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Commercial Naphtha Blends for Partially Premixed Combustion

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ABSTRACT

Partially Premixed Combustion has shown the potential of low emissions of nitrogen oxides (NOx) and soot with a simultaneous improvement in fuel efficiency. Several research groups have shown that a load range from idle to full load is possible, when using low-octane-number refinery streams, in the gasoline boiling range.

As such refinery streams are not expected to be commercially available on the short term, the use of naphtha blends that *are* commercially available could provide a practical solution. The three blends used in this investigation have been tested in a single-cylinder engine for their emission and efficiency performance.

Besides a presentation of the sensitivity to injection strategies, dilution levels and fuel pressure, emission performance is compared to legislated emission levels. Conventional diesel combustion benchmarks are used for reference to show possible improvements in indicated efficiency.

Analysis of the heat release patterns revealed an interesting and strong correlation between the premixed fraction and the amount of soot produced. To be specific, each of the fuels showed a decrease in this fraction as either fuel pressure was lowered or load was increased, showing a transition from more premixed to mainly mixing-controlled combustion, with the corresponding soot emissions.

For one 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.

INTRODUCTION

Conventional diesel engines traditionally suffer from significant emissions levels of both particulate matter (PM) and nitrogen oxides (NOx) [1]. Overcoming these harmful emissions often comprises these engines' relatively high efficiency. The introduction of new technologies, e.g. advanced exhaust gas after treatment [2] and high pressure fuel injection equipment [3], not only added significant extra costs to vehicles, but also introduced a fuel consumption penalty because of higher exhaust gas back pressures, regenerative cycles and an increase in parasitic losses in the fuel system [4].

Partially Premixed Combustion [PPC] [5,6,7] has shown to be able to reduce emissions to similar or even lower values as the aforementioned technologies. However, this concept has shown this emission reduction with a simultaneous efficiency improvement. Conventional fuels, i.e. diesel [8] or gasoline [9] imply a number of challenges for this concept, but fuels in the gasoline boiling range, with relative low-octane-number were shown to be very well suitable for this

concept [10]. The load range over which the concept can be applied was shown to depend on the reactivity. At best this applicable load ranges from idle to full load, without major modifications to the engine setup. Several refinery streams were used by Manente and coworkers [11].

However, such refinery streams are not expected to be commercially available on the short term. For certain applications, the used of currently commercially available naphtha blend 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.

For the present investigation, two commercially available naphtha blends have been selected, with different boiling range, aromatic content and associated reactivity. The blends were sourced from a local chemical supplier, i.e. Remat Chemie, Helmond (The Netherlands). The blends have been analyzed in a gas chromatograph-mass spectrometer to determine their composition and were subsequently tested in a single-cylinder engine for their emission and efficiency

performance. A third blend of 50 vol-% RON95 gasoline and 50 vol-% of the first naphtha blend was also tested and furthermore a comparison is made to a conventional diesel fuel.

The present paper presents a summary of the performance of these three naphtha blends with respect to emissions and efficiency. Besides a presentation of 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

Experimental Apparatus

For this investigation a six-cylinder DAF engine, referred to as CYCLOPS, is used. For more information on the setup the reader is referred to a detailed description [8], of which this subsection is a short summary. Prior to this measurement campaign, the engine has been overhauled with new pistons and liners.

The CYCLOPS is a dedicated engine test rig, see Table 1, based on a DAF XE 355 C engine. 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. Cylinders 4 through 6 of this inline 6 cylinder HDDI engine operate under the stock DAF engine control unit and 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. Apart from the mutual cam- and crankshaft and the lubrication and coolant circuits, this test cylinder operates autonomously from the propelling cylinders and uses stand-alone air, EGR and fuel circuits for maximum flexibility.

Table 1. CYCLOPS test setup specifications

Base Engine	6 cylinder HDDI diesel
Cylinders	1 Test cylinder
Bore [mm]	130
Stroke [mm]	158
Compression ratio	15.7 (original 17.0)

Fed by an air compressor, the intake air pressure of the test cylinder can be boosted up to 5 bar. Non-firing cylinders 2 and 3 function as EGR pump cylinders (see Figure 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 is cooled both up- and downstream of the pump cylinders. Several surge tanks, to dampen oscillations and to 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.
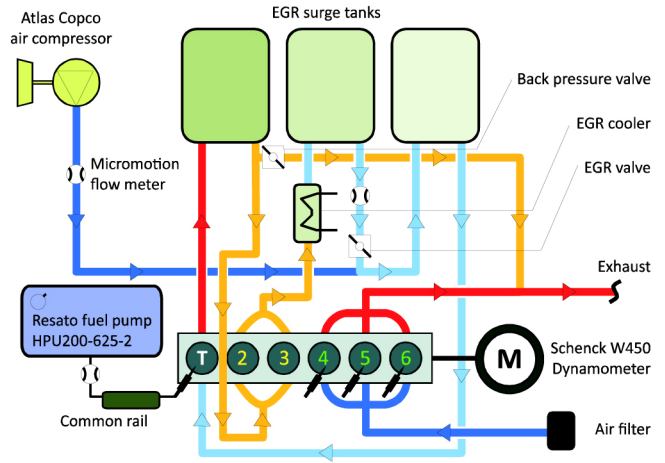

Figure 1. Schematic of CYCLOPS experimental setup: a modified DAF engine using separate fuel, air and EGR systems for one dedicated test cylinder

Fuel is injected into cylinder 1 is by a prototype Delphi common rail injector with a nozzle having 8 holes of 0.151 mm diameter with an umbrella angle of 153 degrees. All steady state flows of fuel, air and EGR, are measured with Micromotion Coriolis mass flow meters.

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) is measured using an AVL 415S smoke-meter. All quasi steady-state engine data are recorded by means of an in house data acquisition system (TUeDACS). A SMETEC Combi crank angle resolved data acquisition system is used to record and process crank angle resolved data. For more information on the setup and the procedures and definitions used, the reader is referred to earlier work by the authors [8].

Fuels Under Investigation

Manente [12] showed that fuels with an octane number (ON) of around 70 are possibly best suitable for PPC as they can be applied over the complete load range without major modifications to the engine.

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 such naphtha blends (NB1 and 2, respectively) have been selected for this investigation. In principle, they are upstream precursors of pump gasoline and consequently, cheaper in production, which is confirmed by Kalghatgi and coworkers [10].

The fuels used are presented in Table 2. The main difference between NB1 and NB2 is their average molar mass, which is substantially higher for NB2 and implies a higher boiling range. The third naphtha blend (NB3) consists of 50 vol-% of NB1 and 50 vol-% of gasoline (RON95). The pump gasoline has been used to decrease reactivity since the naphtha blend 1 might still be slightly too reactive for PPC purposes. A lubricity additive is used with these low viscosity fuels to ensure sufficient lubricity for the components under high fuel pressure.

Table 2. Overview of the fuels under investigation.

Fuel	CN	AFR$_{st}$ [-]	HHV [MJ/kg]	LHV [MJ/kg]	Boiling range [°C]
EN590	52.4	14.6	45.6	42.7	170-360
RON95[1]	14.7	14.7	44.67	41.8	~65-185
NB 1	45 ± 5	14.87	46.52	43.48	94-140
NB 2	50 ± 10	14.74	46.23	43.31	142-200
NB 3[2]	30 ± 10	14.8		42.74	~65-185

NB1, NB2, gasoline and EN590 diesel have been tested according to ASTM D240 (higher heating value or HHV). To obtain the lower heating value (LHV) the heat released by the condensing water (2260 kJ/kg or 40.6 kJ/mole) has been subtracted from the HHV. The properties of Naphtha blend 3 have been calculated from these results.

