinery fuels.

Figure 11–5: Burn duration as a function of load for the refinery fuels.
cially for high loads it will result in increased noise levels and possible damage to the engine. In Figure 11–5 the burn durations of all fuels are presented for the load range.

The middle and end of the combustion event are in a conventional diesel regime governed by the injection event. The start of combustion, on the other hand is obviously directly coupled to the ignition delay. With such spray-controlled combustion a long ignition delay therefore thus results in reduced burn duration, with increased pressure rise rates and higher noise.

From Figure 11–5 can be seen that this also holds for the fuel with the bio-content. This fuel, showing the shortest ignition delay for low to mid load, has increased burn durations at these loads. At higher loads, as ignition delays for all the fuels converge to a common value, the burn duration becomes also comparable. The maximum pressure rise rate, which is known to be a measure for possible hardware damage, is not shown here, but for all points under investigation meets the target values. Note from Figure 11–5 that burn durations increase between 16 and 20 bar. This is a direct effect of the retarded combustion phasing.

**Efficiency THEO fuels**

To investigate the influence of aromatics and oxygenates, a number of THEO fuels are used. Similar to the approach used for the refinery fuels, a constant CA50 of \( 5 \pm 1^\circ\text{CA aTDC} \) is used, except for the highest loads where CA50 is retarded to limit the maximum cylinder pressure. The exact CA50s used are presented in Figure 11–19 in the appendix of this chapter.

The resulting maximum indicated efficiency is shown in Figure 11–6 for all fuel-load combinations. Both the absolute values and trends seen for the refinery fuels are reproduced by the THEO fuels. All fuels, except for PRF70, show an increase in indicated efficiency up to 16 bar IMEP, after which indicated efficiency drops. This was shown to originate from the increased heat losses at the highest loads for the refinery fuels (Figure 11–2). These increased heat losses are induced by retarded combustion phasing and longer burn durations because of a lower achievable fuel pressure. This effect is even more prominent for the THEO fuels due to their low viscosity.

With respect to ignition delay, only marginal differences can be seen between the fuels. Only at the lowest and highest loads, where operating conditions and consequently the stratification are not fully constant between the fuels, the ignition delay values deviate slightly. As trends are similar to those of the refinery fuels in Figure 11–3, they are not shown or further discussed here.

Given that CA50 is near constant between the fuels, their ignition dwell is also quite similar, as is shown in Figure 11–7. Considering the near-constant injection duration this implicitly can also be used to compare the ignition delays of the fuels. For both the ignition delay (not shown here) and the ignition dwell, only slight deviations can be seen at the highest and lowest loads. At the highest injector flow rates, for these low viscous fuels increased leak flows precluded the high pressure pump to maintain fuel pressure at the desired value. This can be seen to result in a more negative dwell. This and other effects of fuel pressure will be further discussed on the following pages.
The concept of Partially-Premixed Combustion has been shown to reduce smoke by elongating the available mixing time, however, with a penalty in combustion efficiency. Throughout the load variation, hardly any fuel related differences are observed, as combustion efficiency is dominated by global conditions. Below a certain load both reactivity (in terms of ignition delay) and volatility (in terms of boiling range) may play a role. Both properties are directly related to the fuel dispersion in the combustion chamber. Over-leaning effects can occur if ignition delay becomes too long or vaporization too fast [100]. Some solutions for reduced unburnt emissions at low loads, which are currently under investigation, are briefly discussed from page 96. At low loads, the fuel having the shortest ignition delay, DBC, shows the highest combustion efficiency, see Figure 11–9. For the other fuels, combustion efficiency is reduced in the same order as ignition delay was increased (Figure 11–3).

As carbon monoxide and unburned hydrocarbons are used for computing the combustion efficiency, they are not shown separately. For all fuels EURO VI legislation levels for CO are only met at 12 bar IMEP and above. At the lower load points, in-cylinder temperatures are not high enough to obtain complete combustion.
fuel pressure is varied from 600 to 1800 bar in increments of 200 bar, while CA50 and load are kept constant at 8 °CA aTDC and 8 bar IMEP, respectively.

One can see that for all fuels smoke increases as fuel pressure is lowered. For fuel DBC this results in the most significant PM levels, presumably induced by its high viscosity and boiling range. This explains its poor behavior with respect to smoke at mid load, where 1000 bar fuel pressure is being used. While it suffers most from such a mismatch, its high response to fuel pressure also means that further improvements may be possible at a slight increase in fuel pressure. From Figure 11–11 one can also see that the fuel in the diesel boiling range (D) tolerates a lowered fuel pressure best. This indicates that the effect of better atomization through increased viscosity is more important than the lower vaporization due to the difference in boiling range. The RON70 diesel was also found to have the longest ignition delay of all, which could explain its excellent smoke propensity. Any changes to the benchmark diesel fuel’s composition, lowering boiling range, less aromatics, or the addition of oxygenates, are shown to worsen the fuel pressure sensitivity.
To enable EURO VI smoke emissions, fuel pressure has to be more accurately matched to the minimum necessary fuel pressure for the various load conditions. The fuel pressure necessary will depend on the fuel, but for all fuels the pressure has to be increased, especially at 12 bar IMEP. For the highest load, viscosity enhancer may have to be added to the fuels. A second option is to adapt the fuel injection equipment to enable either a lower injector leak flow for these low viscous fuels, or a pump which enables high fuel pressures even at high leak flow.

Nitrogen oxides emissions, as shown in Figure 11–12, display little fuel specific trends as they are mostly determined by global conditions (temperature and oxygen concentration). Only at the lowest load, some differences between the fuels can be seen. The impact on NOx emissions at this lowest load is caused by the adapted dilution strategy, which was inevitable for stability reasons. For the rest of the load range, emissions approach or achieve the EURO VI NOx levels. To be EURO VI NOx compliant over this part of the load range, a slight increase in dilution level may be necessary. The efficacy of an increase from 50 to 60 wt-% is shown on page 71.

No clear distinction is reported between the THEO fuels with respect to UHC and CO emissions. The global behavior of the THEO fuels is comparable to the refinery fuels. The indicated specific CO emissions are EURO VI compliant over 12 bar load. However, the hydrocarbon emissions do not meet the EURO VI limit throughout the complete load range. This does not have a big impact on the indicated efficiency. However, a small oxidation catalyst is necessary to be emission compliant.
Smoke emissions as presented in Figure 11–14 show the same trends as the refinery fuels, with the unexpected smoke local maximum between 8 and 12 bar gross IMEP. The chosen load – fuel pressure strategy is concluded to be responsible for this observation, which can be solved by an increase in fuel pressure, reducing injection duration. On the other hand, the OH group of ERF70 is shown to inhibit massive smoke formation and it is therefore that this fuel is below EURO VI legislation for all operation points. This performance is significantly better than was seen for the DBC fuel. Apparently, the effect of the structural position of the oxygen is much more pronounced than actual oxygen content. However, a large part of the increased smoke emissions for PRF70 and especially TRF70 also originate from a higher fuel pressure sensitivity, as will be shown next.

Figure 11–14: Smoke emissions as a function of load for the THEO fuels.

A fuel pressure sensitivity sweep from 600 to 1800 bar is again performed for a single 8 bar load, with CA50 kept constant at 8 °CA aTDC to enable a fairer comparison between the reference fuels. Figure 11–15 correlates with current knowledge, i.e. alcohols reducing and aromatics increasing smoke emissions with respect to a paraffinic fuel. The remarkable difference between ethanol and the effect of the Fatty Acid Methyl Esters (FAME) in fuel DBC might be attributed to structural properties. FAME has a long carbon chain of typically 18 to 20 carbon atoms with a double bonded oxygen atom which apparently is not effective in decreasing smoke. Together with its viscosity and volatility characteristics it is concluded that those long-chained esters are not favorable for smoke reduction.

Figure 11–15: Fuel pressure effect on smoke emissions at 8 bar gross IMEP for the THEO fuels.

The fuels requiring the most improvement over the load range with respect to smoke emissions, luckily also show the highest fuel pressure sensitivity. Therefore, to meet EURO VI smoke emissions over the complete load range, a higher injection pressure might be the best solution. This way, the smoke problem might be solved, at the expense of somewhat higher parasitic losses. Still, the problem of increased smoke emissions at 20 bar IMEP may occur, since the low viscosity of the fuels makes it hard to maintain high fuel pressure at a high mass flow demand.

The reported observations imply that engine parameters have to be selected carefully when using different fuels in Partially-Premixed Combustion. Viscosity is critical when high fuel pressures are demanded. On top of that, solely adding a certain oxygen quantity is not sufficient for smoke reduction; also the position of oxygen in the molecule structure needs to be evaluated. A single or double bonded oxygen atom in an ester group may end up in CO directly, whereas the atomic hydroxyl group in an alcohol may provide an OH radical which is a key species in soot oxidation. As a last remark for discussion...
and to lead the way for further work, it is emphasized that the used smoke detection method utilizes the paper filter method, which provides no information on soot morphology or size distribution. Therefore, additional measurements are required with sophisticated particle sizing equipment.

Like for the refinery fuels, nitrogen oxides are once more fully governed by global conditions (not shown here). From 4 bar load onwards, they are well below EURO V and close to EURO VI limits. The differences at 4 bar load are induced by different dilution strategies, i.e. different EGR rates as can be seen from Figure 11–23 in the appendix of this chapter. Obviously, increasing the EGR rate will reduce NOx emissions even at low loads, although stability might then be affected.

Low speed performance

Part of this work consists of a first study towards idling with the selected fuels. Since the lower load limit is governed by ignition problems, a relative high (2.3±0.2) bar gross IMEP was selected to represent an idling engine (600 rpm). Some other studies have already expanded the low load capabilities by different strategies, i.e. using negative valve overlap (NVO) or rebreathing [101], intake air heating [102] or throttling. All those techniques are deployed to promote ignition when auto-ignition conditions are not met by increasing either the momentary temperature (NVO, rebreathing, heating) or mixture strength (throttling). For the present investigation, none of these measures is used and only the effect of fuel composition is studied.

For the low speed condition, intake pressure is set to atmospheric (1.00±0.05 bara). To meet EURO VI NOx legislation, some Exhaust Gas Recirculation had to be applied, although some fuels required reduced EGR to achieve an acceptable stability. The results in Figure 11–16 depict a moderate difference in stability between the fuels. Only fuels D and DLA differ significantly. Presumably, their reactivity is not high enough at current conditions without any intake air heating (~30°C), yielding over lean conditions due to the large ignition delay. One of the reference fuels (i.e. ERF70) also shows this behavior, albeit to a lesser extent. If the corresponding fuel conversion efficiency is compared with the ignition delay, an almost linear decay up till 10 °CA ignition delay is observed. Beyond this point, control over the combustion event is lost and additionally, a penalty in stability is inevitable. Nonetheless, all fuels have sufficient stability at this particular load following the definitions stated before.

Optimal combustion phasing in terms of unburnt emissions is found to be around TDC (see Figure 11–17), which can be explained by the higher temperatures at this point in the cycle.
and the time available at high temperatures. The exact reason why ERF70 has an improved performance when running with a slightly retarded phasing is not well understood, however, the ignition delay is so long for this blend that the spray-piston alignment is not optimal anymore. Even for CA50 at TDC, a significant part of the fuel ends up in the squish volume and, later in the cycle, in the crevice volume where it harms the combustion efficiency.

**Discussion**

The most striking observations between the fuels are summarized in Table 11–2. Large differences were seen with respect to smoke emissions at mid load. It was shown that this was to a large extent caused by the chosen experimental fuel pressure strategy and the difference of the fuels’ smoke propensity as a function of the fuel pressure. Low fuel pressure sensitivity (FPS) is good, but a high FPS, in its turn, means that too high smoke emissions may be solved, at the expense of higher fuel pressure and the associated parasitic losses. This is especially the case for fuels DBC and TRF.

For the larger part of the load range, NOx levels do not show any differences between the fuels as they are dominated by global conditions. Only at 4 bar IMEP some differences were observed with DBC performing much better and DLA much worse than average. At this low load, also combustion efficiency shows differences between the fuels with DLA performing best and ERF70 worst.

At low engine speed and 2 bar IMEP, ERF70 is again the worst performer with respect to combustion efficiency. DLA also suffers from poor combustion efficiency. For both fuel DLA and D combustion stability is compromised at this low engine speed. Over the rest of the load range, all fuels show similar trends and absolute values with respect to efficiency.

**Table 11–2:** Performance comparison of the seven fuels.

<table>
<thead>
<tr>
<th>Smoke mid load</th>
<th>FPS (+ is low)</th>
<th>NOx 4 bar</th>
<th>$\eta_{\text{comb}}$ 4 bar</th>
<th>$\eta_{\text{comb}}$ low speed</th>
<th>Stability low speed</th>
</tr>
</thead>
<tbody>
<tr>
<td>G</td>
<td>O</td>
<td>–</td>
<td>O</td>
<td>O</td>
<td>O</td>
</tr>
<tr>
<td>D</td>
<td>O</td>
<td>+</td>
<td>O</td>
<td>O</td>
<td>–</td>
</tr>
<tr>
<td>DLA</td>
<td>–</td>
<td>O</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>DBC</td>
<td>–</td>
<td>–</td>
<td>+</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>PRF70</td>
<td>O</td>
<td>O</td>
<td>+</td>
<td>O</td>
<td>O</td>
</tr>
<tr>
<td>TRF70</td>
<td>–</td>
<td>–</td>
<td>O</td>
<td>O</td>
<td>O</td>
</tr>
<tr>
<td>ERF70</td>
<td>+</td>
<td>+</td>
<td>O</td>
<td>–</td>
<td>O</td>
</tr>
</tbody>
</table>

Figure 11–18: Combustion efficiency as a function of ignition delay at low load operation for all fuels.

The aforementioned ignition delay hypothesis is confirmed by the results presented in Figure 11–18. A fuel independent decrease is observed extending the delay from 5 to 10 °CA. With respect to fuel composition, no conclusions can be drawn, although high boiling fuels seem to suffer from poor vaporization.
Summary and conclusion

Given that an octane number of 70 seems to be the optimum reactivity for load range capacity of Partially-Premixed Combustion, seven fuels have been blended, all with the same RON70, but different physical and chemical properties. Four of these fuels are blended from existing refinery streams. For a more fundamental approach, three ternary mixtures of Toluene, n-Heptane, Ethanol and iso-Octane are used, of which the aromatic (toluene) and oxygenated (ethanol) content is varied.

The load range capacity of these fuels is determined based on a number of criteria.

• The mid and high load fuel efficiency is good for all fuels and does not differ too much between them. At the highest load, efficiency can possibly be reduced by shorter injection durations made possible by an increased maximum fuel pressure.

• With respect to smoke emissions, not all fuel perform that well. ERF70 was seen to have lower smoke emissions than all the other fuels. On the other hand, especially the diesel fuel with added bio content and the toluene reference fuel have high smoke emissions. However, it also was shown that these fuels have the highest sensitivity of smoke emissions to fuel pressure. As such, an increase of this fuel pressure may solve their smoke emissions at the cost of higher parasitic losses. Future tests should focus on the fuel pressures necessary for achieving EURO VI particular emissions and the brake efficiency penalty associated with such fuel pressures.

