GTLine – Gasoline as a potential CN suppressant for GTL

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ABSTRACT

The main driver to investigate low temperature combustion concepts, such as partially premixed combustion (PPC), is the promise of low particulate matter (PM) and nitric oxide (NOx) emissions. A critical prerequisite for PPC is to temporally isolate the fuel injection and combustion events. In practice, exhaust gas recirculation (EGR) is applied in order to sufficiently extend the ignition delay to that effect. Hereby, in general, higher EGR rates are necessary for fuels with higher cetane numbers (CN).

Against this background, the objective of this paper is to investigate the efficacy, with respect to PM-NOx emissions and engine efficiency, of gasoline as a potential gas-to-liquid (GTL) CN suppressant in various dosages. The performance of the resulting GTLine blend will be evaluated under PPC operating conditions in a heavy-duty direct-injected diesel engine.

Setting aside for a moment any potential practical issues (e.g., flash point, vapor pressure) that fall outside the scope of this study, our data suggest that blending gasoline to otherwise high CN GTL appears to be a promising route to improve not only the efficiency, but also PM and NOx emissions, particularly when operating in PPC mode. Interestingly, this benefit is notwithstanding the high aromaticity of the gasoline compared to GTL.

Given the ongoing dieselization trend and associated surplus of gasoline in many regions, notably Europe, along with the fact that the cost price of gasoline is significantly lower than that of GTL, the proposed GTLine approach promises to be a cost effective way to accommodate GTL in a world wherein low temperature combustion concepts, such as PPC, appear to be really taking off.

1. Introduction

Low temperature combustion (LTC) concepts such as homogeneous charge compression ignition, premixed charge compression ignition and partially premixed combustion (PPC) are seen as promising routes to achieve both low emissions and high efficiency in future compression ignition engines. For practical reasons, including controllability of the combustion phasing and thermal loading of the engine, fully premixed combustion, as is the case for the former two concepts, is considered here to be less promising in real-life applications. This study will therefore focus on the latter combustion principle, PPC.

PPC can be defined as a combustion process in a compression ignition engine, whereby a temporal separation exists between the fuel injection and combustion events, thereby implying that a long ignition delay (ID) is the single most important prerequisite [1–10]. A shared conclusion found in all these studies is that PPC is most readily realized with a low CN fuel, else prohibitively high EGR rates are likely necessary to adequately extend the ID (Table 1). Other key findings from the before mentioned studies, along with associated data on engine specifications, operating conditions and fuel matricies, are presented in Table 2.

In our previous work [13], we evaluated the performance of two Fischer–Tropsch (FT) GTL diesel fuels with CN’s of 52 and 72 in various combustion modes from high (i.e., conventional diffusion) to low (i.e., PPC) temperature regimes. The results demonstrated that, at equal fuel aromaticity, a high CN yields no discernible benefit in terms of PM-NOx trade-off in high temperature combustion modes and even becomes a serious handicap when transitioning into the low temperature regime.

While GTL is best known and often explicitly marketed for its exceptionally high CN, it is possible to produce GTL with lower, more diesel-like values by means of a combination of shortening and branching the paraffinic chains intrinsic to the FT process [13]. While future GTL plant owners might take notice of aforementioned insights, producers of high CN GTL diesel must necessarily add low CN compounds in order to decrease the CN.

Earlier, we investigated the use of ethanol [14] and oxygenated aromatics [15] as potential CN suppressants for GTL. Shell too acknowledged that for some engine operation conditions the otherwise...
high CN of their GTL product should be lowered and therefore proposed to blend in oxygenated and nitrated aromatics [16]. A well known approach to lower the CN of diesel fuel in general is to blend it with low CN fossil or biofuels [11,17–23].