The exact chemical composition of the two naphtha blends was not known and therefore these blends have been tested in a combined gas chromatography-mass spectrometer (GC-MS). type GCMS-QP5000 from Shimadzu. Di-ethyl ether (DEE) is used as a solvent, because of its high volatility and lower boiling point compared to the test substances.

According to the obtained GC spectra and full compositions as presented in Figure 21 in the Appendix, Naphtha blend 1 mainly consists of low octane components. These components are in accordance with the boiling point range. The supplier's claim of less than 0.5% aromatics can be partially confirmed. In this study it is found that Naphtha blend 1 contains less than 3.4% aromatics based on the fact that no aromatics were found in 96.6% of the mass spectrum that could be specified. The claim about octane and isomers content is also confirmed by the experiments. Based on 96.6% of the blend, the average carbon length is found to be (7.88 ± 0.06) with an H/C ratio of (2.11 ± 0.01)[3].

Originally, Naphtha blend 2 has been selected as being quite similar to Naphtha blend 1 but with additional aromatic components (increase in ON). This is confirmed by the measurements as shown in Figure 22. Based on only 71.8% of the blend, the average carbon length is found to be (10.1 ± 0.6) with an H/C ratio of (2.02 ± 0.06)[4].

Octane or Cetane numbers were not tested for the present fuels. The Cetane number is estimated using a correlation of hydrocarbon type and carbon number to cetane number (see Figure 6 in ref [13]. However, as not all of the blend components are known, 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. Especially at lower cetane numbers this uncertainty (e.g. ± 5) can have significant impact.

According to this method, naphtha blend 1 (with mainly *n*-paraffins and iso-paraffins with an average carbon number of 8, as well as mono-cyclonaphtenes) should have a Cetane number of 45 ± 5.

Naphtha blend 2, on the other hand, contains *n*-paraffins and iso-paraffins with an average carbon number of 10, as well as aromatics. Hence, the component reactivities are more spread, but the average does not differ a lot with respect to NB1. A CN of (50 ± 10) is found for NB2. The error interval of the second naphtha blend is larger due to the relatively large amount of unknown components. Nevertheless, the main conclusion is that both blends have a CN similar to diesel.

Finally, naphtha blend 3 consists of NB1 and pump gasoline. The CN of RON95 has been estimated using the well-known equation of Kalghatgi [14]. Hence, the cetane number of NB3 is estimated to be 30 ± 10.

Conditions and Procedure

Based on the results of Manente [15], the engine speed is set to 1250 rpm, which is typical for a heavy-duty vehicle during highway cruising. An EGR flow of around 50 weight percent is used, both to limit pressure rise rates, as found in previous work [16], and to have nitrogen oxides emissions below Euro VI levels [17,18].

The latter two references have stated that a combustion temperature higher than 1500K is necessary to promote the reactions from CO to CO2, and that on the other hand it is important to be below 2000K to avoid thermal NOx formation (Zeldovich' mechanism). Apart from an EGR weight percentage of around 50%, this also implies the use of a global lambda value of around 1.5. To achieve such an air excess ratio, intake pressure is varied accordingly.

The recirculated exhaust gas is heavily cooled using cold process water, to about 300K and the exhaust back-pressure is regulated to 0.3 ± 0.2 bar higher than the intake pressure to mimic the presence of a turbocharger of finite efficiency and enable the use of external EGR in practice. Depending on turbocharger efficiency, 0.3 bar excess exhaust pressure is considered to be feasible with sufficient high turbine

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[1]Lower heating value has been calculated assuming an average composition of C$_8$H$_{15}$. Boiling range is represented by the temperatures at which 10 (T10) and 90% (T90) of the fuel have vaporized, respectively.

[2]Boiling range equal to that of RON95, only with a different distribution.

[3]Error intervals have been determined by estimating the unknown part of the blend, using both the shortest and longest saturated carbon chain found in the mixture.

[4]Similar error estimation as for Naphtha blend 1, although H/C ratio is very much depending on aromatic/paraffinic content.

efficiency. The error interval given is caused by test bench limitations.

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

• Engine speed = (1250 ± 10) rpm

• λ = (1.5 ± 0.1)

• (50 ± 5) wt-% of EGR

Both single and advanced injection strategies will be tested 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 at 8 bar.

• 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

Fuel pressure increases with load to keep injection duration roughly constant in crank angle domain. 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.

All operating points should have acceptable combustion stability (i.e. σ_{IMEP} < 5%) and preferably 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. These limitations have been specified by Leermakers and co-workers [8], but they have been slightly modified for this research.

• 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. As an indicator for this, the HC emissions have been limited to 2000 ppmC.

Definitions

The calculated crank angle at which 10% of the fuel has been burnt (CA10) is used as main indicator for the start of combustion (SOC). 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 CA10 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$_{main}$) and start of combustion is also evaluated. This so-called ignition dwell, if positive, is thought to be beneficial for reduced soot production since injection has ended before combustion starts. In summary the following definitions are used:

• Ignition delay (ID) is defined as CA10 - SOI$_{main}$

• Burn duration (BD) is defined as CA90 - CA10

• Ignition dwell is defined as CA10 - EOI$_{main}$

Premixed fraction

It has been postulated before that Partially Premixed Combustion can vary in the amount of premixed combustion. This grade of premixing is quantified by comparing the heat released in the premixed combustion phase and the total heat released. The premixed fraction is defined using the method suggested by Solaka and coworkers [19] is followed, where a Gaussian profile is fitted to the rising flank of the premixed peak, between 50% of the maximum and the actual peak. The Gaussian profile is defined as

$$G(x) = h \cdot e^{-\left(\frac{x - x_0}{2\alpha^2}\right)^2},$$

(1)

with x_0 the central position of the peak, and h and α representing the height and width of the Gaussian profile, respectively. From Figure 2 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.
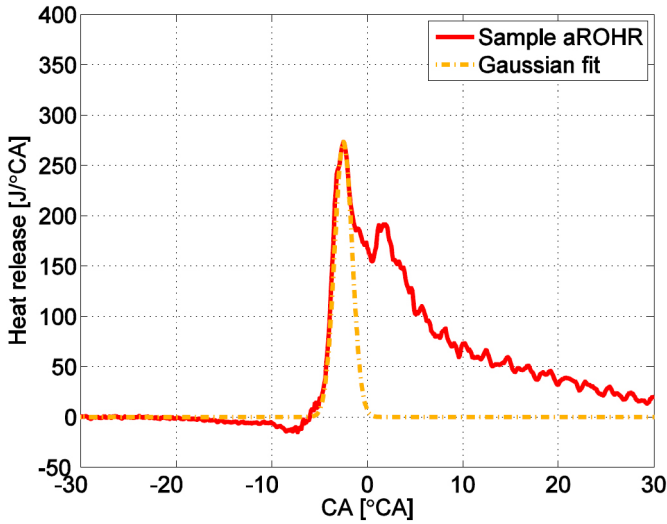
Figure 2. Rate of Heat Release and Gaussian profile as a function of crank angle degree. Gaussian fit is used to define the premixed fraction

Efficiencies

Combustion efficiency provides information about the completeness of combustion and it is used to derive thermal efficiency. In order to calculate the combustion efficiency all specific emissions (i.e. ISCO, ISHC, ISPM and ISH2) 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) represents the way in which combustion efficiency is calculated.

$$\eta_{comb} = \frac{ISCO \cdot LHV_{CO} + ISHC \cdot LHV_{HC} + ISH2 \cdot LHV_{H2}}{ISFC \cdot LHV_{fuel}}$$

(2)