• NOx emissions are for the larger part of the load range determined by global conditions and are little fuel specific. To achieve EURO VI NOx levels, the precise EGR percentage has to be fine-tuned. Only at the lowest loads this might not be possible without compromising combustion stability.

• At low engine speed and only 2 bar IMEP, additional strategies have to be investigated to increase the combustion efficiency of the ethanol reference fuel in particular. At these conditions for the fuels in the diesel boiling range, with and without aromatics combustion stability is compromised.

Summarized, the fuel in the gasoline boiling range is more or less the benchmark, with average performance over the whole load range, except for slightly higher NOx emissions at low load. Fuel D has a better indicated efficiency at this low speed, at the cost of a lower stability at low engine speeds. The diesel fuel with low aromatics, did not give low smoke emissions as was expected. Smoke emissions are even worse than average, as are NOx emissions, and stability and combustion efficiency at low speed. The fuel with added bio-content has particularly high smoke emissions, although it also shows the highest fuel pressure sensitivity of all fuels. Although having the highest smoke emissions, it also displays the lowest NOx levels at 4 bar and good combustion efficiency at low speed.

Like the fuel in the gasoline boiling range, the primary reference fuel performs average over the whole load range. The added toluene in TRF70 does not change this performance too much. The biggest difference can be seen with respect to smoke emissions. While it produces significant smoke emissions, they can be reduced with a higher fuel pressure. The hydroxyl group in ERF70 makes for superior performance with respect to smoke emission, significantly better than the ester group in DBC, at a cost of lower combustion efficiency at lower loads and speeds.

References

Acknowledgements

The supply and testing of all fuels by Shell Global Solutions UK, and in particular the help of Roger Cracknell, Sue Webb and Hyun-Woo Won is gratefully acknowledged.

Additional figures - operation settings

The following graphs are for further reference and validation of the operating conditions.

**Figure 11–19:** CA50 used for all fuels in the load range study

**Figure 11–20:** Intake pressure as a function of load for all fuels

**Figure 11–21:** Fuel pressure as a function of load for all fuels. Note that the low fuel pressure for TRF70 at 20 bar IMEPg was induced by a leaking seal of the fuel pump

**Figure 11–22:** Air excess ratio as a function of load for all fuels

**Figure 11–23:** EGR wt-% as a function of load for all fuels
Further advances in Low-Temperature Combustion strategies are being sustained by a detailed understanding of the underlying phenomena. Laser-based diagnostics, in particular, have helped in probing properties of flow and scalar fields with high precision and accuracy [103].

One such technique is Planar Laser-Induced Fluorescence (PLIF) of radical minor combustion species [104]. This method can give a spatial insight in different intermediate steps of the combustion process, and has helped to understand and improve conventional engine concepts in particular.

As many processes in conventional engines can be seen as statistically stationary, a combination of images of different sampling moments, and in multiple engine cycles is possible. Genzale [105] developed a technique where a single spatially representative image is objectively selected from a set of images, using a statistical image-correlation technique. Besides that, techniques also exist to derive probability density functions, mean values, and variances from such image sets to describe the occurring processes. These methods, however, do not statistically correlate the images in the time domain.

Combustion phenomena in LTC are kinetically dominated. The ignition process occurs more slowly than in diesel engines and possibly at multiple locations simultaneously and also (local) extinction (e.g. quenching) may be more important. Such processes cannot be viewed as statistically stationary, as its statistical parameters (i.e. mean and variance) may vary with time, and can therefore not be described with the aforementioned statistical parameters (e.g. probability density functions).

One option to acquire both spatial and temporal (in-cycle) insight in the combustion process is the use of a laser cluster [106]. Such a cluster, consisting of typically 4-8 conventional laser systems enables images of (short) sequences of radical distributions, typically used at sampling rates up to 10 kHz [107]. An advantage of such an approach is that the laser pulse energies are typically similar to that of low-speed laser systems. However, the number of sequential experiments presented in this chapter have been performed by Maurice Corvers, under supervision of the author.
images is limited by the amount of lasers in the cluster.

Another option is the use of a pulse-burst system [108], where a significantly larger number of pulses is created, also at high pulse energy. To extend such a technique to cinematographic imaging (i.e. sustained multi-kHz sampling over thousands of images) a different type of laser system is necessary. Cinematographic (or temporally-resolved) recording of scalar fields is limited by the rather low pulse energies at multi-kHz repetition rates.

Various fuel tracers can be excited [109] by using for instance the relatively high-power fourth harmonic of Nd:YAG lasers [110]. Formaldehyde (HCHO), which is representative of low-temperature reactions in an engine, can also be excited by using the third harmonic of such a laser system.

Imaging diatomic molecules such as the hydroxyl radical (OH, representative of high-temperature reactions) requires tunable narrowband radiation in the ultraviolet range. Because of the relative abundance of OH and the efficiency of the Rhodamine 6G dye used for this, such an OH imaging technique has been demonstrated at multi-kHz repetition rates [111]. To localize the flame front, or the transition from low-temperature to high-temperature reactions, the methylidene (CH) radical can be used [112].

CH-PLIF at low repetition rates is a well-established technique [113]. However, employing this technique at high repetition rate has not been widely deployed, although it has been shown possible with a pulse burst system by the group of Sutton [114] and with a laser cluster by Miller et al. [115]. In the present investigation a high speed laser system is used for cinematographic imaging of the CH radical. The experimental setup is described in the next section.

The equipment is optimized for CH-PLIF measurements and the limits of the equipment are tested. This is all done using a turbulent Bunsen-type flame. The analysis method of the recorded images is described in more detail, after which results from the technique are presented for three Bunsen burner experiments. Based on the available laser fluence, conclusions are drawn on the applicability range of the present system. Furthermore, the laser power necessary for application under engine conditions is estimated, which is not achieved for the present system.
Experimental setup

Initially, the diagnostic method will be tested using a Bunsen-type flame. The equipment that is used to perform measurements for this research will be described in this section.

Laser setup

A high-power laser system is necessary to obtain a high signal-to-noise ratio. Simultaneously, a high repetition rate is desired in this research, since the goal is to perform crank angle resolved PLIF in an optical engine running at approximately 1000 rpm.

In the present research a single pump-dye laser combination is used, where a multi-kHz pump laser is used to pump a high-speed dye laser. If the laser fluence of such a system is high enough, it enables the cinematographic study of combustion events at high frequency over a large time and cycle domain. The choice for the laser system is based upon the research of Jiang et al. [114], who concluded that the minimum pulse energy for single-shot CH-PLIF is 400 μJ/pulse when using a laser sheet of 50 × 0.2 mm. This equals a laser fluence of 40 J/m²/pulse.

The pump laser used is a frequency doubled EdgeWave IS8II-DE double cavity Nd:YAG high-speed laser, at 532 nm. This is crank angle triggered by a LaVision high speed controller and LaVision DaVis software, which also control the detector setup. The Nd:YAG laser has a net repetition rate up to 10 kHz, with a specified maximum pulse energy of 7 mJ/pulse between 0-3 kHz repetition rate per cavity (so up to 6 kHz net). A 6 kHz repetition rate enables a 1 crank angle degree (CAD) resolution at an engine speed of 1000 rpm. For repetition rates above 3 kHz per cavity, the power of the pump laser has a maximum at 25 W. The pulse energy at higher repetition rates is decreasing proportionally to the repetition rate.

A Sirah Credo high speed dye laser is used for excitation of the CH radicals. Both an oscillator and an amplifier dye cell are used, followed by a doubling crystal and Pellin-Broca prisms to separate the harmonics. Styryl 8 dye is used to transform the pump laser wavelength to wavelengths between 730 - 810 nm. DMSO is used as the dye solvent to red-shift the peak dye efficiency by about 20 nm, compared to using ethanol. This way the peak value of 15% is closer to the desired excitation wavelength (before frequency doubling) of 780 nm.

The day-to-day output power of the dye laser is in the range of 90-130 μJ/pulse. This is one to two orders of magnitude less than in previous research [116], caused by the use of a high speed laser system instead of a low speed laser system. Given the fluence used by the group of Sutton [114], the expectation is that the present laser system would enable CH-PLIF when using a laser sheet with a maximum height of 16 mm.

When the laser beam exits the dye laser, it is 4 mm high and 0.2 mm wide. Two cylindrical UV-coated plano-concave (f=-30 mm) and plano-convex (f=150 mm) lenses are used to stretch the beam to a laser sheet of 20 mm high. This enables a single-image vertical (side-view) cut plane of one of the engines sprays at Top Dead Center. This height is slightly more than the estimated maximum sheet height. The width of the laser sheet is constant at 0.2 mm. At the high quenching conditions expected in the engine, the fluorescence signal is not expected to depend on the thickness of the laser sheet.

Detector setup

The camera that is used is a VisionResearch Phantom V7.1 high-speed CMOS camera. This camera has a maximum frame rate of 4.8 kHz at the full resolution of 800×600 pixels (12 bit monochrome). A high speed image intensifier (Intensified Relay Optics, IRO; LaVision) is lens-coupled to the camera. This IRO allows gating times down to 100 ns and has a spectral range of 190-800 nm. A Nikon manual focus 60 mm f/2.8 glass lens is used.

The CH-fluorescence from the A-X(0,0), A-X(1,1) and B-X(0,1) bands is captured around 431 nm. To obtain an as high as possible signal to noise ratio, a Semrock FF01-427/10 band pass filter with a narrow bandwidth of 10
nm is used. The maximum transmission is 99% as shown in Figure 12–1, which also shows the CH-fluorescence of the three bands described before (arbitrary units) compared to the transmission characteristics of the filter.

**Optimization of equipment**

The equipment described in the previous section has to be optimized for use in this research. Important settings include data handling, laser wavelength, laser power and camera settings.

**Laser wavelength**

Following the theory and the simulated CH-excitation spectrum from LifBase [117], the CH radical will be excited at the B-X(0,0) band using a laser wavelength around 390 nm. To verify that it is indeed CH that is fluorescing and to determine the exact excitation wavelength to be used, an experimental excitation spectrum of the CH-radical in a Bunsen flame is made from 385.00 nm to 393.00 nm. While scanning the dye laser over this wavelength range, 8000 images at a resolution of 288x400 pixels are taken. Each individual image is filtered using a 2D median filter applied over an area of 3x3 pixels (approximately 0.3×0.3 mm) to decrease the noise level. After the filter has been applied, two areas in the image are averaged to determine the background and signal intensities. The ratio of these two average intensities is used as a measure for the signal strength. Although this definition is rather arbitrary, it enables comparison of signal strength of different excitation wavelengths with each other, and to a simulated excitation spectrum.

Figure 12–3 shows both spectra, the experimental spectrum matches the simulated spectrum with CH-emissions peaks on exactly the same excitation wavelengths. The spectrum simulated with LifBase has a resolution of 0.05 nm and a median filter with size 51 (0.05 nm) is applied to the experimental data to improve the clarity of the figure.

![Figure 12–1](image1.png) **Figure 12–1:** Transmission characteristics of optical filter vs. simulated CH fluorescence spectra from LIFBASE [117].

**Layout of setup**

For the experiments using the Bunsen-type flame, the burner is placed close to the exit of the dye laser. The setup used to test the diagnostic method and optimize the equipment and their settings is shown in Figure 12–2.

![Figure 12–2](image2.png) **Figure 12–2:** Experimental setup
Cinematographic imaging of methyldiene radicals using LIF

However, because of the lower pump pulse energy, the system can not reach the specified 130 μJ/pulse.

Detector settings

The camera is placed as close to the observed object as possible, to increase the spatial resolution of the recorded images, which in the current setup is approximately 0.1×0.1 mm per pixel. The numerical aperture of the Nikon lens used is set to its maximum value (f/2.8).

The gate time of the intensifier is set to the shortest possible value, which is 100 ns. Using the shortest possible gate time suppresses any background light as much as possible, while still capturing all fluorescent emission. The timing of the intensifier gate is set such that the intensifier is opened just before the laser pulse, therewith bracketing it. Any elastically scattered laser light is efficiently blocked by the optical filter used.

The IRO gain setting controls this amplification factor on an arbitrary scale of 0-100%. This intensification factor has an influence on the effective resolution of the image. When using a moderate gain (e.g. 60%), even though the signal is weak, a closed flame front with sufficient detail is visible. On the other hand, when using a high gain (e.g. 90%), the images are losing detail and the CH-LIF signal shows much more shot-noise. This effect can be seen in Figure 12–4.

To maintain as much detail as possible in the images, the best setting would be to use a rather low gain, if possible.

Unfortunately, a low gain introduces an intensity level near the limit of detection of the camera and makes the system susceptible to

Figure 12–3: Experimental vs. simulated CH-excitation spectra.

Both vertical y-axes are in arbitrary units and therefore the relative height of the peaks in the experimental and simulated spectra are not matching. The height of the peaks is also influenced by the flame temperature, where for the simulated spectrum a temperature of 2500 K is assumed. The matching excitation wavelengths indicate that it can be concluded that the observed signal is indeed laser-induced fluorescence of CH.

In contrast to the simulated spectrum, the strongest experimental emission occurs when exciting around 387.2 nm. This is also the wavelength that Durie [118] described as the second strongest band. The highest CH-LIF signal occurred at a wavelength of 387.204 nm and therefore this wavelength is used, corresponding to the R_{1}(8.5) transition of the B-X(0,0) CH emission band.

Laser power

The measured day-to-day power of the two cavities of the Nd:YAG pump laser, as measured with a thermal power sensor, is between 5.1 and 6.1 mJ/pulse below 3 kHz and between 3.3 and 4.2 mJ/pulse at 5 kHz. Cavity 1 has slightly lower pulse energy than the second cavity, but both are well below the specified pulse energies of 7 mJ/pulse for repetition rates between 1-3 kHz and 5 mJ/pulse at 5 kHz.

The efficiency of the dye laser system is as specified by the manufacturer, with a maximum pulse energy at 387.204 nm being 90 μJ/pulse at 3 kHz. However, because of the lower pump pulse energy, the system can not reach the specified 130 μJ/pulse.

Figure 12–4: Effect of different IRO gain settings on image quality (gate time 100 ns)

To maintain as much detail as possible in the images, the best setting would be to use a rather low gain, if possible.

Unfortunately, a low gain introduces an intensity level near the limit of detection of the camera and makes the system susceptible to
Cinematographic imaging of methylidene radicals using LIF

'ghosting' [119]. Ghosting is a known issue with high-speed CMOS sensors and is caused by the relatively long time it takes for the signal on the analog busses of the sensor to settle within 12-bit accuracy. Therefore a portion of the information from the previous image can still be present on the current image and the effective time resolution of the camera is reduced.

The only solution for this is to increase the IRO gain and find a compromise between detail and time-resolved accuracy. For the remainder of this research, a gain of 75% is chosen.