When reviewing Table 2, one practical and relatively low cost fuel looks particularly promising, gasoline. Commonly referred to as Diesel–gasoline as TTropsch GTLine blend of GTL and gasoline–EGR exhaust gas recirculation CR compression ratio EGR exhaust gas recirculation FT Fischer–Tropsch GTL gas-to-liquid GTLine blend of GTL and gasoline

Table 1 Minimum required EGR rate to achieve PPC.

| Source | Fuel | CN  | EGR (wt%) |
|--------|------|-----|-----------|
| [1]    | Gasoline | ±15 | 0         |
| [5]    | Gasoline | ±15 | 5         |
| [11]   | Diesel   | ±56 | 25        |
| [2]    | Diesel   | ±42 | 30        |
| [10]   | Diesel   | ±43 | 40        |
| [12]   | Diesel   | ±54 | 48        |
|        |         |     |           |

calculated in wt.% using both CO2 sensors (intake and exhaust). Gaseous emissions, along with common pressure, temperature and mass flow sensors are logged for 40 s at 20 Hz for each operating point. Data acquisition for in-cylinder pressure and heat-release analyses is achieved by a SMETEC Combi system, which logs in steps of 0.1 crank angle degree for 50 continuous cycles. Variables measured by this system are in-cylinder pressure via an AVL GU21C, calibration value 36,87 pC/bar, intake and fuel pressure, and injector current. For each operating point, the FSN is averaged over three measurements.

2.2. Fuel matrix

In total, five fuels will be evaluated in the engine tests: neat GTL, three GTLine blends (e.g., 10, 20 and 50 vol.% gasoline), and EN590 diesel as a reference fuel. Fuel properties, as measured by ASG-Analytik GmbH Germany, can be found in Table 4.

2.3. Experimental procedure

All tests are conducted with a single injection per cycle, at a fixed engine speed of 1200 rpm, and a constant engine oil and coolant temperatures of 90 and 85 °C, respectively. For all fuels, EGR rates are varied from 0 to 50%. Hereby, the CA50 is kept constant at 10° CA after top dead center by adjusting the start of injection (SOI). An overview of the operating conditions is provided in Table 5.

2.4. Repeatability and accuracy

Various engine operation points have been re-measured on a regular basis in order to assess the repeatability. First, the complete data set has been measured, where after some points were repeated. In all cases, new results were in good agreement with older ones. In earlier work [13], the repeatability of the engine setup and data acquisition system used in this study is discussed in greater detail. Associated data on accuracy is summarized in Table 6.

3. Results

3.1. Rate of heat release

Fig. 2 shows the rate of heat release (RoHR) for all fuels at 15 wt% EGR. As might be expected, when maintaining a constant CA50, lower CN fuels yield a longer ID, higher peak rate and shorter combustion duration.

\[ \text{ID} = \frac{\text{heat released}}{\text{rate of heat release}} \]

Time expressed in CA between SOI and SOC, whereby SOI and SOC are defined as the CAD at which the fuel first enters the combustion chamber, as evidenced by RoHR first going negative as a result evaporative cooling, and the moment at which the RoHR first rises above the 50 J/CAD threshold, respectively.
The RoHR signal can be unimodal (e.g., 50/50 blend; steep rise and fall) or more bimodal like (e.g., 100/0; steep rise and slow fall, even with a plateau), whereby the first and second modes represent the contribution of premixed and subsequent diffusion combustion, respectively.

_Ceteris paribus_, wider RoHR curves are indicative of a more dominant role for diffusion combustion, which tends to be slower than its premixed counterpart. A greater prevalence of diffusion combustion, in turn, is to be expected for high CN fuels, owing to their relatively short ID’s.