Gross indicated (η_{ind}) and thermal efficiency (η_{th}) will be calculated according to respectively equation (3) and (4).

$$\eta_{ind} = \frac{P_{ind}}{\dot{m}_{fuel} \cdot Q_{LHV}}$$

(3)

$P_{ind} = W_{ind}n$ is based on the work done W_{ind} in the compression and expansion stroke and *n* engine speed in rev/s, Q_{LHV} represents the lower heating value of the fuel and $\dot{m}_{fuel}$ 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.

$$\eta_{th} = \frac{\eta_{ind}}{\eta_{combustion}}$$

(4)

RESULTS AND DISCUSSION

Below, the relevant results for all fuels will be discussed in five 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. 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 ignition behavior is found to be quite similar to that of diesel (see Figure 3). EGR helps to get a significant ignition delay, although a complete separation between injection and combustion is not obtained. However, the physical properties (e.g. boiling range, volatility) do differ, which might lead to distinctive effects. The heat release for the single injection is typical diesel-like, with a distinct premixed peak followed by some injection-controlled combustion.
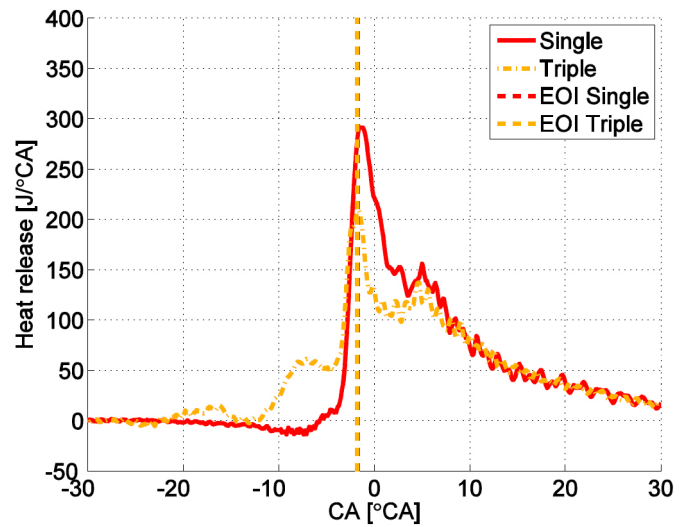

Figure 3. Comparison of NB1 at 800 bar fuel pressure with single and multiple injections with pilots at −60 and −30 °CA aTDC. EOI of last injection and single are almost identical and thus the vertical lines overlap.

Mixing prior to combustion can be promoted with two pilot injections. However, a penalty in combustion efficiency is expected as more fuel might end up in the crevices or in the vicinity of the cylinder wall. The EGR helps to suppress some of (early) low temperature reactions, but the heat release for the triple injections shows that combustion still starts before injection has ended. It proves to be difficult to postpone auto-ignition of high-reactive components such as

n-heptane, *n*-octane and *n*-nonane that are present in NB1, see Table 6 in the appendix.

Some of the emission results have been summarized in Table 3. Although a slight reduction in PM emissions is achieved without a significant NOx penalty, combustion efficiency suffers from the multiple injection strategy. Therefore, indicated efficiency does not benefit from the use of multiple injections.

Table 3. Overview of Naphtha blend 1 results for two different strategies and 50% EGR

		Single	Triple
IMEP$_{gross}$	[bar]	7.8	7.8
CA50	[°CA aTDC]	5.5	4.6
λ	[-]	1.53	1.59
η_{ind}	[-]	0.473	0.468
η_{comb}	[-]	0.993	0.977
ISNOx	[g/kWh]	0.57	0.59
ISPM	[g/kWh]	0.26	0.19

Naphtha blend 2

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 4 clearly visualizes such undesired early combustion, when a double injection strategy at 1500 bar is used.
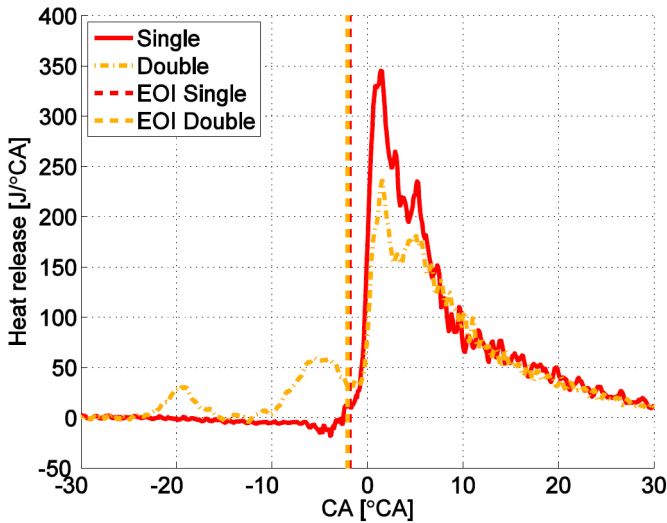

Figure 4. Three phase compared to single phase heat release for double and single injection, respectively. NB2 @ 1500 bar fuel pressure and 50% of EGR. EOI are almost identical for the single and last injection, respectively.

Apparently, 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 4). 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.

Table 4. Overview of engine parameters and results during NB2 combustion characterization

		Single	Double
IMEP$_{gross}$	[bar]	8.0	7.8
CA50	[°CA aTDC]	6.1	5.5
SOI$_{pilot}$	[°CA aTDC]		-61
SOI$_{main}$	[°CA aTDC]	-6.1	-2.6
MPRR	[bar/°CA]	7.4	4.8
λ	[-]	1.61	1.61
η_{ind}	[-]	0.496	0.481
η_{comb}	[-]	0.994	0.966
ISNOx	[g/kWh]	0.48	0.39
ISPM	[g/kWh]	0.049	0.033

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 5 shows that the increased resistance to auto-ignition for NB3 results in a distinctly different heat release pattern compared to NB1 and NB2, for both single and double injection strategies.
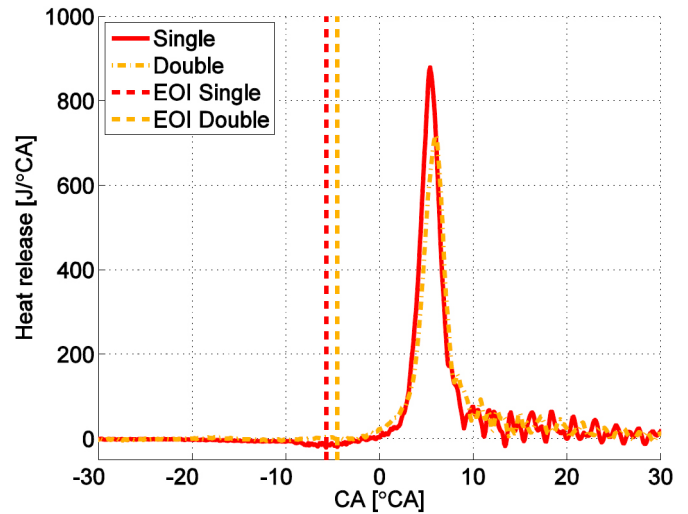

Figure 5. Both single and double injection yield a similar heat release for NB3. NB3 at 1500 fuel pressure and 50% EGR.

Even for the double injections, ignition is postponed until TDC, by the reduced reactivity. 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 5), it remains doubtful whether significant benefits will be obtained with such early pilot injections.