Image correction

Despite the use of an optical filter, there is still noticeable background and flame noise present in the images taken with the high speed camera. For both quantitative and qualitative analysis, this noise has to be reduced or in the ideal case, removed completely. For this research the filter methods of Dronnieu and Dec [120] have been examined. They use a set of filtering methods to improve image quality and compensate for laser fluence variations. The following set of filtering methods is applied, loosely based on the work of Dronnieu and Dec.

By placing a black screen behind the Bunsen burner and using a narrow band pass filter, there is no noticeable background present in the recorded images. However, to correct for the offset of noise in the CMOS, this image is still used as a background removal filter. In such a filter, the average background image when not using a laser is subtracted from each image during the following measurements. This step is only useful for static background disturbances, or those reproducible in a cyclic domain.

For noise reduction a 2D Wiener filter is used. This filter uses the fact that, even though the intensity level of the noise can be of the same order of magnitude as the intensity level of the signal, there is a difference in their spatial variances (i.e. how fast and how often the signal changes over a small spatial domain). The Wiener filter uses a local neighborhood size of 5×5 mm (50×50 pixels) to reduce background noise, without affecting the signal area too much.

After application of the Wiener filter, most of the noise outside of the flame region is removed, but the image still looks granular. The image can be smoothed using a 2D median filter. This non-linear filter is particularly useful for reducing noise while preserving edges. A side effect of this filter is that the signal area is somewhat enlarged, which means the flame front will appear slightly wider than it actually is. The main advantage of this filter over an averaging filter is that outliers (low and high) in the intensity have no influence on the result. The median filter uses a local neighborhood size of 5×5 pixels (0.5×0.5 mm) to reduce the graininess of the image, while retaining sufficient signal at the flame front.

Lastly, the image can be corrected for variabilities in the laser profile, as the fluence is not uniform over the height of the laser sheet. This is tested using a cuvette filled with a dye solution that can be excited at the wavelength used. For the present research, Coumarin 1 is used, which has the extra benefit that the emission wavelength is close to that of the CH-radical (431 nm). Therefore, the detector setup does not have to be adapted. The Coumarin 1 dye is solved in ethanol (1 mg/L) in a cuvette which is placed at the location of the burner.

Figure 12–5 shows the recorded Coumarin 1 LIF signal (inverted) in the left. The laser sheet is entering from the right and excites the Coumarin 1 molecules inside the cuvette. At the vertical green line an intensity profile is measured and plotted on the right side of Figure 12–5. Both sides of Figure 12–5 show that the laser fluence, which has proven to be reasonably stable from shot to shot, has an approximate Gaussian shape. This intensity profile of the laser sheet can be used to correct the images for the varying fluence. However, for the first investigations on the applicability of the technique, the variances in laser profile are not corrected for.
Cinematographic imaging of methylidene radicals using LIF

The flame from the propane-fueled Bunsen burner shows turbulent motion. Figure 12–7 shows 8 consecutive chemiluminescence images recorded at 1000 Hz to show this behavior. For capturing the CH-chemiluminescence, the band pass filter FF01-427/10 is used in front of the IRO. The IRO gate time is set to 20 μs and the IRO gain is set to 55%. In the visible range, the Bunsen-type flame is identical to the flame shown in Figure 12–6. The CH-chemiluminescence is a measure for the spatial distribution of the CH-radicals. In the premixed flame, two flame fronts can be distinguished. The first flame front occurs when part of the fuel reacts with the oxygen in the premixed air, this is the inner blue cone. The second flame front occurs when the remaining fuel reacts with oxygen in the ambient air. The CH-chemiluminescence images show that only the inner cone of the Bunsen-type flame has a high CH-radical concentration. The inner cone is bright blue in the visible range. The concentration of CH-radicals in the flame front of the outer cone, dark blue in the visible range, is assumed to be too low to be detected by the camera.

Results

To validate the applicability of the aforementioned optical diagnostic method, a number of experiments has been conducted. The results of these experiments are discussed in three parts:

• CH distribution in a turbulent flame
• CH distribution in flames with varying air/fuel ratio (AFR)
• CH-PLIF signal versus laser fluence

The shown images are the results after filtering the recorded images with the filters as described before. The first set of experiments is conducted using the turbulent Bunsen flame starting with a laser beam of 4×0.2 mm and subsequently using a laser sheet.

CH-radical distribution in a turbulent flame

Figure 12–5: Non-uniform fluence of laser sheet shown by means of Coumarin 1 fluorescence.

An overview of the effects of the filters in sequence (with the exception of the laser profile correction) is shown in Figure 12–6. While the Wiener filter retains the full resolution of the signal in the base image, the median filter might reduce both the spatial and gray scale resolution somewhat. Still, a spatial resolution better than 0.2×0.2 mm is achieved.

Figure 12–6: Step-by-step improvement of recorded images through filtering.

In Figure 12–7 the imaging of chemiluminescence results in the CH-signal integrated over the line-of-sight. Figure 12–8, on the other hand, shows 14 consecutive CH-PLIF images (i.e. a cross section of the CH-signal in the flame). The images are recorded at 1000 Hz, using a laser sheet of about 20 mm in height and a resulting fluence of 22.5 J/m²/pulse. The IRO is used at 75% gain with 100 ns gate width. The turbulent behavior of the Bunsen-type flame is clearly recorded in the CH-PLIF images. The images also show a good resemblance with the
CH distribution in flames with varying air/fuel ratio

It is of obvious interest to study the fluorescence signal yield at varying air/fuel ratio. The CH-radical concentration can be very low during fuel-rich, diffusive combustion, as the flame front is wider and more spread out. To increase the local laser fluence, a laser beam of 4×0.2 mm instead of a sheet is used for this experiment. The air/fuel ratio is varied by adjusting the air hole opening of the Bunsen burner and thereby adjusting the amount of air mixed with the fuel. When this air hole is closed, a fuel-rich yellow diffusion flame is visible. When opening the air hole, the diffusion flame transforms into a blue premixed flame.

Figure 12–9 shows the results of these measurements. The middle column shows photographs of the actual flames for varying AFR values. The AFR is increasing from top to bottom. The right column shows the CH-chemiluminescence of the same type of flames, these show the CH-radical concentration in the line of sight of the camera (inverted colors). The left most column shows the CH-LIF results, where the CH-radical concentration is clearly captured. The location of the CH-radicals corresponds to the inner flame front as seen in the middle pictures.

The CH-LIF images of the fuel-rich flames show a reasonable CH-fluorescence intensity, however, only at high air fuel ratio. At the locally fuel rich regions, as seen in a diesel engine, this might be a problem. Even for the more fuel-lean conditions, the reduced laser fluence when using a bigger laser-sheet has shown to be a problem. Due to divergence of the laser and the optics used, the laser fluence of the laser sheet is only 14.5 J/m²/pulse at 6 m from the dye laser (where the engine for possible application is
positioned), which decreases the signal-to-noise ratio to 2:1 and lower. This makes it impossible to distinguish the CH-PLIF signal from the background noise in the image. To verify the necessary laser fluence, in the next section the signal response to increasing laser fluence is investigated.

**CH PLIF signal versus laser fluence**

While some CH-fluorescence can be seen in the experiments described in the previous section, the laser fluence has been shown to be just on the edge of feasibility.

To acquire a relation between the CH-PLIF signal and the laser fluence, the laser sheet dimensions are decreased to 5×0.2 mm, resulting in a maximum laser fluence of 58.3 J/m². The power of the Nd:YAG pump laser is varied by adjusting the current through the photodiodes, with the repetition rate set to 3 kHz. Figure 12–10 shows some of the results of these measurements. From left to right the currents used to produce the images are 0%, 96%, 98%, and 100%. The laser fluence is not a linear response to the diode current, because of both the pump and dye lasers responses. Above each image the actual laser fluence is shown.

![Figure 12–10: CH-LIF signal with varying laser fluence.](image)

After visual inspection of the images, it seems that a laser fluence of about 40 J/m²/pulse could be the minimum to distinguish the CH-PLIF signal from the flame noise. This result resembles the results of Sutton and coworkers [114], who concluded that 40 J/m²/pulse is the minimum required laser fluence. To further verify the necessary laser fluence, all images from this experiment (100 per pump laser current setting) are examined. In each image an area is selected where CH-PLIF might be visible, see the left most image in Figure 12–10. In Figure 12–11, the average intensity of this area in each of the images, is plotted versus the corresponding laser fluence.

![Figure 12–11: Averaged CH-fluorescence intensity as function of laser fluence. Horizontal line denotes maximum background level.](image)

The averaged intensity levels of this area are scaled between 0 and 100%. The intensity of the images recorded without laser excitation is equal to the flame background signal. The horizontal line represents the maximum background signal, without any laser excitation, which has an intensity of 15%, whereas the average signal at maximum laser fluence is only 20%. This, however, does not mean that the signal-to-noise ratio is maximized at 1.3:1, as it merely represents the average of the selected area. Locally, the intensities are much higher than this average.

With the current setup the maximum energy per pulse that can be delivered to the engine is 58.3 μJ/pulse. This would yield a maximum possible laser sheet height of only 6.5 mm. Furthermore, the engine uses additional optics, and depending on the operating conditions, beam blocking, quenching and signal trapping may reduce the available signal significantly. It can
Cinematographic imaging of methylidene radicals using LIF

therefore be that 1 to 2 orders of magnitude more pulse energy may be necessary if the engine's full combustion chamber is to be imaged.

However, for cinematographic imaging of CH in burner applications, depending on operating conditions, the discussed technique has shown to be a feasible option. Depending on the domain under investigation, the present system allows imaging up to 10 kHz, with the maximum amount of images only dependent on camera memory.

Conclusions

The goal of this research was to develop a cinematographic PLIF diagnostic for the methylidene (CH) radical, that could be used for crank angle resolved measurements in an optically accessible engine. A high-speed Nd:YAG laser has been used to pump a high-speed dye laser.

The wavelength used for excitation of the CH radical has been found by comparing an experimental excitation spectrum with a simulated one. An image processing procedure has been described, which has been shown to reduce background noise and improve signal quality.

With the high speed dye laser system, it has been shown to be possible to image the CH radical distribution in a turbulent Bunsen flame. This was possible up to 6 kHz (when using two cavities of the pump laser), both using a laser beam of 4 mm and a laser sheet of 20 mm high.

When reducing the air to fuel ratio of the bunsen flame, the fluorescent signal strength decreases significantly. Still though, the flame front can be distinguished when using a laser beam. For two-dimensional imaging, however, higher laser energy is necessary.

For engine conditions, pulse energies of 1 to 2 orders of magnitude more than the present setup may be necessary. For cinematographic imaging of the flame front in burner applications, depending on operating conditions, the discussed technique has shown to be a feasible option. Depending on the spatial domain under investigation, the present system allows imaging at sustained repetition rates of up to 10 kHz.

References

[117] Luque and Crosley (1999), Lifbase: Database and spectral simulation (version 2.0.64).
Because high-speed CH-LIF was shown to have a very limited applicability under engine conditions, the same setup was used for more feasible imaging of the OH radical.
Cinematographic imaging of hydroxyl radicals in an optically accessible engine

As discussed in the previous chapter, laser based diagnostics can help in understanding the underlying phenomena in Low-Temperature Combustion. In particular the cinematographic imaging of minor combustion species, such as the methyldiene (CH) and hydroxyl (OH) radicals, can give both spatial and temporal (in-cycle) insight in the combustion process. In the previous chapter it was shown that with the setup used it was possible to image the CH radical distribution in a turbulent Bunsen flame, up to a repetition rate of 6 kHz. However, at reduced air to fuel ratios, the fluorescent signal strength decreased significantly. For engine conditions, it was shown that higher pulse energies were necessary.

Instead of imaging the methyldiene radical, which indicates the transition from low-temperature- to high-temperature reactions, in this chapter the OH radical is probed. This hydroxyl radical is representative of high temperature reactions and can be excited using narrow band radiation in the ultra violet range. This implies the use of UV-suitable optics, but the relatively abundant presence of OH and the efficiency of the Rhodamine 6G dye used make a significantly higher signal possible. Given the higher dye efficiency the frequency doubling is also more efficient. All of this makes that this radical may be more suitable for probing under engine conditions, using the present laser setup.

To develop and test the diagnostic technique, a similar approach is followed as was used in the previous chapter. In the following section the experiment setup is discussed, outlining the test setup with a Bunsen burner and the optically accessible engine, and the detector and laser systems. Using the Bunsen burner, a measured excitation spectrum is compared to a simulated spectrum to verify that it is truly OH which is being excited. Furthermore, this excitation spectrum is used to find the most effective excitation wavelength.

Subsequently the Bunsen burner is used to image both the chemiluminescence and the OH distribution using LIF at varying laser power and air-fuel ratio. As the results of these measurements were very satisfactory, subsequently also measurements in the optically accessible engine are obtained. Two sets of measurements are presented. In the first set, images taken at different crank angles without any laser excitation are compared to images taken at the same crank angles using either a laser beam or a laser sheet for OH excitation. As using a laser beam proved to be most viable under the conditions used, this is further applied to test the performance of the diagnostic technique at varying engine load.

Experiment setup

Throughout this chapter, results are presented from two experimental setups. The optically accessible engine setup and Bunsen burner, as indicated in Figure 13–1 are presented next. This is followed by a description of the excitation and detection systems that both setups use. To conclude this section, an experimental excitation spectrum is acquired to verify with a simulated spectrum and to obtain the most effective excitation wavelength.

Optically accessible test engine

The optically accessible engine is a single cylinder Ricardo test engine driven by an electric motor, with the cylinder head derived from a DAF MX engine. More information on the

Figure 13–1: Layout of the experimental setups
setup can be found in the work of Zegers [121] from which some specifications are repeated in Table 13–1. The position of the cylinder head relative to the piston position at TDC can be adjusted to change the effective compression ratio of the engine. For the present investigation an effective compression ratio of 17.2 is used.

Table 13–1: Optically accessible engine specifications.

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore</td>
<td>130 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>156 mm</td>
</tr>
<tr>
<td>Connecting rod length</td>
<td>270 mm</td>
</tr>
<tr>
<td>Displacement volume</td>
<td>2.07 liter</td>
</tr>
<tr>
<td>Combustion chamber shape</td>
<td>Pancake</td>
</tr>
<tr>
<td>Combustion chamber height at TDC</td>
<td>6.3 mm</td>
</tr>
<tr>
<td>Effective compression ratio</td>
<td>17.2:1</td>
</tr>
</tbody>
</table>

To obtain optical access to the pancake-shaped combustion chamber, three quartz windows are placed in the cylinder liner. This optical liner is shown in Figure 13–2 together with the detector setup and the sheet-forming optics for the laser sheet. Two opposite windows are used to send a vertical laser sheet through the engine, and a window placed perpendicular to this sheet enables imaging of the plane illuminated by the laser. The plano-concave windows follow the cylinder bore on the inside and have a height of 38 mm and a width of 61 mm. This enables studying the center plane of the combustion chamber over the full width and height, from 25 °CA before through 25 °CA after TDC. Outside of this crank angle domain the piston top is located below the bottom of the liner window. To correct for the distorted image resulting from the plano-concave windows, a correction lens can be used. However, for the initial investigations described in this chapter, this lens is not used.