Table 2
Summary of literature review on PPC.

| Ref. # | Engine specifications | Operating conditions | Fuels | Key findings |
|--------|-----------------------|----------------------|-------|--------------|
| [1]    | HD, CR = 14           | 4-9 bar IMEP, CR = 14 | Diesel, Gasoline | Engine can run on gasoline in PPC mode with a much higher IMEP while maintaining low NOx and smoke |
| [2]    | HD, CR = 16.1         | 4 bar IMEP, 5-60% EGR | Diesel | The LTC models show a longer liquid-fuel penetration and longer ID for PPC. Moreover, reduced and altered soot formation regions are observed |
| [3]    | LD, CR = 16.1         | 5 bar IMEP, 0-65% EGR | Diesel, Gasoline, n-Heptane, n-Butanol | Soot emissions are strongly related to injection timing Higher intake pressures counteract EGR soot penalty |
| [4]    | LD, CR = 15.5         | 5 bar IMEP, 20-35% EGR | Diesel, Propane | NOx and particulate matter (PM) emissions are reduced with early split injection strategy using high propane ratios |
| [5]    | LD, CR = 14.7         | 3-7 bar IMEP, 5-15% EGR | Gasoline | Double injection improves PPC spark assisted combustion efficiency Lower pilot fuel mass injection reduces CO and UHC emissions |
| [6]    | LD, CR = 16.5         | 1-5 bar IMEP, 0% EGR | Diesel, Ethanol | Combustion mode moves from two-stage to three-stage increasing the premixed ratio |
| [7]    | HD, CR = 17.1         | 4-12 bar IMEP, 0% EGR | Diesel, Methane | Start of injection (SOI) significantly affects emissions in LTC mode Heat release shifts from two-stage to Gaussian profile when advancing SOI |
| [8]    | LD, CR = 15.0         | 6 bar IMEP, 0% EGR | Diesel, DME | Dual injection strategy shows extremely low NOx emissions while maintaining moderate engine output |
| [9]    | LD, CR = 17.5         | 8 bar IMEP, 0-20% EGR | Diesel, n-Butanol | The joint action of a longer ignition delay and a better fuel volatility reduces smoke at moderate injection pressures |
| [10]   | LD, CR = 16.0         | 4 bar IMEP, 40-45% EGR | Diesel | Theoretical analysis of the reaction rates suggests that soot formation is insensitive to equivalence ratio at temperatures below 1500 K |

Table 3
Test engine specifications.

| Engine type | HDDI |
|-------------|------|
| Engine model | XE355C |
| Cylinders | 6, with 1 isolated for research purposes |
| Capacity [l] | 12.6 |
| Bore [mm] | 130 |
| Stroke [mm] | 158 |
| Compression ratio [-] | 15.7 |

Table 4
Fuel properties.

| Property | Unit  | 100/0 | 90/10 | 80/20 | 50/50 | Ref. (EN590) |
|----------|-------|-------|-------|-------|-------|--------------|
| GTL [%V/V] |       | 100   | 90    | 80    | 50    | 0            |
| Gasoline [%V/V] |   | 0     | 10    | 20    | 50    | 0            |
| CN (IQT) [-] |   | 79.8  | 68.2  | 62.6  | 45.5  | 51.6         |
| LHV⁎ [MJ/kg] |     | 44.6  | 44.4  | 44.3  | 43.7  | 42.5         |
| Density⁎ [kg/m³] |   | 777.3 | 773.5 | 769.7 | 758.3 | 835.4        |
| Cw [%wt] |   | 84.6  | 84.6  | 84.5  | 84.4  | 85.1         |
| Hw [%wt] |   | 15.1  | 14.9  | 14.7  | 14.1  | 13.1         |
| Aromatic content, [%V/V] |   | <0.1  | 2.6   | 5.1   | 12.5  | 16.3         |
| AFNstoch⁎ [-] | | 14.9  | 14.8  | 14.7  | 14.5  | 14.2         |
| Sulfur⁎ [mg/kg] |   | 0.5   | 0.9   | 1.3   | 2.4   | 14.2         |

* Blend values calculated from those measured for neat compounds

Table 5
Engine operating conditions.