Table 5. Overview of engine parameters and results during NB3 combustion characterization

		Single	Double
IMEP$_{gross}$	[bar]	7.7	7.6
CA50	[°CA aTDC]	6.1	6.2
SOI$_{pilot}$	[°CA aTDC]		-61
SOI$_{main}$	[°CA aTDC]	-8.9	-4.5
MPRR	[bar/°CA]	16.3	13.8
λ	[-]	1.48	1.47
η_{ind}	[-]	0.476	0.457
η_{comb}	[-]	0.987	0.959
ISNOx	[g/kWh]	0.85	0.52
ISPM	[g/kWh]	0	0.0035

2. Total Dilution and Combustion Phasing Variation

In this results section, all three naphtha blends will be compared. Even though the previous sections have 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. Injection timing has been adjusted to reach the target combustion phasing and it was found that all SOI were in the frame of −15 to −5 °CA aTDC. The most important results are discussed below.

Controllability

One of the challenges of (Partially) Premixed Combustion can be (a lack of) controllability. In earlier work by the authors [20] it was proposed to use the sensitivity of the ignition delay (S_{ID}) as means to quantify the controllability, i.e. the derivative of CA50 with respect to a change in injection timing:

$$s_{ID} = \frac{\partial CA50}{\partial SOI}$$

(5)

At very early injection timings, where ignition is dominated by global parameters, the response of 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.

The sensitivity of ignition delay for the Naphtha blends is shown in Figure 6. Blends 1 and 2 show stable and similar performance for both air excess ratios. Even the less reactive NB3 has acceptable controllability.
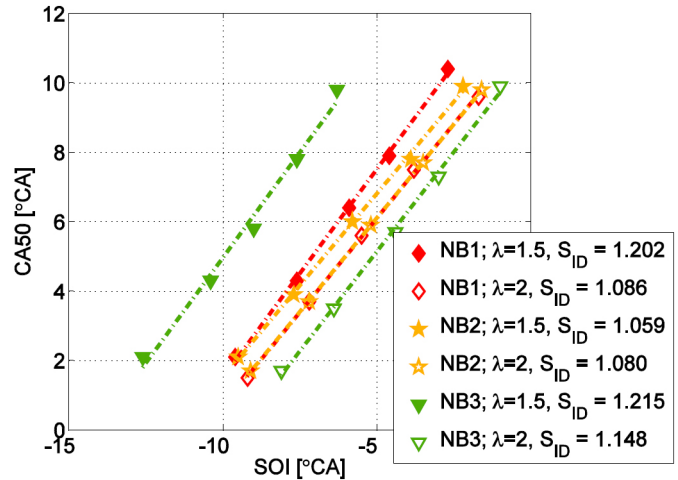

Figure 6. Combustion phasing response varying injection timing

Heat release parameters

Having a near unity S_{ID} implies that over the sweep, the time between injection and CA50 remains nearly constant. Figure 7 shows that for all fuels, also the ignition dwell and burn duration remain near constant with injection timing.

Furthermore, the expected trends with reactivity and dilution level can be observed. The low reactive NB3 gives longer ignition dwell, but because of larger premixed phase also shorter burn durations. Higher dilution levels also increase the amount of premixed burn and as such, reduce the burn duration.
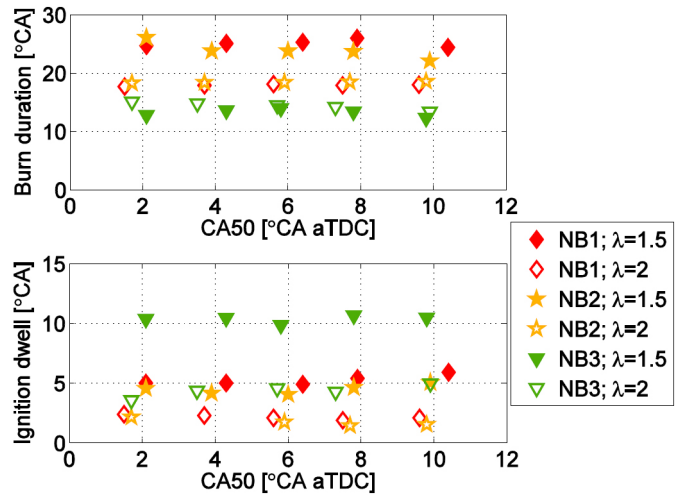

Figure 7. Burn duration and ignition dwell as a function of combustion phasing resulting from an injection timing variation.

Emissions

Hydrocarbon and CO emissions, seem to correlate with the boiling range, as can be seen from Figure 8. 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. This effect might also influence nitrogen oxide emissions. Confinement of the fuel closer to the center of the combustion chamber will increase the temperature locally and as such the NOx formation. This seems to be not counterbalanced by the increase in heat capacity.
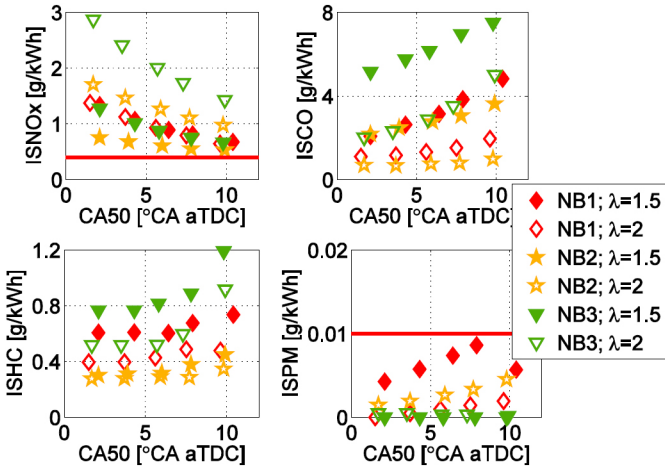

Figure 8. Overview of emissions for combustion phasing variation

Volatility is furthermore expected to heavily influence soot formation. In Figure 8, the λ = 1.5 NB2 series has been omitted from the ISPM plot in order to obtain a better view on tiny differences for the other series. Note that for the present conditions, all fuels are within ISPM EURO VI emissions levels

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. However, for none of the series EURO VI levels are achieved. An increase in EGR level might solve this problem since some margin exists with respect to PM emissions. This will be further discussed below.

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 for all fuels.

However, the lower boiling 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. With somewhat retarded combustion phasing (10 °CA aTDC) the

penalty in efficiency is limited. Further retarding combustion, however, is to be really detrimental to efficiency.
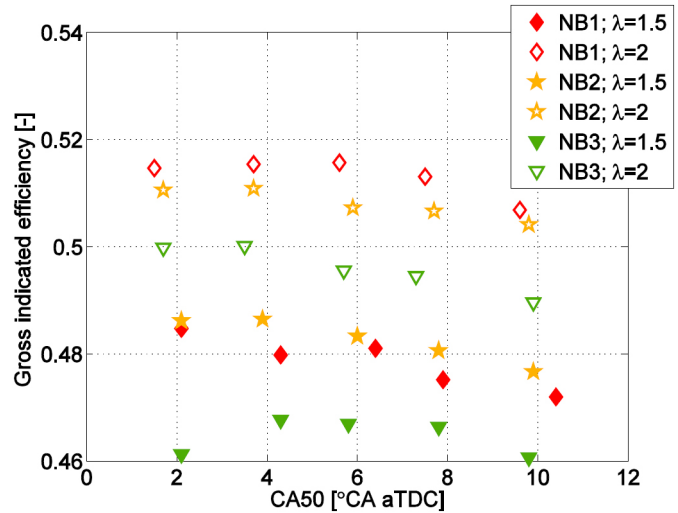

Figure 9. Gross indicated efficiencies for combustion phasing variations

3. EGR Level Increase Variation

The previous section showed somewhat too high emission levels for NOx were experienced with an EGR level of 50 wt-%. 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 10. Although the lower global temperatures give rise to a slightly reduced combustion efficiency, it is still acceptable.
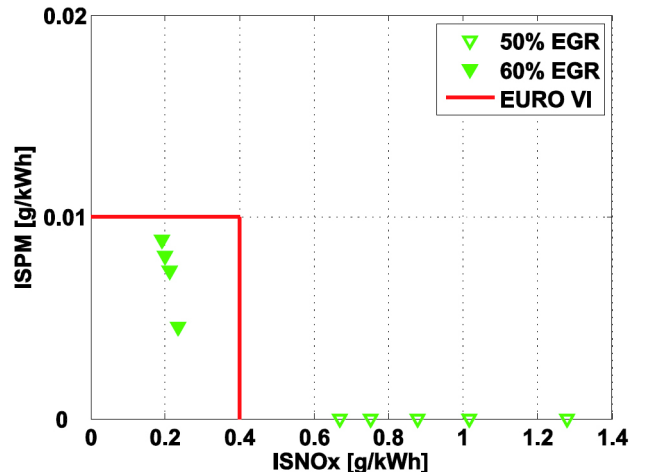

Figure 10. Increased EGR levels to obtain Euro VI compliant nitrogen oxides emissions.