To enable an unobstructed side-view of a single fuel jet, a custom asymmetric 5-hole injector nozzle is used. Of this injector nozzle, one hole is pointed in the radial direction of the incident laser sheet. The other four injector holes are located at relative angles of 105, 155, 205 and 255°, away from the jet of interest. >99% pure n-heptane is provided to the injector by a Resato P200-635-2 fuel pump, similar to the one used for the CYCLOPS test setup.

Detector setup

To perform crank angle resolved measurements, the Phantom v7.1 high speed camera, as described in the previous chapter, is used. One of the benefits of the Phantom camera is that it can be triggered at irregular time intervals by a crank shaft encoder. During experiments on the optically accessible engine this is useful because of minor changes in rotation speed that occur throughout an engine cycle. Like in the previous chapter the camera is lens-coupled to a LaVision IRO image intensifier to enable short gating times for reduction of the background signal recorded. The lens used for imaging the
OH fluorescence is a UV lens with a focal length of 100 mm and a numeric aperture of f/2 (B. Halle Nachfl.).

To further limit the background signal two filters are used. The first filter is a T166-09 band pass filter of 310±10 nm. While the maximum efficiency of this filter is less than 15%, it does offer relatively effective blocking of wavelengths outside this range. During the engine experiments, a second WG-305 high pass filter is used to further eliminate elastically scattered laser light. The filters enable the capturing of the fluorescence emission, while effectively blocking the laser wavelength of around 283 nm, as will be discussed next.

Laser setup

For excitation of OH radicals the same laser is used as was described in the previous chapter. For excitation of OH radicals, the dye laser uses a Rhodamine 6G dye solution in ethanol. The maximum efficiency of this dye solution is approximately 28% at a 567 nm. After frequency doubling, this corresponds to a wavelength 283.5 nm, which is near the peak of the A-X(1,0) excitation band. The maximum obtained power from the dye laser is 830 mW @ 3 kHz. The laser beam has a height of 12 mm and a width of 3 mm at 4 m from the dye laser.

The experiments on the Bunsen burner are executed closer to the dye laser, where the beam profile is still small. To stretch the laser sheet in vertical direction, for these experiments only a UV-coated negative lens (f=-30mm) is used. For the experiments in the engine, a cylindrical lens (f=100 mm) compresses the divergent laser beam in horizontal direction. The resulting laser sheet is 10 mm in height and less than 1 mm thick. To achieve the highest possible laser fluence, in some experiments a laser beam is used instead of a laser sheet. For these experiments a spherical lens with a focal length of 100 mm is used.

Excitation wavelength

To verify that the excited molecules are truly OH and to find the most effective excitation wavelength, an experimental excitation spectrum is obtained. For this spectrum, the laser sheet is directed through the bottom part of a propane-fueled Bunsen flame. The wavelength of the dye laser is varied from 280 through 284 nm and the excited Bunsen flame is recorded with the high speed camera system. Of each recorded image, an area of the flame is averaged into an intensity value which represents the amount of fluorescent signal. In Figure 13–3 this measured excitation spectrum is compared to a spectrum simulated with LifBase.

While the relative heights of the peaks do not all comply between the spectra, their positions clearly match. This indicates that the fluorescence is indeed from excited OH radicals. The measured excitation spectrum is also used to obtain the most suitable excitation wavelength. The Q1(6) transition at 282.895 nm shows the highest emission intensity and will therefore be used for excitation throughout this chapter.
Cinematographic imaging of hydroxyl radicals in an optically accessible engine

Bunsen burner results

To develop and test the diagnostic technique, the described equipment is first tested on a propane-fueled Bunsen burner. In the following subsections OH LIF images are first compared to chemiluminescence images. After this, the signal dependence on a laser power variation and on an air-fuel ratio variation are shown, before the technique is applied in the engine.

Chemiluminescence

As a first step, the Bunsen flame is imaged without any laser excitation. Figure 13–4 is composed of one image taken with a regular digital camera and four subsequent images taken with the high speed camera equipped with the band pass color filter. This first image shows the flame as it is visible to the human eye. The other four images, show the line-of-sight natural emission of the Bunsen flame projected on the camera.

Because of the rather rich air/fuel mixture, not all fuel is able to combust in the inner cone. The remaining fuel ignites when it mixes with ambient air. This combustion can be observed in the bigger almost colorless flame front at the edge of the larger flame in the first image. The emitted light from the OH*-radicals in the outer cone can be seen in the gray scale images in Figure 13–4 as the dark grey flame structure, with lower intensity.

While images clearly display the OH* distribution, all images represent a 3-dimensional flame projected on a plane. As such, no conclusions can be drawn on the location of the visible species in the depth of the image. And the images merely show excited OH*, not all OH. Planar laser-induced fluorescence, PLIF, can be used to solve these problems in the following sections.

High speed OH-PLIF in a Bunsen flame

Planar LIF can be used to image the cross-sectional distribution of OH radicals. The laser sheet which is used for this measurement has a height of 15 mm, a thickness of 0.25 mm and the energy was 217 μJ/pulse. This results in a laser fluence of 58 J/m²/pulse.

The first image of Figure 13–5 again shows a photograph of a Bunsen flame made with a regular digital camera. The other images however show a cross section of the bottom part of the Bunsen flame, displaying fluorescing OH radicals. These OH-PLIF images clearly show that OH is not present inside the inner cone, but high concentrations can be seen in both the inner and the outer flame front. Both flame fronts can be determined from the steep signal rise at the boundaries. Between the two flame fronts, OH concentrations are significantly lower, although there is still some OH present.

Combustion in the inner cone of the Bunsen flame occurs when a rather rich air/fuel mixture comes out of the burner and ignites. In this flame front OH*-radicals are produced. OH*-radicals return to their ground energy level and emit light during this transition. The high-speed camera, equipped with the color filter, is able to capture this light which results in the light grey waving flame structure visible in the four gray scale images. These images show some indication of a turbulent flame structure where the OH*-radicals can be observed at the edge of the inner cone.

Figure 13–4: Regular photo of the Bunsen flame followed by four subsequent high speed chemiluminescence images of OH* recorded at 3 kHz. Spatial domain of all images approximately 28×57 mm.

Figure 13–5: Regular photo of the Bunsen flame followed by four subsequent high speed OH-PLIF images of the bottom part of the Bunsen flame (fluence = 58 J/m²/pulse). Dimensions of the OH-LIF images are approximately 22×21 mm (w×h).
Laser power variations

To relate the intensity of the OH-PLIF in the Bunsen flame to the laser fluence used, the laser power is varied in a series of experiments. Figure 13–6 shows the influence of this laser fluence variation.

![Figure 13–6: OH-PLIF signal for varying laser fluence. The window for calculating the averaged intensity is indicated in the left most picture.](image)

For each laser fluence tested, the intensity of the window shown in Figure 13–6 is averaged both spatially and over 400 images. The averaged intensities for varying laser fluence are shown in Figure 13–7. In this figure, the first two measurement points do not show any OH fluorescence signal. At 8.5 J/m²/pulse some signal occurs, but this is too low to be seen in the figure. The three higher fluences, however, show very strong fluorescence signal. The relation between fluence and intensity shows a linear resolution, although this is not directly visible in Figure 13–7, as at the higher fluences some pixels of the frames were overexposed. Consequently, the true values of these measurements should lie slightly higher.

Though not directly compared here, it should be noted that signal values are at least an order higher for OH fluorescence than for CH, which was used in the previous chapter.

Varying air-fuel ratio

As conventional diesel combustion in an engine does not combust in a premixed way like the Bunsen flame, but in a more diffusive mode, the air-fuel ratio of the Bunsen flame is varied to test the influence on the fluorescence signal. The premixed flame, as shown to the left of Figure 13–8 clearly displays both the inner and outer flame fronts. However, as the air-fuel ratio is decreased, the inner flame front disappears and only the dimmer outer flame front remains visible. A high air-fuel ratio results in much broadly distributed OH which makes both their presence and the position of the flame front harder to detect, as the concentration (gradients) are lower. Although this raises some concerns for applicability under engine conditions, in the following section the technique will be applied in the optically accessible engine.

![Figure 13–7: Averaged intensity for varying laser fluence.](image)

![Figure 13–8: Images of the Bunsen flame for varying air/fuel ratios. Top: Photographs taken with a regular camera. Bottom: High speed OH-PLIF images of approximately 27x51 mm. The red lines indicate the laser sheet edges.](image)
High speed OH-PLIF in an optically accessible engine

To test the applicability of the laser diagnostic under engine conditions, initially three different loads are selected. All three are in the lower end of the engine’s load range to protect the optical components. For all cases, the engine speed is 600 rpm, intake pressure is ambient, and no EGR is used. Results are presented for loads from 0.9 through 3.0 bar gross IMEP. This load is varied by varying the injection duration while keeping the fuel pressure constant at 1000 bar. For all tests, start of injection (SOI) is at TDC. Settings can be found in Table 13–2.

<table>
<thead>
<tr>
<th>Gross IMEP [bar]</th>
<th>Inj. dur. [°CA]</th>
<th>CA50 [°CA aTDC]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.9</td>
<td>2.2</td>
<td>5.0</td>
</tr>
<tr>
<td>1.6</td>
<td>3.6</td>
<td>4.5</td>
</tr>
<tr>
<td>3.0</td>
<td>5.4</td>
<td>5.0</td>
</tr>
</tbody>
</table>

At the lowest load, injection duration is only 2.2 °CA. For this load, the ignition delay is 2.5 °CA meaning that combustion only starts when injection has already stopped. This results in a largely premixed combustion. At a load of 1.6 bar and higher, injection and combustion overlap which causes the injection to result in more diffusive combustion.

Laser configurations

At the lowest load (0.9 bar) three measurement sets are considered: without laser, with laser sheet, and with laser beam. The former is used for background correction, the latter for maximizing fluence. The relevant parameters are listed in Table 13–3; the effective laser power is measured inside the cylinder liner.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Without laser</th>
<th>Laser sheet</th>
<th>Laser beam</th>
</tr>
</thead>
<tbody>
<tr>
<td>IRO</td>
<td>75% gain, 100 ns (min)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(P_{\text{laser,eff}})</td>
<td>300 ± 50 mW</td>
<td>475 ± 50 mW</td>
<td></td>
</tr>
<tr>
<td>Sheet</td>
<td>6.3 x 0.25 mm</td>
<td>0.50 x 0.25 mm</td>
<td></td>
</tr>
<tr>
<td>Fluence</td>
<td>64 J/m²/pulse</td>
<td>1.3 kJ/m²/pulse</td>
<td></td>
</tr>
</tbody>
</table>

In Figure 13–9, for each of the cases 6 consecutive images are shown. Starting from the start of injection the sequences span 7.5 °CA with a 1.5 °CA interval. The left column shows the sequence without a laser, the middle column with a laser sheet and for the right column a laser beam is used. In all images the yellow vertical line represents the edge of the cylinder wall, the red lines represent the cylinder head and piston top, and the yellow dot represents the location of the injector tip. In these images, the laser enters from the right first passing through the isolated jet of interest. The crank angle is shown in the top left of each image, with 360 being TDC.

The measurements without a laser are executed to visualize any background emission captured by the camera, in spite of the short gating time and the filter used. It is obvious that the first three frames in the left column do not show any emission. The first signs of combustion can be noticed in the fourth frame at 364 CAD. The isolated jet is visible as a cloud at the right side of the combustion chamber, whereas the other four jets form a bigger cloud to the left. The intensity is the highest shortly after start of combustion after which it decreases gradually.

When using a laser sheet, as shown in the middle column of Figure 13–9, several differences can be seen. First, one can notice that in the first frame, even before injection has started, laser light induces some background signal. Furthermore, the heavy scattering during injection, in images 2 and 3, is not sufficiently being blocked by the band-pass filter. After injection...
and during combustion, there is only a marginal difference between using a laser sheet or not. Especially on the right side of the combustion chamber, the signal is slightly higher than when not using a laser, but this difference is hard to distinguish and no conclusions can be drawn about whether this is fluorescence or just elastically scattered laser light. The laser fluence may be too low to achieve a noticeable difference between the two measurements under the present conditions.

To increase the laser fluence for the experiments shown in the right column of Figure 13–9, the laser power is optimized and the sheet is compressed into a small beam. Furthermore, an additional WG305 high-pass filter (HPF) with a tipping point between the excitation and emission wavelengths is used to further reject scattered laser light. And while using the same 1.5 °CA interval, the phasing is shifted half a crank angle degree, starting from TDC. A major difference can be observed in the first three images, where elastic scattering is effectively reduced by the additional high pass filter.

The first sign of OH-LIF is visible at 363.0 °CA. A bright horizontal line occurs at the location where the laser beam crosses the right combustion cloud, and can clearly be distinguished from the background signal. This indicates that the increased laser fluence is necessary for detecting OH under the present conditions. During the first crank angles of combustion, no fluores-

![Figure 13–9: Temporal selection of image sequences taken at 0.9 bar gross IMEP, all using the same settings. Without a laser (left), with a laser sheet (middle) and with a laser beam and an additional HPF (right).](image)
Cinematographic imaging of hydroxyl radicals in an optically accessible engine

ence is seen on the left side of the images. The laser beam is aligned with the isolated spray and therefore does not cross any of the other sprays. At later crank angles, visible in the last couple of images, one or more of the four sprays in the left part of the combustion chamber move into the laser beam, through the swirl and spreading of the jets.

Most importantly, it can be concluded that a very high laser fluence is necessary. This means that for imaging the complete combustion chamber, under the present conditions the high-speed laser system does not provide sufficient pulse energy for cinematographic imaging.

Figure 13–10: Temporal selection of the image sequences taken with a laser beam and HPF at 0.9 (left), 1.6 (middle), and 3.0 (right) bar gross IMEP.
Load dependency of OH-LIF

All measurements in the previous section are executed with a rather low load of 0.9 bar gross IMEP. This load is close to idling and not representative of normal operation of the engine. OH-LIF also needs to be applied at higher loads to gain more insight in the applicability of high repetition rate OH-LIF in an optically accessible heavy duty engine. This section describes the OH fluorescence for varying loads. Again a laser beam is used for excitation and an additional high pass filter (HPF) is used to suppress elastically scattered laser light.

The left column of Figure 13-10 is the same 0.9 bar condition as presented in the previous section. For the middle column the load is increased to 1.6 bar and for the right column the load is 3.0 bar. For all cases injection ends before 365 °CA and is therefore only visible in the first two images of each column. The image sequence obtained at the lowest load shows clear emission of OH-radicals at the locations where the laser beam crosses the combustion cloud. The intensity of the emitted light decreases strongly as the load increases for the second and the third sequence of frames. The third sequence hardly shows any LIF of OH anymore.

Two possible causes can be indicated for the decrease in OH-LIF emission for increasing load. Firstly, increasing load means that injection behaves more and more like a diffusion flame instead of premixed combustion. For the Bunsen burner it was shown that emission of OH-radicals is high for premixed flames and that emission decreases heavily when the flame becomes more diffuse. Only for the two lowest loads, some OH emission is visible. Combustion is largely premixed for these loads since the injection duration is shorter than the ignition delay. Only the loads with rather premixed combustion show any signs of OH-LIF.