| Parameter | Unit  | Value |
|-----------|-------|-------|
| Engine speed [rpm] | | 1200 |
| IMEP [bar] | | 5.5-6.0 |
| CASO [CAD aTDC] | | 10 |
| Intake pressure [bar] | | 1.0 |
| Exhaust pressure [bar] | | 1.3 |
| Intake temperature [°C] | | 40 |
| EGR [%w%, CO2/CO2] | | 0-50 |
| Lambda (I) [-] | | 2-1 |
| Injection pressure [bar] | | 1500 |
| Injection duration [μs]/[CAD] | | 950-1050/ 6.9-7.6 |

As the CN drops, however, the premixed phase begins to play a more dominant role in the heat-release event. In fact, particularly for the GTLine fuels with the highest blend ratios of gasoline, the very nature of the RoHR curve changes from bi- to unimodal as the contribution of diffusion combustion wanes and the combustion type gradually shifts into PPC territory.
3.2. Ignition dwell

An important drawback of diffusion combustion is the so-called diesel dilemma or PM-NOx trade-off. Measures to decrease diffusion flame temperature (e.g., by using EGR) tend to curb NOx and promote PM emissions, and vice versa. LTC concepts therefore aim to switch to a new paradigm, wherein this trade-off no longer manifests. To this end, measures are undertaken to increase the role of premixed over diffusion combustion.

The rationale for this is quite straightforward; as fuel is more widely dispersed in the combustion chamber, local equivalence ratios drop and combustion heat is released more homogeneously throughout the cylinder. Former and latter phenomena, in turn, generally result in lower PM and NOx formation rates.

In order to measure the relative importance of both combustion modes, we will evaluate the so-called ignition dwell (IDw) of the combustion event. The IDw is defined as the difference (e.g., expressed in CA) between the end of injection (EOI) and the start of combustion (SOC) (Eq. (1)). Hereby, a negative and positive value signifies classical (i.e., lifted diffusion flame) and PPC diesel combustion, respectively [25].

\[
IDw = CA(SOC) - CA(EOI)
\]  

(1)

Fig. 3 shows the IDw as function of EGR. Data points below the dashed line indicate diffusion combustion is more dominant. Conversely, data points positioned above this line will most likely be void of this combustion mode and are considered to be of the PPC type. As discussed earlier when reviewing the PPC literature and is further evidenced in Fig. 3, all investigated fuels can be pushed into PPC territory by means of EGR, irrespective of their CN.

Nevertheless, as found in literature (Table 1), the data in Fig. 3 demonstrate that far less EGR is required for the lower CN fuels (e.g., those with a higher concentration of gasoline). As can be seen in Fig. 4, a minimum ID (e.g., 7–8 CAD) is required to breach this threshold, with associated EGR levels falling with CN.

Note that for the remainder of this paper, only measurements with IDw values greater than zero will be considered. Complete EGR sweeps are provided in Appendices A–D, and associated data on HC and CO emissions in Appendix E.

### Table 6
Data acquisition accuracies.

| Data type                   | Brand          | Type         | Unit       | Accuracy                        |
|-----------------------------|----------------|--------------|------------|---------------------------------|
| Temperatures                | Omega          | k-type thermocouple | °C         | ±1.1 °C                         |
| Pressures                   | GE PMP 1400    | g/s          | ±0.25% of value |
| Air mass flow               | Micro Coriolis Motion CMF200 | g/s | ±0.35% of rate |
| Diesel mass flow            | Micro Coriolis Motion CMF010 | g/s | ±0.2% of rate |
| In-cylinder pressure        | AVL O2U1C      | bar          | ±0.3 % FS (250 bar) |
| Gaseous analyzer            | HORIBA 7100 DEGR | %, ppm | ±0.5% Full Scale |
| Smoke meter                 | AVL 415S/ Filter method | FSN | ±0.01 FSN (<6 FSN) |

Fig. 2. RoHR as a function of CAD at 15% EGR.

Fig. 3. Ignition dwell as a function of EGR.