4. Fuel Pressure Variation

Over the last decade, automotive manufacturers have strived for higher and higher fuel pressures to decrease

particulate matter emissions. However, alternative fuels with completely different characteristics (e.g. ignition behavior and structural effects) might be able to break with this tendency. Therefore, for each of the fuels under investigation, the fuel pressure is reduced while all other parameters were kept constant. The differences in ignition behavior however, lead to minor adjustments in injection timings in order to keep CA50 at a constant 4 °CA aTDC.

Particulate emissions

When comparing all of the naphtha blends to EN590 diesel, one can see from Figure 11 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.
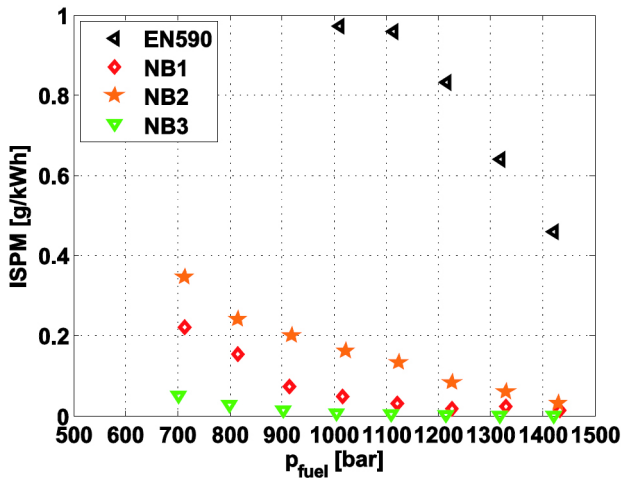

Figure 11. Soot production effects at constant operating conditions for lowered fuel pressures.

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 12 for 1000 bar fuel pressure. One should note that for all fuels, the load and CA50 are constant. However, the combustion with constant CA50 is quite different for all fuels, due to the diffusive trails.
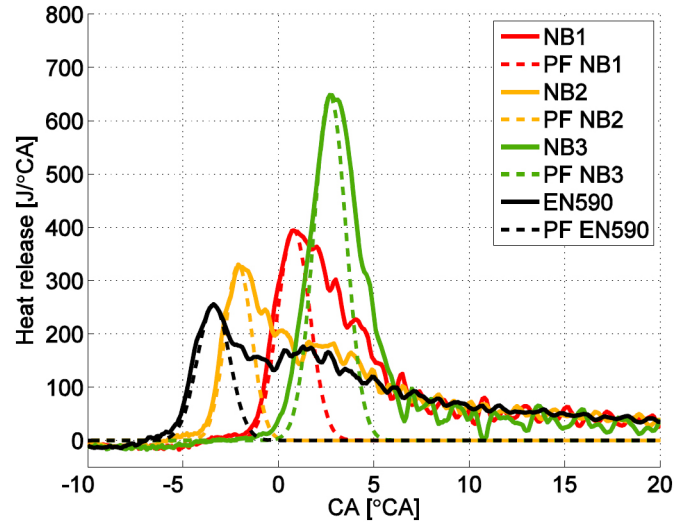

Figure 12. Heat release patterns at 1000 bar. 8bar IMEP CA50 = 4degCA aTDC. (Premixed fraction Gaussian fits shown with dashed lines.)

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. 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 overlap is often said to correlate with the aforementioned soot emissions. However, Figure 13 only shows only marginal differences of this dwell time with respect to fuel pressure.
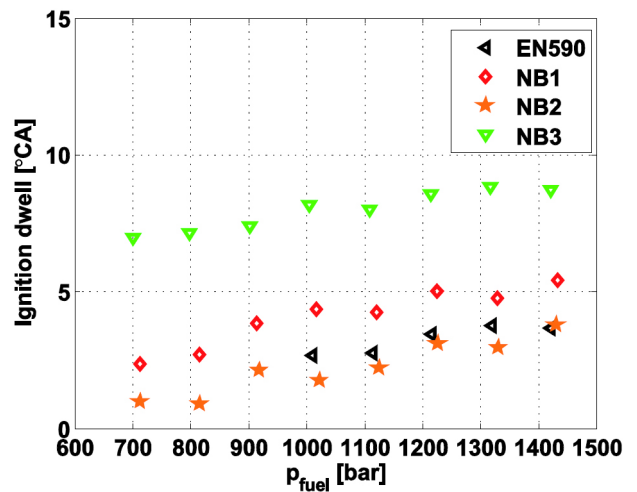

Figure 13. Ignition dwell as a function of fuel pressure.

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 drop 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.

This effect of volatility on the amount of premixed is even more evident from Figure 14, where the premixed fraction of the heat release is computed for all operating points.
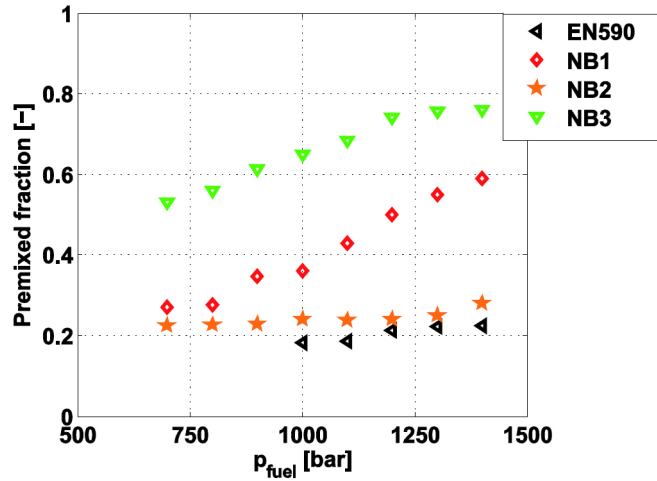

Figure 14. Premixed fraction as a function of fuel pressure

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 fuel pressure. The more this premixed fraction is reduced, the higher the smoke emissions are expected to be. For the least reactive NB3 blend, even at 700 bar fuel pressure, more than half of the fuel burns in premixed mode, which keeps soot emissions at a minimum.