The second cause is the formation of soot particles at higher loads which block the laser light as well as trapping any signal emitted from the OH-radicals. Load is increased by increased injection duration while air intake pressure remains constant. Therefore, with a load increase also equivalence ratio increases which intensifies the production of soot.

What can be concluded from these tests is that the present laser system is not suitable for imaging OH over a wide operating range.

Conclusions

In this chapter, a high-speed dye laser system was used for multi-kHz repetition rate imaging of the hydroxyl (OH) radical, indicative of high temperature reactions during combustion.

Using a Bunsen burner, it was verified that the laser truly excites this OH radical and the most effective excitation wavelength was determined. Using this excitation wavelength on the Bunsen burner, clear images can be made of the OH distribution in a turbulent flame. From these images it is possible to determine the flame front location accurately. The available signal was shown to depend nearly linearly on the laser fluence.

When the air-fuel ratio of the burner is decreased, the brightest flame front disappears and only the dimmer outer flame front remains visible. A high air-fuel ratio results in much broadly distributed OH which makes both their presence and the position of the flame front harder to detect.

When applied in the engine at an idling condition, laser power needs to be optimized and the sheet has to be focused to a small beam to get a laser fluence which enables a sufficiently high signal level. Under more sooting and more diffusive conditions at slightly higher loads, even the maximum possible laser fluence is not sufficient to obtain a distinguishable signal. From this can be concluded that with the present laser system, cinematographic imaging of minor combustion species is not viable under engine relevant conditions.

References

A third laser diagnostic technique to study early stages of soot formation is developed. This technique uses simultaneous laser-induced incandescence of soot and fluorescence of poly-cyclic aromatic hydrocarbons (PAH).

Photo courtesy of Mark Musculus at Sandia National Laboratories
Laser diagnostics of early soot formation (PAH)

The high-speed laser diagnostic techniques discussed in the previous chapters have proven to be of limited applicability under engine conditions. Therefore, in this chapter a technique is developed which is not cinematographic, but images from separate engine cycles and test runs are combined to resolve the images in the crank angle domain. Consequently, 2-3 orders higher laser pulse energies can be used, from which the signal to noise ratio benefits significantly. More specifically, the developed technique aims at studying soot formation mechanisms.

Soot formation (i.e. the rate of formation, particle size and number density) depends on a large number of parameters. Amongst others, the operating conditions have an impact on these formation processes. During the first steps of soot formation, a fuel like \( n \)-heptane is mostly broken down to \( C_1 \)- and \( C_2 \)-hydrocarbons [122]. From these smaller hydrocarbon fragments, higher hydrocarbons may be formed under fuel-rich conditions. An important class of these higher hydrocarbons is the poly-cyclic aromatic hydrocarbons (PAH), who are important precursors in soot formation [123]. Starting from single aromatic rings the molecules grow through different size classes of an increasing number (2-12) of aromatic rings, before they transition into (larger) particles through particle inception, surface growth and coagulation [124]. In the present investigation, however, we focus on the first steps of the soot formation (i.e. the growth in PAH size).

Low-temperature combustion conditions offer a particularly useful platform for studying this early soot formation. Under these conditions, the diluent effect of recirculated exhaust gas lowers peak temperatures but also broadens the temperature history in time, with a slower, more kinetically controlled progression through different intermediate combustion species. As such, the intermediate temperature regions where PAH species reside are more broadly distributed, both spatially and temporally.

The laser-induced emission and absorption spectra of PAH molecules depend on their size and structure, which can be very diverse for combustion-generated PAH. As such, absorption wavelengths are not unique according to size and therefore the size of these PAH cannot be defined very precisely. However, spectral analysis of broadband PAH-Laser-Induced Fluorescence (LIF) emission shows a transient red-shift prior to the onset of soot formation, implying a growth of PAH size [125]. This red shift of its broad band absorption (or emission) spectrum can be used to some degree to determine the size distribution of the PAH. Laser-induced fluorescence with ultraviolet excitation (e.g. 266 or 355 nm) has been shown to excite small PAH species, whereas visible excitation at 532-nm should excite only larger PAH molecules with at least five rings [126]. The smaller PAH species can be either present in the fuel, or synthesized by combustion. The larger PAH species with five or more rings are mostly due to synthesis during combustion (fuel aromatics are typically 1-5 rings [127]).

This chapter is a follow up on the work of Bobba and Musculus [128], who have shown a technique to image PAH at 532-nm excitation and distinguish this PAH signal from soot incandescence. Extending Bobba’s work over a broader wavelength range should enable studying the spatial and temporal evolution of both smaller and larger PAH species even farther. 633 nm HeNe lasers have been widely used for laser extinction measurements of soot. As a side study, using 633 nm LIF we can check if PAH absorption occurs along with extinction by soot when using 633-nm laser light.

Excitation at these wavelengths using high-fluence laser pulses, however, can also lead to laser-induced incandescence (LII) of soot. As such the resulting signal is a combination of contributions by both PAH and soot. Indeed, LII is commonly used both in laboratory flames as well as engine applications to detect soot [129]. To distinguish between PAH fluorescence and soot LII, in atmospheric-pressure flames a strategy was used to separate the signals based on their respective lifetimes [130]. Under high-pressure
engine conditions with strong fluorescence quenching and rapid conductive heat transfer, however, the lifetimes of both PAH fluorescence and soot LII are much shorter, both close to the 10-ns laser pulse, so temporal separation is not possible.

In this study, to discriminate between PAH fluorescence and soot LII, a second shot of another laser beam at 1064 nm is taken virtually simultaneously to probe the spatial presence of soot only. 1064 nm light is used for excitation because PAH fluorescence arising from excitation in the near infra-red is not expected to be significant, even for very large PAH [131] [132].

In the following section, the engine setup and the operating conditions used are laid out, followed by a detailed description of the excitation and imaging setups. Using the techniques described, in the subsequent results section the spatial and temporal evolution of both PAH and soot are explored. First for a single LIF excitation wavelength this evolution is studied for varying operating conditions (i.e. ambient oxygen mole fraction). Based on the natural luminosity signal and heat release patterns, it is shown which stage of combustion is being investigated. Both the LII and the LIF signal are also spectrally resolved to further discriminate between fluorescence and soot incandescence.

The condition with the lowest oxygen concentration is investigated at multiple excitation wavelengths. At this condition PAH evolves most slowly and as such the most significant difference in temporal PAH size evolution may be expected. In addition to laser-induced emission spectra obtained for these different excitation wavelengths, quantitative chemiluminescence spectra are obtained to further validate the working of the technique. Conclusions on the applicability and limitations of the technique are drawn for its application for present as well as for future investigations. The acquired data, which are not all shown here, serve as a possible benchmark for modeling and investigations for a more detailed understanding of early soot formation.

**Experiment set-up**

**Test engine**

The engine used in this study is an optical single-cylinder variant of a Cummins N14 engine. Research on this engine has over the last two decades contributed to a better understanding of both conventional diesel combustion [133] as well as low-temperature combustion [134]. As such, the engine and its specifications have been described extensively many times. Therefore, in this section only a brief description of the engine is given and for further information the reader is referred to [135] and [136].

In the present configuration, the engine uses a Bowditch piston with an open, right-cylindrical bowl and a flat fused-silica piston crown window. This window provides imaging access to the bowl, viewing from below. A 30-mm-wide curved window matching the contour of a portion of the bowl wall, and a flat rectangular window installed in a ring at the top of the cylinder, allow laser access into the bowl, even when the piston is near top dead center.

![Figure 14–1: Schematic of the single-cylinder engine, laser configuration, and optical detector system. The camera and spectrometer field-of-view are shown in the upper right corner.](image-url)
A custom, high-pressure diaphragm pump specially designed for low-lubricity fuels is capable of pressurizing the fuel rail up to 2000 bar. For the experiments presented here, a lower pressure of 1000 bar is intentionally selected to slow the jet penetration so that PAH and soot formation processes can be observed with less impingement of the jet on the piston bowl. A Cummins XPI common-rail injector with a low flow-rate 8-hole nozzle (nominal 140-micron orifices) is used. Relevant engine data such as cylinder pressure, injector actuation signal and fuel-rail pressure are acquired at quarter crank-angle resolution, simultaneously with the acquisition of optical data. Some engine specifications are given in Table 14–1, and a schematic of the experiment is shown in Figure 14–1.

**Table 14–1: Major engine and fuel system specifications**

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore</td>
<td>139.7 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>152.4 mm</td>
</tr>
<tr>
<td>Bowl width</td>
<td>97.8 mm</td>
</tr>
<tr>
<td>Displacement</td>
<td>2.34 L</td>
</tr>
<tr>
<td>Geometric compression ratio</td>
<td>11.2:1</td>
</tr>
<tr>
<td>Fuel injector</td>
<td>Cummins XPI</td>
</tr>
<tr>
<td>Nozzle hole arrangement</td>
<td>8 x 14°</td>
</tr>
<tr>
<td>Nozzle processed flow rate</td>
<td>1.24 L/min</td>
</tr>
<tr>
<td>Nominal orifice diameter</td>
<td>140 μm</td>
</tr>
</tbody>
</table>

**Conditions and fuel**

Geometrical compromises have to be made to implement optical access in the engine. As a result, the geometric compression ratio of the optical engine is only 11.2:1. To mimic charge conditions at top dead center (TDC) typical of those in the production engine (compression ratio 16:1), elevated intake air pressures and temperatures are required, see Table 14–2.

At an engine speed of 1200 rpm, a target load point of 6 bar gross IMEP is investigated. To achieve this target load, a single 1000 bar fuel injection is used, of which the logical start of injection is set to 8 °CA before TDC for all imaging measurements. Fuel is injected for 2500 microseconds, or 18 CA degrees at 1200 rpm. This actuation command signal is kept constant over changing operating conditions, resulting in changes in the exact load due to variations in fuel conversion efficiency. To avoid excessive thermal loading of the optical engine, fuel was only injected every 10th cycle. The XPI injector used has a delay between start of actuation and the actual start of fuel injection (i.e. when fuel first emerges from the injector) of approximately 460 microseconds [128], or 3.3 CA degrees at 1200 RPM.

For testing the diagnostic technique, HPLC grade n-heptane is used. Under conventional diesel combustion conditions n-heptane (CN=52.5-56, depending on the test procedure used [137]) displays similar ignition behavior as European diesel fuel, but being composed almost entirely of alkanes, it is spectrally more “pure” than aromatic-containing diesel fuel, in that it does not fluoresce under ultraviolet excitation like diesel does.

Imaging measurements were performed with different excitation wavelengths, but also at different oxygen mole fractions, with the in-

**Table 14–2: Engine operating conditions**

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>TDC motored density</td>
<td>16.6 kg/m³</td>
</tr>
<tr>
<td>TDC motored temperature</td>
<td>975 K</td>
</tr>
<tr>
<td>Intake pressure</td>
<td>177 kPa (abs)</td>
</tr>
<tr>
<td>Intake temperature</td>
<td>155 °C</td>
</tr>
<tr>
<td>(Simulated 16:1 intake pressure)</td>
<td>116 kPa (abs)</td>
</tr>
<tr>
<td>(Simulated 16:1 intake temp.)</td>
<td>118 °C</td>
</tr>
<tr>
<td>Engine speed</td>
<td>1200 rpm</td>
</tr>
<tr>
<td>Load</td>
<td>~6 bar gIMEP</td>
</tr>
<tr>
<td>Fuel pressure</td>
<td>1000 bar</td>
</tr>
<tr>
<td>Start of actuation command</td>
<td>-8 °CA aTDC</td>
</tr>
<tr>
<td>Injection command duration</td>
<td>2500 μs</td>
</tr>
<tr>
<td>Intake oxygen mole fractions</td>
<td>21 – 18 – 15</td>
</tr>
<tr>
<td>Air excess ratio @ 21 % oxygen</td>
<td>2.39</td>
</tr>
<tr>
<td>(Simulated EGR rates)</td>
<td>0 – 30 – 45</td>
</tr>
<tr>
<td></td>
<td>55 – 59%</td>
</tr>
</tbody>
</table>
Laser diagnostics of early soot formation (PAH)

take stream diluted by a metered flow of nitrogen. An oxygen mole fraction of 21% represents conventional diesel combustion with undiluted air. An oxygen mole fraction of 18% mimics typical current diesel combustion using exhaust aftertreatment, while 15% represents commercial LTC applications with little or no aftertreatment. 12 and 10.5% oxygen mole fractions are examined for very low-temperature conditions where both soot and NOx formation are so low that exhaust aftertreatment may not be required for those emissions. Additionally, the low combustion temperatures further slow down reactions so that the soot formation pathway can be studied in more detail. The EGR rates that would be required to achieve such intake oxygen mole fractions are also listed in Table 14–2.

Excitation setup

Two independent 10-Hz Spectra Physics Quanta Ray Nd:YAG laser systems provide the two excitation beams.

One (model GCR-250) is tuned down using a thin-film polarizer and a half wave plate polarization attenuator to provide 400 mJ/pulse at 1064 nm for soot-LII. This wavelength is used, as this is expected not to result in any fluorescence emission, even of very large PAH [131] [132]. As a result, the images recorded using this LII laser can be interpreted to be solely soot incandescence.

A second YAG laser (PRO-200) produces different laser wavelengths to induce the fluorescence of different PAH size classes. For this purpose the second (532nm) and fourth harmonic (266 nm) are used. Additionally, the third harmonic (355 nm) of this YAG laser pumps a Spectra-Physics mirror-less optical parametric oscillator (MOPO) to excite PAH fluorescence using 633 nm laser light. This wavelength has been chosen intentionally because it matches the wavelength of commercial Helium-Neon lasers, which are commonly used for extinction techniques [129]. As described earlier, very large PAH may absorb at 633 nm, which would confound extinction techniques using 633 nm laser light that are intended to measure soot only. Here, signal resulting from excitation at 633 nm (i.e., PAH fluorescence) without any corresponding soot LII from 1064-nm excitation would provide evidence of the presence of very large PAH. Laser pulse energies are adjusted to 100 mJ at 266 (tuning quadrupling crystal) and 532 nm (half-wave-plate polarization attenuator). For 633 nm, the maximum available pulse energy of 70 mJ is used.

For the fundamental YAG wavelength and its harmonics, dielectric mirrors direct the laser beam to the engine. For the MOPO wavelength of 633 nm, broadband coated right angle glass prims are used. The two laser beams are combined and co-aligned using narrow-band reflective dichroic mirrors when using the YAG harmonics, or a broadband transmitting dichroic beam splitter when using the parametric oscillator (663 nm).

The co-aligned laser beams are angled at 14 degrees relative to the fire deck, to probe both PAH and soot along the approximate symmetry plane of one of the eight fuel jets (152-degree included angle for injector spray pattern). The beams are formed into sheets that are less than one mm thick over the region of interest using a cylindrical (f=-50 mm) and a spherical lens (f=500mm).