Fig. 4. ID as a function of EGR.

3.3. Indicated efficiency

Indicated efficiency is calculated as follows:

\[
\eta_{ind} = \frac{P_{ind}}{(m_{fuel} \cdot LHV)},
\]

(2)

where

- \( P_{ind} \) is the indicated power,
- \( m_{fuel} \) is the mass flow of the fuel, and
- \( LHV \) is the lower heating value.

The penalty of heavy EGR use is quite tangible in Fig. 5. As might be expected, EGR weighs on efficiency. Particularly for rates in excess of 35–40 wt%, efficiency drops rapidly when approaching stoichiometric conditions, coinciding with a rapid increase in both CO and HC emissions (E).

Accordingly, in our data set at least, the higher the CN, the higher the drop in efficiency when operating in PPC mode. Note that the authors have not attempted to further optimize the efficiency by, for example, modifying the CAS50 or intake pressure. Interestingly, comparable efficiencies are found for all fuels at any given EGR level.
3.4. PM and NOx

Notwithstanding taking into account only higher than zero IDw data, aforementioned PM-NOx trade-off is still present in varying degrees for all fuels (Fig. 6). Nevertheless, striking differences can still be observed, with generally more favorable curves found for the lower CN fuels. In fact only the two lowest CN fuels, EN590 and 50/50 GTLine, are found capable of achieving combined Euro V engine out emissions for PM and NOx. The number of fuels drops to one for Euro VI.

For all fuels, there appears to exist a tipping point, whereby the emissions trade-off no longer holds and even goes into reverse. The significance of this tipping point with respect to the validity of the aforementioned IDw boundary between classical and PPC diesel combustion will be discussed in the next section.

4. Discussion

4.1. PPC threshold

The PPC threshold of zero in the IDw equation has been defined in accordance with the literature consensus with respect to the definition of this combustion concept. Judging from the PM-NOx emissions data (Fig. 6), however, a classical trade-off is still clearly present in many data points for which the aforementioned IDw criterion has been met. As the PPC concept is praised by the combustion community for the very absence of this trade-off, its existence here suggests that diffusion combustion may still play a role even well after the EOI.

Although detailed optical engine experiments would be required in order to fully comprehend this discrepancy, a possible contributing factor might be attributable to the last fraction of fuel injected near the EOI still burning as a lifted diffusion flame. Given that the onset of auto-ignition is generally a local event in the spray, this theory would appear to be a promising candidate for further scrutiny in optical experiments.

4.2. Cetane number and aromaticity

Going against conventional wisdom, the two best performing fuels, both with respect to efficiency and emissions, are those with the higher aromaticity and lower CN. This is in line with the conclusions of our previous work [13], which stated that both high CN and aromaticity have a negative impact on aforementioned parameters when operating in PPC mode, although the latter fuel characteristic appears even more detrimental than the former. In other words, purposefully increasing aromaticity with the objective to lower CN appears to be a sound approach for this particular LTC concept.

Looking at the PM-NOx trade-offs shown in Fig. D.1 in the Appendix, it would appear that neat GTL performs worst of all fuels. This trade-off improves with higher concentrations of gasoline and thus even in the face of falling CN and increasing aromaticity. Interestingly, the 80/20 blend and reference fuel show comparable behavior, notwithstanding a lower CN for the latter fuel (e.g., 63 vs. 52, Table 4).

A plausible explanation for this performance parity, achieved here at dissimilar CN values, might be found in the associated aromaticity of the fuels in question. As it happens, the lower CN reference diesel fuel contains more than three times the amount of aromatics as is true for the 80/20 GTLine blend (e.g., 16.3 vs. 5.1%, Table 4).

As concluded in an earlier study [13], given an equal CN, the fuel with the lowest aromaticity will generally yield the more favorable PM-NOx trade-off. It would appear here that a higher aromaticity can be offset by a lower CN, whereby the respective negative and positive impacts on the trade-off cancel each other out. As the results in Fig. D.1 would suggest, this is indeed the case for the reference diesel fuel and the 80/20 GTLine blend.