The correlation of particulate emissions with the premixed fraction is shown in Figure 15. This graph shows that increasing the premixed fraction, either through operating conditions, or through the use of a higher volatile, or lower reactive fuel, is a very efficient way of reducing PM emissions. In this case an exponential reduction is shown, as the PM emissions are given on a logarithmic scale. The correlation of the PM emissions is shown to be much stronger to this newly introduced premixed fraction, than with the conventional ignition dwell approach.
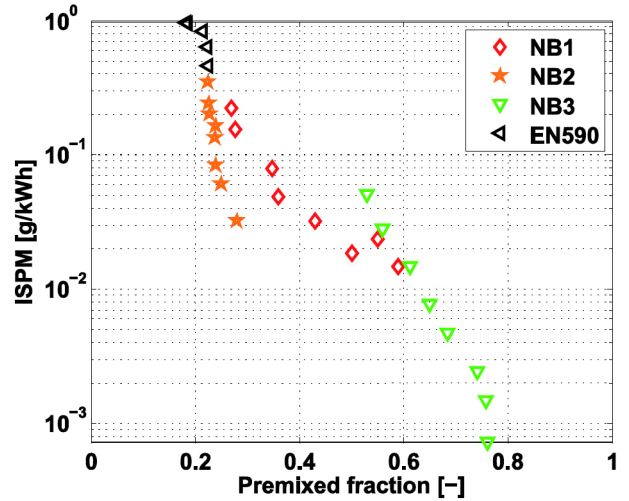

Figure 15. PM emissions on a logarithmic scale as a function of the premixed fraction

5. Load Variation

Given the results above for one single load, all fuels have been investigated for a broader load range, i.e. 8 through 16 bar IMEP. This load range represents the range from about one-third to two-thirds of the engine's rated torque output.

Heat release parameters

As shown above 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, was also shown to change when altering the fuel pressure. Also for a change in load these parameters are expected to change, as will be shown below for the naphtha blends as well as diesel.

Looking at the low load part in Figure 16 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 converges to 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 is reduced as load is increased, even for the highest load it exhibits significantly higher premixed fraction.
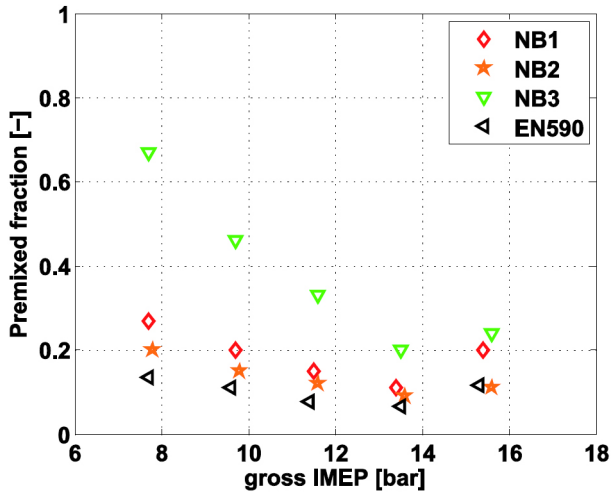
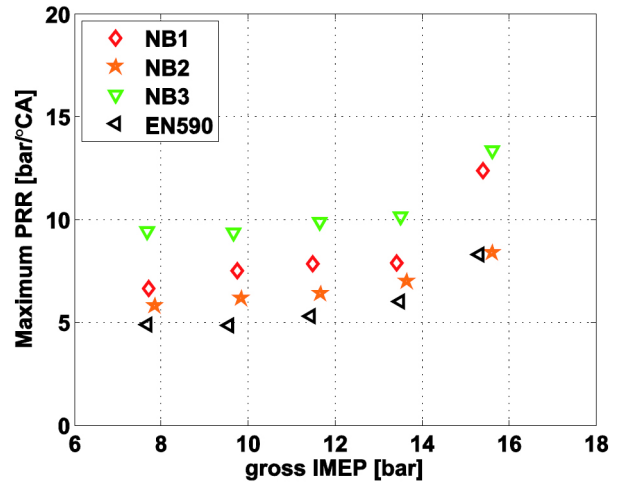*Figure 16. Premixed fraction as a function of load for each of the fuels.*

A different trend is visible for the ignition dwell, or the amount of overlap between the injection and combustion events, as is shown in Figure 17. Each of the fuels shows a reduction in ignition dwell as load increases. Where at the lower load end a clear difference between diesel and the low reactive NB3 can be observed, this difference disappears as load increases. It should be noted that for all of the fuels, the ignition dwell becomes negative over 10 bar load.
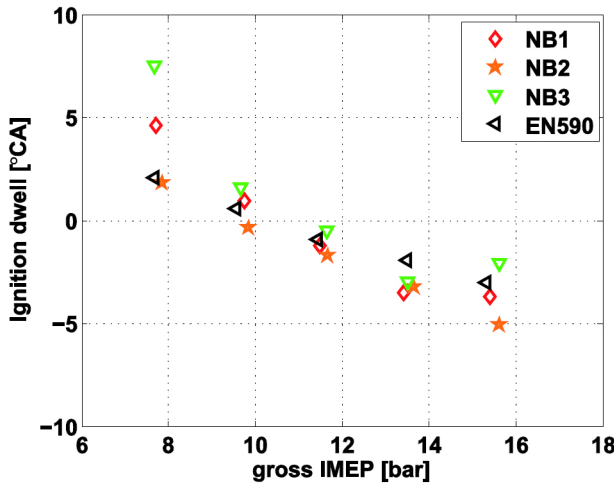

Figure 17. Ignition dwell as a function of load for each of the fuels.

For all of the fuels, the maximum pressure rise rate increases with load, as can be seen in Figure 18. 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 the low boiling fuels have somewhat higher pressure rise rates.

Figure 18. Maximum pressure rise rate as a function of load.

Emissions

One of two 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 19. 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.
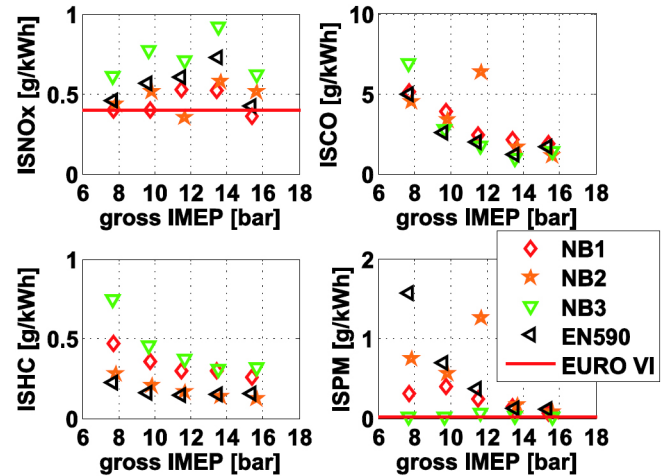

Figure 19. Emission levels as a function of load for all naphtha blends and diesel.

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 significant effects in 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.

Efficiency

Figure 20 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.
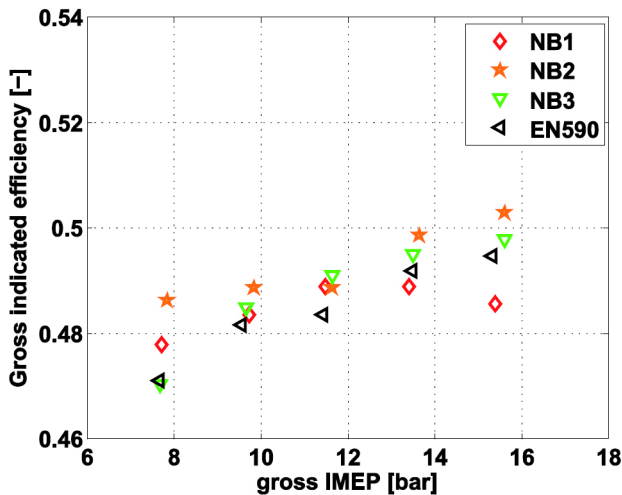

Figure 20. Gross indicated efficiency as a function of load for all naphtha blends and diesel.