In the near-horizontal direction the beam is expanded such that the sheets overfill the width of the engine window. This way only the reasonably uniform parts of the laser sheets, making up approximately two thirds of the present laser power, enter the cylinder at 30 mm width. This overfilling and losses on the path to the engine result in a delivery of 50-60% of the laser power into the engine. For LII this yields a laser fluence above 0.8 J/cm² over the path of the laser inside the engine. A laser power variation has shown that under the present conditions this laser fluence is above the LII saturation threshold, with only a small increase in LII signal upon an increase in laser fluence.
Detector setup

The soot-LII signal from 1064-nm excitation is imaged through the piston-crown window and directed by the 45-degree mirror and a 50-50 visible-range beam splitter to a gated, intensified CCD camera manufactured by Xybion Electronic systems (model ISQ-350-W-3) with a Gen-III intensifier. The camera is equipped with a 105-mm focal-length glass lens, used at f/4. The light entering this camera is spectrally filtered using SWP450 and GG385 filters. As described in [133], the laser-heated soot (LII) emits more strongly at shorter wavelengths than the combustion-heated soot, so the soot-LII emission is spectrally filtered to the shorter band-pass spectral range of 385 - 450 nm to improve the signal-to-noise ratio. Furthermore, these filters withhold any scattered light from either laser from disturbing the image or damaging the intensifier. The laser pulse is bracketed with a gate width of ≈60 ns, the practical minimum of this intensifier.

The signal originating from the shorter wavelength excitation is imaged through the beam splitter and a removable aluminized mirror, using a PI-MAX 3 ICCD camera with an HQf (GEN-III) intensifier. This camera uses the same type of lens, also at f/4. The gate width of the intensifier is set to the minimum value of 2.47 ns, and positioned on top of the laser pulse, maximizing signal to noise ratio. To prevent any scattered 1064 nm from damaging the photocathode of this camera, a short wave pass filter with a 50% cut-off near 850 nm (CVI/Melles-Griot FSWP-850) is used. Furthermore, matching narrow-band notch filters reject elastically scattered light at 532 or 633 nm. To reject scattered light from the 266 nm source, a WG285 filter is used. Instead of only looking at blue-shifted fluorescence as was done in earlier work [128], here the whole visible spectrum is observed, with the exception of notch filters that remove the laser wavelengths. This way, also the significant red emission can be imaged.

For spectral measurements of either the incandescent or fluorescent emission, the aluminized mirror can be removed and an Oriel 77250 monochromator is used as a spectrograph by lens-coupling it to a Xybion Gen-II intensified CCD camera (model ISG-250-UX-3). Unlike the two-camera imaging setup, spectral information cannot be obtained at two excitation wavelengths simultaneously from the single spectrograph. Alternatively, the minimum usable gate time of 110 ns is set to bracket either one of the laser pulses to obtain the resulting spectrum.

A grating of 300 lines/mm (Oriel #77939) resolves a broad spectral range (i.e. 400-700 nm). With a slid width of 0.280 mm, this yields a spectral resolution of 8 nm at 500 nm. This grating has a blaze wavelength of 500 nm and a peak efficiency of 80%, with a primary wavelength regime (≥20%) of 250-1150 nm. For calibration of the wavelength range, an Oriel 6035 Hg(Ar) pencil style spectral calibration lamp is used. The recorded spectral images are matched to the manufacturer-specified emission spectrum of the lamp.

A glass 50 mm lens is mounted in front of the spectrometer’s entrance slit and using the same numerical aperture of the spectrometer (f/4). The slit is aligned with the spray of interest, as indicated in Figure 14–1. In every experimental run, a series of 20 spectral images is acquired at a fixed crank angle. For every fourth image, the laser pulses are delayed by 1 CA degree to acquire a background luminosity image (the laser pulses cannot be skipped, only delayed slightly so that they are outside the spectrograph gate). Acquiring background images this way largely allows correction for a possible bias for laser attenuation though soot deposited on the windows. Following this procedure, every experimental run yields 15 signal deposited on the windows. The obtained spectra are ensemble-averaged for
Laser diagnostics of early soot formation (PAH)

Each crank angle. As a last step, all spectra all quantified by correcting for the transmission of the respective filters used and the spectral response of the intensified camera. The spectral radiance calibrations are obtained for the optical path and all filter combinations used, using a Hoffman integrating sphere, model LR-6Z. Spectral ranges with high filter absorption are masked for clarity.

In addition to the laser-based imaging and spectral measurements, a large-area (1 cm²) photodiode viewing through the piston-crown window records the natural combustion-luminosity. Because the natural luminosity signal is attenuated somewhat so that the photodiode does not saturate when soot is present, signals from chemiluminescence are quite weak, and down in the noise. Therefore the natural combustion luminosity is interpreted as being only soot luminosity.

For imaging experiments (using two cameras instead of the spectrometer), in every experimental run also 20 image pairs are acquired, with the laser delayed for every fourth image. Images for LIF and LII are acquired nearly simultaneously, with LII trailing LIF by only 1 μs. This separation is considered to be short on engine relevant time scales, but long compared to fluorescent and incandescent time scales, so these do not give any interference. In [128] it was also shown that the order of the two pulses does not have any influence on the acquired images.

For every crank-angle, one experimental run is done, except for the oxygen mole fractions of 21 and 18%, where 2 runs are done. This is necessary as at these high oxygen concentrations attenuation of the signal by accumulated soot deposits on the windows is severe and two runs are necessary to yield at least 15 usable signal images. After subtracting the ensemble-average background from each signal image, every LII image is overlaid on the corresponding LIF image. Alignment of the overlay of the two cameras, as well as the object position corresponding to the slit of the spectrometer, are determined by imaging a luminescent target.

From the resulting 15 image pairs for every condition and crank angle, a single representative image pair is objectively chosen using a statistical image-correlation technique similar to the one used by Genzale [138]. This image-correlation algorithm selects the image pair of which both components have the strongest correlation with 80% percent of the other single-shot image pairs in the set (but not necessarily with an ensemble-averaged image pair). For each image pair, both components are cross correlated with the respective components of all other image pairs. Then for each image pair the correlation coefficients are ranked and the product of the 20% lowest value of both components is taken. This product is taken as the representativeness of that image pair, with 80% of the images having a higher correlation coefficient for both components. The image with the highest representativeness is thus objectively selected by the algorithm as the “representative” image pair that is most like most (in this case 80%) of the other image pairs in the set. Additional details may be found in [138].

Results and discussion

Crank-angle-resolved luminosity signals and sequences of single-shot images are presented throughout this results section. These images are used to simultaneously visualize laser-induced signals from different excitation wavelengths and are examined throughout the results section to study the early soot-formation process. After further explaining the display of these images, results of the technique are shown for engine operation at varying intake-oxygen mole-fractions, with 532-nm light exciting PAH. Subsequently these images are spectrally resolved and conclusions are drawn about the validity of the technique.

In the subsection after that, for a single operating condition, the PAH excitation wavelength is varied. These results will show if changing the excitation wavelength allows for distinguishing different size classes of PAH and whether a
transient growth in PAH size can be shown using this technique. Again spectral information is used to understand the photo-physics of the technique. The results are concluded with application of the technique to investigate the effects of the injection strategy on the early soot formation.

**Image processing**

In the following sections, post-processed image pairs of both the LII and LIF signals are presented, of which an example is shown in Figure 14–2. The respective signals are combined in false-colored images, with the green color representing the LIF emission intensity and the red color indicating the intensity of LII emission. Areas where the two signals spatially overlap appear as yellow. As neither of the signals is to be interpreted as being quantitative, nor is the ratio between them. Therefore, not all overlapping areas will have the same intensity of yellow, and the ratio cannot be used as a quantitative measure for the ratio between PAH and soot presence. These areas may still have PAH present, but certainly have significant soot signal. As such, any areas that are red or yellow are indicated to represent soot, whereas the bright green areas represent PAH-LIF.

![Figure 14–2: Example false-colored image indicating field-of-view and relevant specifications. Red = LII (soot), green = LIF of large PAH. Yellow is where the signals spatially overlap (soot).](image)

The injector position and bowl rim position are indicated in the figures, with one of the eight fuel jets propagating horizontally from left to right through the image. The area outside of the piston bowl on the right side of the images, from where the laser enters, is masked. The laser sheets expand slightly over their path from right to left, because of the curvature of the bowl rim window.

Because of the different dynamic ranges of the cameras and to make initial soot formation visible, both the LII and the LIF signal images are artificially amplified such that 0.1 percent of the pixels in the area of interest saturates. For this procedure, the injector area is excluded to limit the contribution of any scattered laser light. The effective gains (including post-processing) are displayed in the upper right corner of each image.

At a given crank angle, the LII and LIF images are taken virtually simultaneous from the same engine cycle. Images sets spanning different crank angles are not from the same cycle but composed from different engine runs. The following image sets have varying crank angle ranges and step sizes, depending on when the formation of PAH (and soot) starts. The crank angle at which an image pair is recorded is also indicated in the top right corner of each image.

**Demonstration of technique at 532-nm excitation and varying ambient oxygen concentration**

As a first verification of the laser diagnostic technique, 532-nm LIF excitation is used to study engine operation at two different ambient oxygen concentrations. In Figure 14–3 the results of these tests are given. In the top of this figure the measured injection rate, the post-processed apparent rate of heat release (ROHR) and the photodiode signal are shown. These results indicate that even for the lowest oxygen mole fraction of 10.5% there is significant overlap between the injection and combustion events, because of the long injection durations. After the ignition delay, for both dilution levels the heat release has a distinct peak, followed by a mixing-controlled combustion phase and burn-out (not fully shown in the graphs).

The vertical lines in the two top graphs of Figure 14–3 indicate the crank angles for which image sequences are presented. For the lower oxygen concentration, the crank angles range
from just after the premixed heat release peak until after the luminosity signal has risen significantly. At higher oxygen mole fraction (i.e. 18%) chemical kinetics are much accelerated, with a shorter ignition delay and heat release starting well before top dead center. Also, after the premixed heat-release peak, the luminosity signal rises much more quickly. Because of the faster soot kinetics the crank angle range over which images are acquired is advanced and compressed.

All images in Figure 14–3 show significant scattering of the LII laser on the injector and other in-cylinder surfaces on the left side of the images. As the camera should not detect any 1064-nm light, the laser light may have been blue shifted in some way, which is not fully understood. The scattering appears more significant at the earliest timings, which is because of the high gains used in these images to show any possible early soot LII. At later acquisition CA, where LII signal is actually present, the scattered LII laser light is less disturbing.

In some images, signal outside the area reached by the laser sheet is significant, especially at high sooting conditions. To some extent this is background signal of natural and soot luminosity. To remove this background interference to the degree possible, the ensemble averaged background signal is subtracted from

![Figure 14–3: Top: Apparent rate of heat release (ROHR), measured injector rate, and natural soot luminosity signals for engine operation at two oxygen mole fractions, 10.5% (left) and 18% (right). Crank angles for which LII-LIF measurements are presented are indicated with vertical lines. Bottom: Single-shot image sequences, recorded virtually simultaneously with 532 (false colored green) and 1064 nm laser excitation (false colored red).](image)
For higher oxygen concentration (18% intake $O_2$), for which images are shown in the right of Figure 14–3, a clear diesel jet is visible which is near symmetrical around the spray axis. Over the more limited range of crank angles compared to the low oxygen concentration images on the left, it is only transported upward slightly by swirl. At this condition, first PAH are again detected just after the premixed burn, (here 1 °CA aTDC). Within one crank angle degree, the PAH area is surrounded by soot, after which the sooting jet stabilizes at around 5 °CA aTDC. While some images display pure PAH, the rapid increase in soot presence (as can also be seen for the ‘red’ gains used) quickly overwhelms any present PAH signal. The high presence of soot is also displayed in the significantly higher levels of natural luminosity, saturating the detector. Like was discussed for the high-dilution case, the first detection of soot LII corresponds with the rise in the detected luminosity.

To some extent, the signal presence of both LII and LIF can be interpreted as the reciprocal of the gains used. This gain is calculated automatically to saturate a certain fraction of the signal area, in this case 0.1 percent and subsequently rounded to a single significant digit. Therefore, the inverted gain will occur in quantized steps. Furthermore, as such this inverted gain does not define the signal presence spatially, but merely the maximum signal level. However, this enables a more objective determination of the first occurrence of soot or PAH signals. The signal level is normalized for both excitation wavelengths and plotted in Figure 14–4 for operation at 10.5% $O_2$. For reference, in this graph also the corresponding heat release rate, soot luminosity signal, and injector rate are given.

For determination of the first presence of PAH and soot signal, the first crank angle is taken at which their respective signal level differs from the background level. This procedure is followed for all oxygen percentages and combined in Figure 14–5 with the crank angles of first heat release and first luminosity. For all oxygen concentrations, soot luminosity and LII sig-
Spectral information from 532-nm excitation

To verify the laser-induced spectral composition of the emission recorded in the images from the previous subsection, a number of spectra are acquired. In Figure 14–6, for each of the conditions shown in Figure 14–3, three quantitative spectra are given. These spectra are corrected for the filters used. However, spectral ranges where the filters have high absorbance are artificially masked for clarity.

For the 10.5% O$_2$ condition, the LII spectrum is sampled at 16 °CA aTDC, or the first crank angle where a significant amount of soot was visible. This spectrum is taken as the benchmark for LII signal. The broadband LIF spectrum (which also likely contains some LII) obtained at the same crank angle shows similarity with the LII spectrum, although it is somewhat more blue-shifted. As explained earlier, the emission from 532-nm excitation likely includes laser-induced incandescence of soot when soot is present, so the similarity to the soot LII spectrum from 1064-nm excitation is not unexpected. The spectrum does not show any significant narrow peaks that would be characteristic of emission from small combustion intermediate molecules such as CH or C$_2$. At even later timings, the LIF spectra are even more similar to the soot LII spectra. This will be further discussed for 266-nm excitation, in a later subsection.
At an earlier crank angle (14 °CA) with significantly less soot LII signal, the LIF spectrum is weaker but even more shifted to shorter wavelengths, with the peak only slightly blue shifted from the excitation wavelength of 532-nm. Also significant fluorescence at wavelengths shorter than the excitation wavelength is visible. The origin of this blue shifted fluorescence will be further investigated. It is unlikely that at these early crank angles there is soot LII from particles not yet absorbing 1064 excitation but only 532-nm light. More probable is that PAH already in an excited state by combustion, are excited even further by the laser light and subsequently fall back to a lower energy level, yielding blue shifted emission. This is only visible at the early crank angles, when the signal is not yet dominated by soot LII.

Overall, the LIF signal can be seen to yield broadband spectra, like the LII does. At later crank angles, the contribution of LII in the LIF signal is more important or may even be the only visible contribution. Even at early crank angles, the spectra are difficult to distinguish as their (virtual) peaks lie close to each other.