4.3. Equivalence ratio and temperature

The origin of PM and NOx emissions are often discussed in the context of a $\phi$-T diagram. Herein, $\phi$ and $T$ denote the local fuel/air ratio and temperature, respectively. In an optically accessible engine, these fundamental parameter that lead to NOx and PM, can be determined with (advanced) laser diagnostics. However, for a full metal engine the local $\phi$ and $T$ can not be measured. Nevertheless, when it is assumed that for PPC, ceteris paribus, the impact of CN and EGR on local $\phi$-$T$ conditions is qualitatively similar to that measured for the charge as a whole, some insights might emerge that could help explain aforementioned PM-NOx behavior (Fig. 6, IDw = 0).

In Fig. 7, the bulk equivalence ratio is plotted against the bulk gas temperature, which has been estimated from application of the ideal gas law to the measured pressure and volume history.

From Fig. 7 it becomes clear that temperatures at the SOC are all similar and slightly below 700 K. After the auto-ignition event, temperatures rise rapidly to the respective apices. Here, obvious differences are visible amongst the fuels, as well as a clear trend with CN. As discussed earlier, the higher the CN of the fuel, the higher the amount of EGR required to breach the zero IDw threshold (Figs. 3 and 8).

EGR, which has been cooled to approximately ambient conditions in our experiments, so as to maintain a constant charge temperature, has a cooling effect on the combustion process, owing to the relatively high

2 As determined via air/mass flow meters and in-cylinder pressure sensor.

3 Derived from engine geometry and crank angle position sensor.
specific heats of CO₂ and H₂O. Moreover, given that EGR suppresses oxygen-rich fresh air, the equivalence ratio naturally increases with its dosage.

Combining Figs. 6 and 7, it is fair to assume that the high PM and NOx values seen at IDw = 0 for the high and low CN fuels can at least in part be traced back to a less favorable equivalence ratio and temperature, respectively.

4.4. Indicated efficiency

The main drawback of using high CN fuels in combination with PPC is most evident in Fig. 9. Here, the indicated efficiency is plotted for the various fuels at IDw = 0. A sharp drop in efficiency can be observed for the two fuels with the highest CN (e.g., >60). Note that the penalty is even more pronounced for IDw values in excess of the zero threshold; a fact which, given the previous observation that a higher ignition dwell than IDw = 0 is necessary to have an appropriate PPC border, appears all the more relevant now.

To complicate matters even further, recall that the emissions trade-offs for the higher CN fuels are far less favorable than those measured for the less reactive fuels (Fig. 6).

5. Conclusions

Careful analysis of the experimental engine data for various GTL-gasoline blends in PPC mode has led to the following conclusions:

- The higher the CN, the higher the amount of EGR required to sufficiently extend the ID (Fig. 4) into PPC territory (Fig. 3) and achieve associated low PM-NOx emissions (Fig. 6), whereby the ignition dwell should be somewhat greater than zero.
- A CN higher than 60 eq. EGR rates above 30–40 wt% have a negative impact on indicated thermal efficiency (Fig. 5), most likely as a result of incomplete combustion (Figs. E.1 and E.2).
- Blending in relatively low cost and abundantly available gasoline thus improves the efficiency and emissions behavior of GTL when operating in PPC.

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Appendix A. Ignition delay

![Ignition delay as function of EGR.](image1)

Fig. A.1. Ignition delay as function of EGR.

Appendix B. Indicated efficiency

![Indicated efficiency as function of EGR.](image2)

Fig. B.1. Indicated efficiency as function of EGR.

Appendix C. PM and NOx emissions

![PM emissions as function of EGR.](image3)

Fig. C.1. PM emissions as function of EGR.
Appendix D. PM-NOx trade-off

Appendix E. HC and CO emissions
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