The low reactive Naphtha blend 3 was shown to have a much larger premixed fraction at low loads. This has helped 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.

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 phase. 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 sensitivity s_{ID} 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 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. 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 for 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 EUROVI soot levels.

It should be noted that the premixed fraction was shown to correlate better with this increase in particulate emissions than the traditionally accepted method 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 50% clearly indicating the potential of this concept.

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DEFINITIONS AND ABBREVIATIONS

AFR$_{st}$ - stoichiometric air fuel ratio

aTDC - after top dead center

BD - burn duration

CA - crank angle

CAXX - crank angle at which XX% of the fuel has been burnt

CN - cetane number

CO - carbon monoxide

CO$_2$ - carbon dioxide

DEE - di-ethyl ether

EGR - exhaust gas recirculation

EN590 - European diesel fuel

EOI - end of injection

EURO VI - 2013 European heavy duty transport emission legislation

FSN - filter smoke number

GC-MS - gas chromatography-mass sprectrometer

H/C ratio - atomic hydrogen carbon ratio

H2 - hydrogen

HC - hydrocarbon

HDDI - heavy duty direct injection

HHV - higher heating value

ID - ignition delay

IMEP - indicated mean effective pressure

ISXX - indicated specific XX emissions

LHV - lower heating value

MPRR - maximum pressure rise rate

NB - naphtha blend

NOx - nitrogen oxides

ON - octane number

PM - particulate matter

PPC - Partially Premixed Combustion

ppm - parts per million

ppmC - parts Carbon per million

PRR - pressure rise rates

RON - research octane number

RON95 - European gasoline fuel

S_ID - sensitivity of ignition delay

SOC - start of combustion

SOI - start of injection

TXX - temperature at which XX% of the fuel has vaporized

UHC - unburned hydrocarbons

λ - air excess ratio

σ - standard deviation

η_{comb} - combustion efficiency

η_{ind} - gross indicated efficiency

η_{th} - thermal efficiency

APPENDIX

Fuel Analysis of Naphtha Blend 1

According to the supplier, Naphtha blend 1 consists of octane and isomers. It has also been specified that it should contain less than 0.5% of aromatics. Figure 21 depicts the GC-MS spectrum found for this blend. Obviously, peaks are well separated except for the middle section. Nevertheless, more than 96 % of the mass fractions could be determined with acceptable accuracy. Even though, isomers are hard to distinguish because of their similar boiling point and similar spectrum in the mass spectrometer.
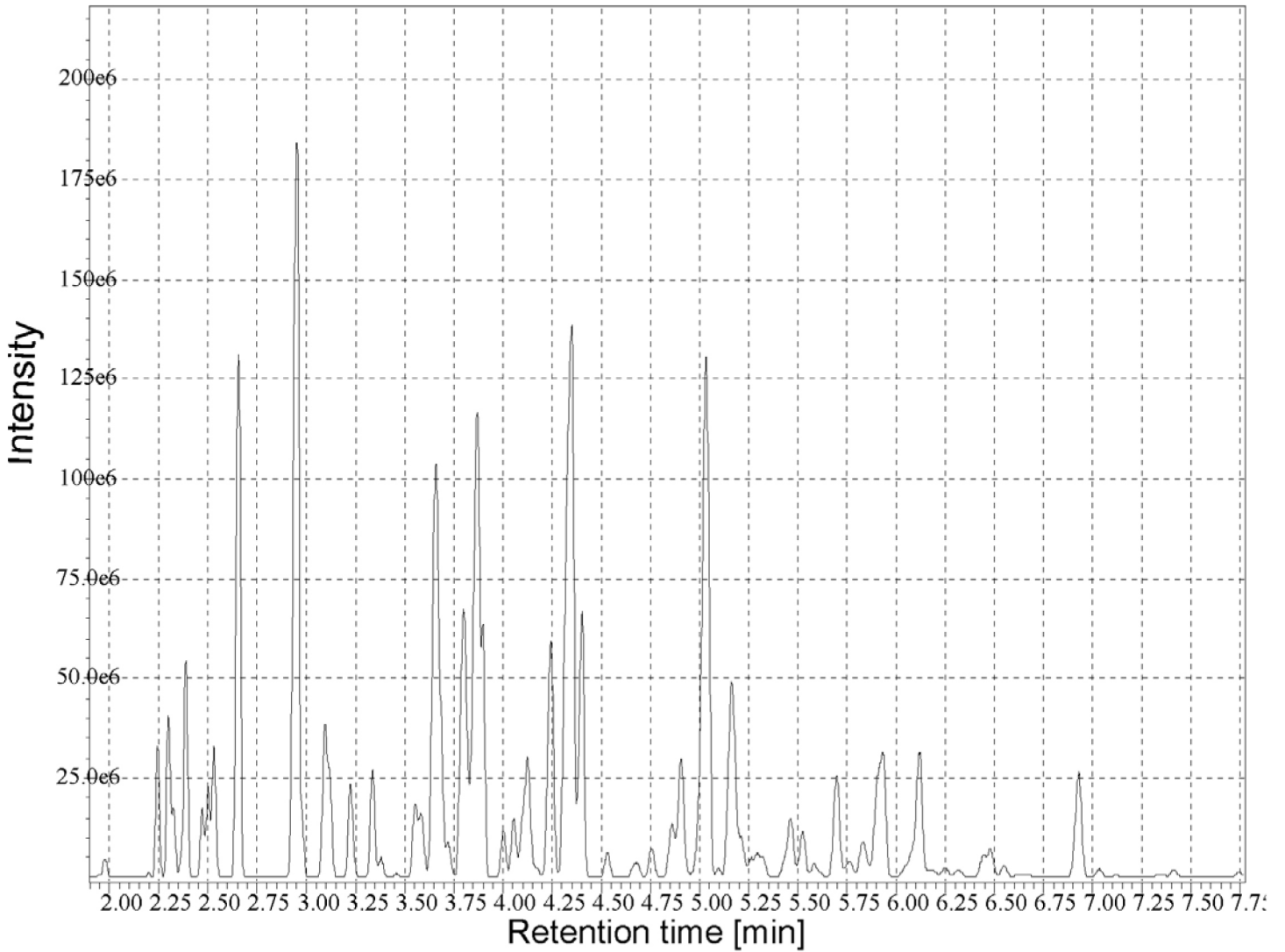

Figure 21. GC-MS spectrum obtained for Naphtha blend 1

Table 6 is an overview of the composition of Naphtha blend 1. As expected, roughly half of the blend consists of saturated paraffins whereas the other half consists of mainly naphthenes. It can be assumed that the supplier's statement of less than 0.5% of aromatics is true. The strange appearance of one olefin (1-nonene) might be related to incorrect correlation as the blend is said to be completely saturated.