Chemiluminescence spectroscopy

The blue shifted fluorescence observed in the previous section was hypothesized to occur through excitation of PAH already in an excited electronic state due to combustion reactions (akin to chemiluminescence). To test this hypothesis, natural emission spectra are acquired for the 10.5% O₂ case. To enable a sufficient signal to noise ratio, the gate time of the spectrometer is increased to 140 microseconds, or about 1°CA. No filters are used, but the aperture of the camera and gate time are adjusted to prevent saturation at higher signal levels (at later CA), for which the obtained spectra are subsequently corrected.

In Figure 14–7 the obtained spectra are shown for an early crank angle range, ranging from first heat release to the last crank angle before soot LII signal and luminosity appears. From the earliest crank angle, a broadband emission spectrum is visible, with the peak in the blue. This broadband emission spectrum is consistent with the CO₂* emission [139] spectrum, ranging from 340 to about 650 nm with its peak around 400 nm. From this start we can see the signal rising at later timings, and a slight hump is visible around 431 nm, corresponding to the excited CH* radical [140]. A distinct chemiluminescence peak is also visible around 580 nm. This peak, which remains visible throughout most of the crank angle range, has also been found by Guyot et al. [141], and may be from sodium impurities in the fuel, as sodium flames are known to have a strong isolated line near 589 nm (Na*, [139]). However, no possible hypothesis exists on the origin of these sodium impurities.

The chemiluminescent spectrum acquired from 8 degrees CA shows the first signal rise towards a broadband red spectrum. The gate time used at this crank angle is a full CA degree. As such, the spectrum obtained may be associated with the laser-induced images of both 8 and 9 °CA aTDC. At these crank angles, in Figure 14–3 no fluorescent emission from 532-nm excitation was visible. However, it is probable that this first rise in PAH chemiluminescence is due to the smaller sizes which cannot be excited with 532-nm light.
Laser diagnostics of early soot formation (PAH)

After this initial potential PAH chemiluminescence, its red-peaked broadband emission rises until around 12 °CA when apparent soot luminosity becomes significant. This onset of soot formation also corresponds to the timing found in the LII images from Figure 14–3. The soot signal eventually becomes orders of magnitude stronger than the chemiluminescence and is therefore not shown here for clarity. Narrow-band features disappear, as the soot luminosity has much higher signal level, and the spectral peak shifts further towards the infrared.

Multi-wavelength comparison

As was shown in Figure 14–5, the temporal difference between signals arising from LIF and LII was the most significant for operation at the lowest oxygen mole fraction of 10.5%. Expecting that PAH formation would be slowest and most extended and therefore more easily studied, the fluorescent signal originating from the three different excitation wavelengths (i.e. 266, 532, 633 nm) is compared at this lowest oxygen concentration. Figure 14–8 shows three time sequences of representative composite images from excitation at these three wavelengths (false-colored green) with simultaneous excitation at 1064 nm (false colored red).

The left and middle sets of images in Figure 14–8 show that PAH can be detected earlier with 266-nm than with 532-nm excitation. The onset of fluorescence resulting from excitation at 266 nm occurs between 8 and 9 °CA, which also corresponds to the start of natural emission found in Figure 14–7. In the images of the crank angles just after this initial formation (i.e. 10, 11 °CA) the signal originating from UV (266-nm) excitation is also stronger than for green (532-nm) excitation. Recall that the images use different gains as indicated in the top right corner of each image.

Excitation with light at 633-nm shows signal only at even later crank angles, starting from 11 °CA. However, there is still detection of PAH before any soot signal is detected. This implies that (large) PAH do absorb light at HeNe wavelengths. While this to some extent may open possibilities for fluorescent detection of such species, absorption by large PAH may be significant compared to absorption by soot particles only in a narrow crank angle range, especially at higher oxygen concentrations. Furthermore, at later crank angles where LII signal is high compared to the fluorescent signal, PAH absorbance may be less significant compared to soot extinction.

Figure 14–8: Composite image sequences for LII excitation at 1064nm (red) and LIF excitation (green) at 266, 532 and 633 nm. Crank angle range and operating conditions correspond to Figure 14–3 (10.5% O2). Images in each pair are virtually simultaneous, but image pairs are from separate engine runs.
All three image sequences show a consistent PAH signal development. A clear temporal redshift in excitation absorption wavelength, and hence growth in PAH size, can be detected before the onset of soot formation. The temporal range constitutes only 3-4 crank angles, however, even at this lowest oxygen concentration. Spatially, no clear differences can be seen between the different excitation-wavelength/size classes. At crank angles where significant signal is present for longer wavelength excitation, also signal is present for shorter wavelength excitation. This indicates that from onset of PAH formation, smaller size classes are still being formed while the larger classes are synthesized, or that large PAH also absorb the laser light to some extent.

For detection of the onset of the smallest PAH formation and its spatial progression, 266-nm laser light is the most obvious choice. However, the UV laser light as well as the corresponding emission are more readily attenuated by soot, PAH, and other in-cylinder substances than laser light and signal of larger wavelengths. While most of the soot on the bowl rim window is blown off by incident laser pulses, attenuation from the soot cloud as well as from the piston window can be significant, especially at high-sooting conditions. As a last remark, ultraviolet fluorescent emission is much more sensitive to signal trapping in the soot cloud [142].

The spatial images shown in Figure 14–8 are spectrally resolved for two different crank angles. The crank angles at which spectra are presented are the same as in Figure 14–6, either at or shortly before the first visible LII signal. The quantitative spectra using 266-nm LIF excitation are shown in Figure 14–10. The spectrally resolved range is also kept constant in the visible, from 400 to 700 nm. As such, a significant part of the emission (in the ultraviolet) is not resolved. Even though the peak of the LIF emission spectrum may lie in the ultraviolet, significant emission is resolved in the visible range. At the early crank angle of 14 °CA aTDC, the LIF signal is spectrally significantly different from any LII signal, with far too short wavelength emission to be attributed to incandescence at the soot vaporization temperature. As such, the 266-nm excited signal at this and earlier crank angles can be interpreted as being almost solely LIF, not having significant LII. At later crank angles, the signal is likely composed of both contributions, resulting in a red-shift of the spectral peak. The more soot signal is present, the more the spectrum starts to resemble the LII signal.

The 633-nm induced LIF spectra, as shown in Figure 14–9 are somewhat weaker than seen before for 266 and 532-nm excitation, especially...
Laser diagnostics of early soot formation (PAH)

at 14 °CA aTDC. Nonetheless, the spectrum displays significantly more light above 650 nm, red-shifted from the 633 excitation. While at the later crank angle (16 °CA aTDC) the shape of the LIF and LII spectra are so similar that no signal can be distinguished in the 633-nm spectrum, the spectrum at the earlier crank angle does verify that even at 633-nm excitation absorption and fluorescence do occur.

Summary and conclusion

In this chapter a technique is developed which aims at studying the first steps of the soot formation (i.e. the growth in PAH size). Low-temperature combustion conditions offer a particularly useful platform for studying this early soot formation, as the intermediate temperature regions where PAH species reside are more broadly distributed, both spatially and temporally. Imaging PAH using a broad wavelength range of excitation has enabled studying the spatial and temporal evolution of what is most likely a range of PAH species of different size classes. At many conditions, especially later in the combustion event, the resulting signal from excitation at these wavelengths using high-fluence laser pulses, however, is likely be a combination of both PAH LIF and soot LII. To discriminate between PAH fluorescence and soot LII, a second shot of another laser beam at 1064 nm is taken virtually simultaneously to probe the spatial presence of soot only, since only soot is expected to absorb at 1064 nm.

At the highly diluted condition, PAH is first detected just after the premixed heat release peak. From this crank angle, the area over which PAH manifest themselves grows until soot LII is first detected. After this delay, soot quickly invades the PAH surface and soot signal dominates the signal from both cameras, as could be seen from the relative gains used. For higher oxygen concentration in the PAH LIF images a clear diesel jet is visible which is near symmetrical around the spray axis. Also at this condition, first PAH are detected just after the premixed burn, in this case just after top dead center. Within one crank angle degree, the PAH area is surrounded by soot. While some images display pure PAH, the rapid increase in soot presence quickly overwhelms any present PAH signal.

To verify the laser-induced spectral composition of the images, a number of spectra are acquired using 532-nm LIF excitation and compared to spectra acquired with 1064-nm excitation. Overall, the LIF signal can be seen to yield broadband spectra, like the LII does, but typically with a greater blue-shift. At later crank angles, the contribution of LII in the LIF signal is more important or even the only discernible contribution. Even at early crank angles, the spectra are difficult to distinguish since they are both broadband. This separation is much less difficult with 266-nm, with the LIF spectrum spectrally significantly different from any LII signal. As such, the 266-nm excited signal at this and earlier crank angles can be interpreted as being almost solely LIF, not having significant LII. At later crank angles, the signal is composed of both contributions, resulting in a red-shift of the spectral peak. The more soot signal is present, the more the spectrum starts to resemble the LII signal. The 633-nm excited LIF signal is somewhat weaker than for 266 and 532-nm excitation. Nonetheless, the spectrum displays significantly more light above 650 nm, red-shifted from the 633-nm excitation. While at the later crank angle no LIF signal cannot be distinguished from the 633 spectrum, the spectrum at the earlier crank angle does verify that even at 633-nm excitation, absorption and fluorescence does occur.

Quantitative chemiluminescence spectroscopy also has shown a clear emission spectrum, probably from PAH chemiluminescence, temporally coinciding with first detection of LIF signal using ultra violet excitation. At later crank angles, the soot signal is orders higher and therefore in the spectra narrowband features disappear and the spectral peak shifts further towards the infrared. This onset of soot formation also
Laser diagnostics of early soot formation (PAH)

Corresponds to the timing found in LII images. From this quantitative chemiluminescence spectra, the likely onset of (excited) PAH can be seen, as well as the development of soot.

The fluorescent signal originating from the three different excitation wavelengths (i.e. 266, 532, 633 nm) is compared at the lowest oxygen concentration, as this displayed the largest temporal difference between signals arising from LIF and LII. PAH can be detected earlier with 266-nm than with 532-nm excitation, indicating a likely temporal growth of PAH size. Excitation with light around 633-nm shows signal only at even later crank angles. However, there is still detection of PAH LIF with 633-nm excitation before any soot LII signal is detected with 1064-nm excitation. This further verifies that (large) PAH apparently do absorb light at HeNe wavelengths. While this to some extent may open possibilities for fluorescent detection of such species, absorption by large PAH is significant compared to extinction by soot particles only in a narrow crank angle range. At later crank angles, where LII signal is high compared to the fluorescent signal, PAH absorbance may be less significant compared to soot extinction.

While a clear temporal redshift is observed in the excitation wavelength absorbed by PAH, implying growth in PAH size before the onset of soot formation, the temporal range is small, even at this lowest oxygen concentration. Spatially, no clear differences can be seen between the different PAH size classes. At crank angles where significant signal is present for longer wavelength excitation, signal is also present for shorter wavelength excitation.

For detection of the onset of the smallest PAH formation and its spatial progression, 266-nm laser light is the most obvious choice. However, the UV laser light as well as the corresponding emission are more readily attenuated by soot than laser light and signal of larger wavelengths. Furthermore, at this wavelength several fuel components as well as (intermediate) combustion products may be excited when commercially available fuels are used.

References

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Summarizing discussion and conclusion

In this thesis the fuel effects on new combustion concepts have been investigated. Furthermore, laser diagnostic techniques have been developed to gain further understanding of the underlying processes. To conclude, in this last chapter the results are summarized and discussed.

Low-Temperature Combustion concepts (LTC, see page 10) aim at reaching or exceeding fuel conversion efficiency of contemporary diesel engines, while reducing engine-out emissions of nitrogen oxides and particulate matter considerably. These LTC concepts vary in the way this goal is achieved.

One such option is PCCI (page 11) where early injections are used with a low compression ratio in order to delay ignition. To apply this concept in the short term, a conventional diesel fuel has to be used, and operating conditions have to be optimized, as described in chapter 3.

In the PCCI regime, NOx and smoke have been shown to be efficiently reduced as a result of an extended mixing time. For viable PCCI combustion, one thus would require a mixing time that is long enough to bring both NOx and smoke levels down to acceptable values. For HC and CO emissions and the associated fuel consumption, however, mixing time should be as short as possible. The mixing time can be increased by increasing the EGR level, lowering intake pressure and/or temperature and by advancing injection timing.

Even when using a low compression ratio, when a fuel as reactive as current diesel is used not every mixing time can be chosen, especially at higher loads. Even at low loads, very high EGR levels and a low intake pressure and temperature are necessary to allow combustion to be phased correctly.

Changing the composition of the diesel fuel, by varying its cetane number, volatility and biocontent, can give an extension of this operating range, which was shown in chapter 4. At the relatively low compression ratio under investigation, the US diesel, having a somewhat lower Cetane Number than European diesels, was shown to effectively increase Combustion Delay.

When comparing fuels of different composition in the PCCI regime, the mixing time was also seen to be the dominant parameter. While other differences between fuels, for instance in volatility and reactivity, have their own effects on emissions and performance, the major impact was related to the combustion phasing and the resulting available mixing time. Indicated efficiency was shown to be at best 45%, partly attributed to the low compression ratio of 12:1.

In the following chapter, a higher compression ratio was used, which enables a higher efficiency. However, a less reactive fuel is required to delay auto-ignition and phase combustion correctly.

For the low reactivity blends used in chapter 5 it was shown that the reduction in Cetane Number has the desired effect of increasing combustion delay, even at a higher compression ratio. To be able to choose the mixing time according to the operating conditions, especially at this higher compression ratio, a low reactivity blend is necessary. The blend with an estimated cetane number of 25 was found to be the most flexible in being able to choose the optimum combustion phasing. This high flexibility enables the possibility for meeting NOx and smoke targets simultaneously, without suffering from too high a loss of combustion efficiency.

To gain more control of combustion phasing, more control of reactivity and/or mixture stratification is necessary. A dual-fuel approach can help in this aspect. However, the combustion chamber shape of contemporary diesel engines is not well suited for very early (port) injection, as fuel may end up in crevices (chapter 6). A cost-effective fuel can help in achieving economic advantages, be it direct- or port-injected.
For direct-injected butane, hydrocarbon emissions were found to be an order of magnitude lower than for port-fuel-injected butane, clearly substantiating the hypothesis that crevices are the main source of these hydrocarbon emissions. Furthermore, carbon monoxide and nitrogen oxides are not negatively affected compared to the diesel baseline. Because a high combustion efficiency is retained, fuel-cost savings can be significant.

A second way to use the additional control variable when using two fuels is the RCCI concept (chapter 7), where a large part of the fuel is well mixed and the desired level of both reactivity- and mixture stratification is achieved by one or more early direct injection(s) of a high-reactive fuel. Although hydrocarbon emissions are somewhat increased compared to a conventional diesel engine, due to higher thermal efficiencies the indicated efficiencies are significantly increased. These higher thermal efficiencies are experienced because short burn durations at high gasoline fractions enable CA50 to be phased closer to TDC, without combustion occurring too much before TDC. This and lower heat losses through increased dilution enable a more efficient thermodynamic cycle.

To determine the possible viability of the concept for on-road application, a determination of the control space of injection parameters with respect to combustion phasing has been presented in chapter 8. The RCCI concept has been shown to give a broad range of control with the added control variables. In particular the sensitivity of the late injections of high-reactivity fuel is positive and larger in absolute value compared to an early-injection strategy. Furthermore the sensitivity correlates with the amount injected in the second injection. As such the variation of a relatively large second injection (e.g. 20 mg) is most favorable for control.

The control over reactivity (stratification) in the RCCI concept enables shaping of the heat release profile such that thermal efficiency can be optimized. However, the very early injection of the low-reactive fuel mixture may result in increased combustion losses due to fuel getting trapped in crevice volumes. Therefore an alternative concept was investigated which attempts to shape the heat release rate using a single fuel. This so-called PPC concept (page 12) uses advanced injection strategies to achieve the desired mixture stratification.

Because in this concept reactivity can not be varied in real time, the reactivity of the fuel should be chosen such that it is suitable for the larger part of the engine's load range. This means that, like in contemporary diesel engines, low loads are more premixed and as load is increased combustion becomes more and more mixing-controlled. In PPC, the premixed range is broadened and specific fuel aspects are used to ensure that when at higher loads combustion becomes more mixing-controlled, emissions are still satisfactory.

As an example, commercially-available naphtha blends can help to make the transition from fully mixing controlled combustion (as in a conventional diesel engine) to more premixed regimes. The application of such naphtha blends was described in chapter 9. All of these naphtha blends showed sufficient controllability with respect to injection timing.

The analysis of the heat release pattern revealed an interesting and strong correlation between the premixed fraction and the amount of soot produced, irrespective of how this premixed fraction was realized. To be specific, each of the fuels showed a decrease in this fraction as fuel pressure was lowered and correspondingly an increase in the emission of particulates. When load is increased, all fuels show a transition from more premixed to mainly mixing-controlled combustion.

For the lowest-reactivity naphtha blend, over the whole load range EURO VI PM levels were approached or achieved, combined with a peak gross indicated efficiency of 50% clearly indicating the potential of this concept.

The application of certain bio-fuels (blended with regular diesel fuel) can also enable the fur-
ther use of the PPC concept. Moderate diesel-butanol blends (i.e. with 50, 60 or 70% butanol, presented in chapter 10) are a viable approach to partially-premixed combustion, with the added diesel increasing burn durations to acceptable values, and enabling stable operation.

All butanol-diesel blends have shown an extremely high soot reduction potential compared to diesel-only, even at moderate fuel pressures easily achieving EURO VI particulate matter levels. At higher loads, all blends show a transition to more mixing-controlled combustion and the load at which this transition occurs depends on reactivity. However, for the butanol blends, this transition comes without a significant soot penalty.

Moderate blends were shown to give the best indicated efficiency over the whole load range; with the best blend having an average gross indicated efficiency of 50% over the whole load range. If possible with high efficiency turbochargers, using a higher total dilution a pathway to even higher indicated efficiencies has been identified, with peak efficiency estimated at 55%.

Given that an octane number of 70 seems to be the optimum reactivity for load range capacity of the PPC concept, seven fuel mixtures have been blended that represent different physical and chemical properties, as presented in chapter 11. Four of these fuels are blended from existing refinery streams. For a more fundamental approach, three ternary mixtures of toluene, n-heptane, ethanol and iso-octane are used, of which the aromatic (toluene) and oxygenated (ethanol) content is varied.

The mid and high load fuel efficiency is good for all fuels and do not differ too much between them. With respect to smoke emissions, fuels or different composition show differences in sensitivity to the fuel pressure used. Future tests should focus on the fuel pressures necessary for achieving EURO VI particulate emissions and the brake efficiency penalty associated with such fuel pressures.

NOx emissions are for the larger part of the load range determined by global conditions and are little fuel specific. To achieve EURO VI NOx levels, the precise EGR percentage has to be fine-tuned. Only at the lowest loads this might not be possible without compromising combustion stability. At idling conditions, additional strategies have to be investigated to increase the combustion efficiency and stability.

In general, it was shown that low-temperature concepts can open great possibilities for simultaneous emission reductions and efficiency gains. Which of the concepts to use depends on the specific application and the fuels available. The dual-fuel RCCI concept faces some challenges with respect to combustion efficiency, but has the advantage of working well with conventional fuels. Furthermore, the reactivity can be optimized in real-time and over a broad range, for maximum efficiency. For the single-fuel PPC concept, fuel composition effects are more important, but also for this concept many possible fuels (blends) were shown. If the conditions are well known and do not vary too much, the concept is certainly applicable.

Challenges for both concepts lie in the controllability, high efficiency air handling necessary for the high amounts of EGR used, and further optimization of the fuel. These further improvements or optimizations are being sustained by a detailed understanding of the underlying phenomena. Laser-based diagnostics, in particular Planar Laser-Induced Fluorescence (PLIF) of radical minor combustion species, has helped to understand and improve conventional engine concepts in particular.

Imaging diatomic molecules such as the hydroxyl radical (OH) can give an idea of where the high temperature reactions occur in the combustion chamber. To localize the flame front the methylidine (CH) radical can be used. The goal of chapter 12 was to develop a cinematographic PLIF diagnostic for the CH radical, that could be used for crank angle resolved measurements in an optically accessible engine.

With a high speed dye laser system, it has been shown to be possible to image the CH rad-
Imaging PAH using a broad wavelength range of excitation has enabled studying the spatial and temporal evolution of what is most likely a range of PAH species of different size classes. A second laser shot is taken virtually simultaneously at 1064 nm to probe the spatial presence of soot only, to compare the fluorescence signal to the signal originating from Laser-Induced Incandescence (LII).

At a highly diluted condition, PAH is first detected just after the premixed heat release peak. From this crank angle, the area over which PAH manifest themselves grows until soot LII is first detected. For higher oxygen concentrations, within one crank angle degree the PAH area is surrounded by soot.

The separation between laser-induced spectral contribution of LIF and LII is shown to be least difficult with 266-nm excitation, with the LIF spectrum spectrally significantly different from any LII signal. From quantitative chemiluminescence spectra the likely onset of (excited) PAH can also be seen, as well as the development of soot. PAH can be detected earlier with 266-nm PLIF than with 532-nm excitation, indicating a likely temporal growth of PAH size. Excitation with light around 633-nm shows signal only at even later crank angles. While a clear temporal redshift is observed in the excitation wavelength absorbed by PAH, implying growth in PAH size before the onset of soot formation, the temporal range is small, even at the lowest oxygen concentration.

The successful development of this PAH detection technique opens the way to a better understanding of soot formation pathways, especially under low-temperature combustion conditions.

The understanding acquired with such laser diagnostic techniques and single-cylinder metal engine tests, combined with additional modeling results, provides a pathway for the development of future engines. Using efficient (bio-derived) fuels a significant CO₂ reduction is possible, which entails a great societal impact.
List of publications

Verba volant, scripta manent (Titus)

Journal and technical papers


Leermakers, Bakker, Nijsen, Somers and Johansson. Low octane fuel composition effects on the load range capability of Partially Premixed Combustion. Submitted for publication in Fuel.


(Proceedings of) conferences, workshops, meetings, symposia and colloquia

VIV Symposium “Fuel for thought”, 10 October 2013 (oral presentation and panel discussion)


SAE World Congress, 16-18 April 2013, Detroit, USA (oral presentation).


SDF World Congress 2011, Detroit, USA (oral presentation).

KIC workshop, 2012, Karlsruhe, Germany (oral presentation).


From the author

The past three and a half years have been a great time, not in the least because of a great cooperation with many different people. Many of the results presented in this dissertation are from students who accepted the challenge of being supervised by me. I am very thankful of their effort and dedication.

The *mutua fides* attitude of my ever-growing group of supervisors has helped my development a lot. You have supported me to transform the laziness trained during my studies into an intrinsic motivation for cooperative research. I appreciate the contributions by each of you, Bart requesting physical understanding, Bengt being an authority in engine research, and Nico with his wild ideas on the application of laser diagnostics. I particularly wish to thank Philip for giving me the possibility of teaching many different courses related to my experience.

One of my personal highs during the project was the visit to Sandia National Laboratories in Livermore, California. I am very grateful to Sandia's technical staff for having me, with Mark Musculus in particular. Mark, I have learned incredibly much during this short stay and I hope to work with you again. And Dave, you really helped me get the results I wanted, even when this was boring for you.

I would not have loved my job as much as I have done without the coffee, music and sports with my colleagues, most of which have left Eindhoven by now. My mates Bram, Eric, Ruudje, Snader en Tom and their better halves also helped me get through by making fun of me and stimulating me to find a real job now.

*Sağol, gracias, bedaank, dagebedankztzetdawitte!*

I am most indebted for the stimulating environment of my family and in-laws who all recognize the power of education. Above all, I wish to thank Marleen for her support and love.

Niels
Apart from the presumable challenge of future crude oil shortage, internal combustion engines are associated with problems regarding local emissions, like Nitrogen Oxides (NOx) and Particulate Matter (PM), as well as carbon dioxide (CO\textsubscript{2}), which is generally thought to have a global impact. For local emissions many solutions exist. However, these solutions come with either additional investment costs, a fuel consumption penalty (higher in-use costs), or both. Therefore, often a choice has to be made between local or global emissions. To avoid this trade-off, a simultaneous reduction is preferred.

The reduction of carbon dioxide in road transport depends on a large number of factors. Both bio-fuels and crude-based fuels can reduce the CO\textsubscript{2} footprint of the fuel, depending on production methods, and the upgrading necessary. Furthermore, the fuel can act as an enabler for certain high efficiency combustion regimes. The combustion regime can have an intrinsic benefit in the energy conversion efficiency. Both the combustion regime and the fuels impact the local emissions and can save CO\textsubscript{2} emissions, by avoiding the formerly mentioned trade-off.

In this dissertation, both various alternative combustion concepts are investigated, as well as a variety of fuels (or fuel combinations) to use in either conventional or these alternative combustion concepts. The concepts are mostly compared using experimental tests.

As a first investigation, a short term solution for using Premixed Charge Compression Ignition combustion is presented. In such a short term scenario, engine hardware and fuels would be conventional, and the combustion concept would be made possible by a smart choice of operating conditions, with possible improvements through the composition of conventional diesel fuels. In a somewhat longer term scenario, fuel reactivity can be tailored to the demands of the combustion concept, of which a first investigation is given.

Besides tailoring a single fuel’s reactivity, other researchers have also shown remarkable results using the Reactivity Controlled Compression Ignition concept. This concept uses in-cylinder blending two fuels with different reactivity to a desired value. This concept is first evaluated after which also the controllability, required for real-life use, is shown.

Also commercially available naphtha blends can help to make the transition from fully mixing controlled combustion (as in a Diesel engine) to more premixed regimes. The application of such naphtha blends is described after which also a number of \textit{n}-butanol/diesel blends are presented. Such bio-fuels (be it blended with Diesel fuel) can enable the further use of aforementioned concepts. Given an optimum reactivity for the latter concept, a number of fuels have been blended both from refinery streams and from surrogate fuel components, of which the differences are presented.

Further improvements of the combustion regimes described earlier rely on detailed knowledge and understanding of the underlying processes. The development of both high speed, and statistically correlated laser diagnostic techniques is described after which an attempt is shown to apply these techniques to both conventional and advanced combustion regimes, to gain the aforementioned understanding.

The body of this dissertation is concluded by a general discussion on the results and their respective conclusions.
Author’s Curriculum Vitae

Niels Leermakers was born on January 2nd 1983 in Wintelre, in the South of the Netherlands. After finishing his pre-academic education on the Sondervick College in Veldhoven, he studied Mechanical Engineering at the Eindhoven University of Technology, with a major in Automotive Engineering Science. In March 2010 he graduated from the Combustion Technology group, where one month later he started a PhD project. The results of this work are presented in this dissertation.
Theses

belonging to the dissertation

**Efficient Fuels for Future Engines**

by

Cornelis Antonius Johannes Leermakers

I. Legislation should focus also on fuels’ performance, rather than that of engines alone, because the emission reductions and CO$_2$-efficiency gain possible with future fuels greatly surpass those achievable with engine(-related) technologies.

*Efficient fuels for future engines. (This dissertation)*

II. Engine hardware and technologies used in diesel power trains will become more like those used in gasoline engines and vice versa, resulting in technologies which are universally applicable.

*(This dissertation)*

III. The optimal mixed- or dual-fuel strategy and fuel type(s) to be used for practical application of low-temperature combustion concepts depend on the conditions (engine speed, load, transiency, ambient conditions) specific to such applications.

*(This dissertation)*

IV. The introduction of high-cost, low-energy-density *Diet* fuels can decrease the energy used in transport.

*di-et [dahy-it] - adjective
having a smaller number of calories than usual
from Medieval Latin *dieta*, literally, daily regimen, diet
(taken as a derivative of Latin *dies* day)*

V. To evaluate the performance of fuels, whenever possible dedicated test rigs should be used instead of engines.

*Engines are not made for testing, but for moving people and goods around. (Kleijwegt)*
VI. One who compares dissertation-related complications with those that may occur during childbirth, forgets the lack of a caesarean-equivalent for the former.

*Can PhD candidates be “too posh to push”?*

VII. The use of non-standardized units, such as football fields, elephants, and Eiffel-towers-to-the-moon does not add clarity for one who does not have any sense of magnitudes and obscures information for one who does.

“If you took all the veins out of your body and laid them end to end, you would die.” (N.N.)

VIII. For a student, it’s impossible to keep track of progress in an assignment as unfamiliar as a PhD project. Therefore, long-term planning should be exclusively the promoter’s responsibility.

“Tijdens de Tachtigjarige Oorlog zei echt niemand na 40 jaar: ‘Hè-hè, we zitten op de helft, pfieuw.’” (Maassen)

IX. The term “Sunday’s clothing” has lost its meaning in modern-day Eindhoven.

“Een goed huispak is voor mij een huispak met veel glitters, steentjes, pailletjes, ritsjes, satijnen lintjes, goud, studs.” (Donders)

X. Success is not required to keep trying, but it helps to stay motivated.

“Point n’est besoin d’espérer pour entreprendre, ni de réussir pour persévérer” (William of Orange)

XI. While most garden-shed-inventors’ ideas may be irrational, all combined they are more important for technological breakthroughs than well-performed research is.

“Ja, ik zat te denken dat volgens mij niet de moraliteit de vooruitgang van de samenleving bepaalt, maar juist haar immoraliteit en haar verdorvenheid. De vitaliteit of de verandering van de samenleving is nooit beheerst geweest door het goede of het deugdzame in de ideële en de platonische zin van de moraal of in de objectieve zin van de wetenschap en techniek. De sturende impuls is de losbandigheid; of het nu die van de beelden is, de ideeën of de tekens, dat maakt niet uit. De rationele systemen van de moraal beheersen alleen de lineaire evolutie, hun zichtbare geschiedenis. Maar de fundamentele energie, die zelf deze dingen aandrijft, die komt volgens mij heel ergens anders vandaan.” (Maassen)