Table 6. Composition of Naphtha blend 1

name	weight-%	time [min]	M [g/mole]
n-octane	10.43	4.36	114
1,4-dimethylcyclohexane	8.88	3.87	112
ethylcyclohexane	8.85	5.04	112
methylcyclohexane	8.78	2.96	98
2,5-dimethylhexane	7.55	3.66	114
3-methylhexane	5.63	2.66	100
3-methylheptane	4.35	3.80	114
ethylcyclohexane	3.80	5.17	112
1,2-dimethylcyclohexane	3.21	4.25	112
1,4-dimethylcyclohexane	2.93	4.40	112
2,6-dimethylheptane	2.85	5.93	128
1,3-dimethylcyclopentane	2.68	2.53	98
2,4-dimethylhexane	2.60	3.10	114
2,4-dimethylheptane	2.41	4.91	128
2,5-dimethylheptane	2.28	6.12	128
1-ethyl-2-methylcyclopentane	2.20	4.13	112
n-heptane	2.12	2.39	100
2-methylhexane	2.00	2.30	100
2,3-dimethylhexane	1.64	3.56	114
n-nonane	1.58	6.93	128
2,3-dimethylheptane	1.49	5.70	128
1,2,3-trimethylcyclopentane	1.35	3.34	112
cyclohexane	1.15	2.25	84
1,2,4-trimethylcyclopentane	1.05	3.23	112
1-nonene	1.02	5.47	126
1,3 diethylcyclopentane	0.76	5.30	126
1 ethyl 4 methyl cyclohexane	0.73	6.48	126
1 ethyl 2 methylcyclopentane	0.70	4.06	114
1,3,5 trimethylcyclohexane	0.64	5.53	126
	0.64	5.83	>110
1,1dimethylcyclohexane	0.55	4.00	140
1,2diethylcyclobutane	0.39	4.76	112

Fuel Analysis of Naphtha Blend 2

This blend is said to be based on heavy naphtha components together with 14 to 20 wt-% of aromatics. Figure 22 represents the spectrum corresponding to Naphtha blend 2. As can be seen in this Figure, Naphtha blend 2 contains more components than blend 1. This resulted in a smaller total fraction which could be determined. All peaks representing less than 0.7 wt-% of the blend have been omitted, which results in only 74 wt-% of specified components.
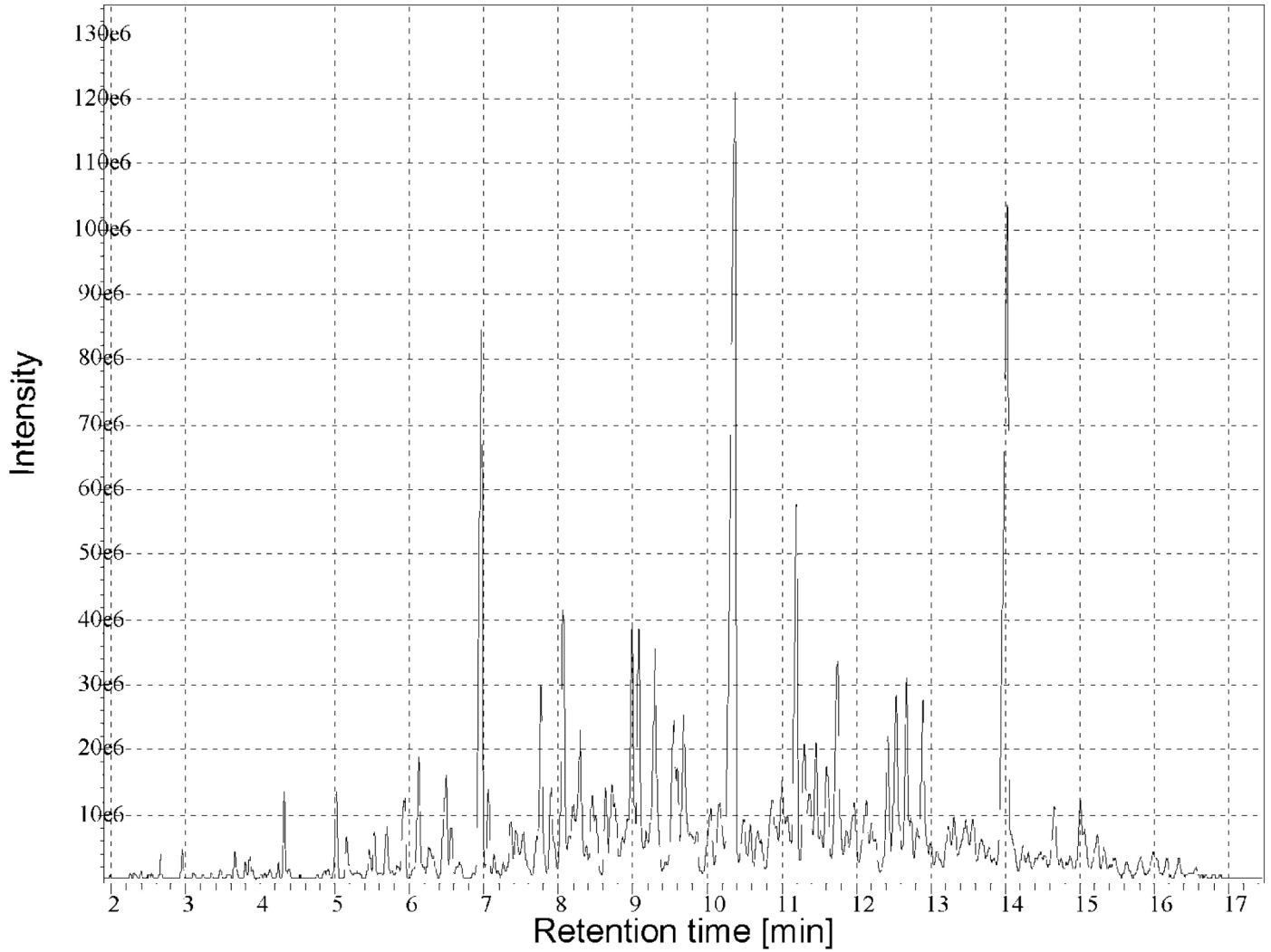

Figure 22. GC-MS spectrum obtained for Naphtha blend 2.

Table 7 is the overview of the retrieved mass fraction of different components. Aromatic components have been denoted in italics. Not all of these aromatic components could be correctly attributed. Therefore, some species have only been determined in terms of hydrocarbon type.

Table 7. Composition of Naphtha blend 2

name	weight-%	time [min]	M [g/mole]
n-decane	11.14	10.38	142
n-undecane	9.14	14.03	156
n-nonane	4.64	6.97	128
2-methyldecane	3.33	11.20	156
3,5-dimethyloctane	2.7	8.99	142
3-methylnonane	2.7	9.30	142
aromatic	2.5	11.75	
2,6-dimethyloctane	2.38	8.07	142
2-methylnonane	2.1	9.08	142
aromatic	2.1	12.54	134
6-methyl-1-octene	1.9	7.77	126
1-isobutyl-3-methylcyclopentane	1.81	9.69	140
3-methyl-decane	1.76	12.90	156
2-methyl-decane	1.75	12.68	156
1,2,3-trimethyl-benzene	1.63	9.55	120
3-ethyl-2-methyl-heptane	1.55	8.29	142
propylbenzene	1.46	8.72	120
-	1.43	10.88	
(2-methylpropyl)-cyclohexane	1.38	11.30	140
5-methyl-decane	1.36	12.43	156
2-methyl-undecane	1.25	15.01	170
3-undecene	1.2	11.46	154
1-methyl-2-propyl-benzene	1.19	11.61	134
(1-methyl-propyl)-benzene	1.1	12.14	134
1-decene	1.07	11.01	140
aromatic	1.06	13.47	
aromatic	1.04	10.17	
-	1.04	14.67	152
1-ethyl-4-methyl-cyclohexane	1.03	6.50	126
naphthalene	1.03	11.98	138
2,5-dimethylheptane	1.01	6.13	128
-	0.92	7.90	126
aromatic	0.92	8.20	120
1-methyl-4-(1-methylethyl)cyclohexane	0.91	10.05	140
butylcyclohexane	0.84	11.37	140
1-ethyl-2-methylbenzene	0.78	10.49	120
2-methyloctane	0.74	5.94	128
1,3,5trimethylbenzene	0.71	8.46	120
1-methyl-4-(1-methylethyl)cyclohexane	0.69	9.60	140