

Contents lists available at ScienceDirect

Fuel

journal homepage: www.elsevier.com/locate/fuel



Full Length Article

Naphtha vs. dieseline – The effect of fuel properties on combustion homogeneity in transition from CI combustion towards HCCI



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ARTICLE INFO

Keywords:
Naphtha
Dieseline
Combustion homogeneity
Diesel engine and stratification

ABSTRACT

The scope of this research study pertains to compare the combustion and emission behavior between naphtha and dieseline at different combustion modes. In this study, US dieseline (50% US diesel + 50% RON 91 gasoline) and EU dieseline (45% EU diesel + 55% RON 97 gasoline) with derived cetane number (DCN) of 36 are selected for experimentation in an optical engine. Besides naphtha and dieseline, PRF60 is also tested as a surrogate fuel for naphtha. For the reported fuel with same RON = 60, the effect of physical properties on combustion homogeneity when moving from homogenized charge compression ignition (HCCI) to compression ignition (CI) combustion is studied.

The combustion phasing of naphtha at an intake air temperature of 95 °C is taken as the baseline data. The engine experimental results show that higher and lower intake air temperature is required for dieseline mixtures to have same combustion phasing as that of naphtha at HCCI and CI conditions due to the difference in the physical properties. Especially at HCCI mode, due to wider distillation range of dieseline, the evaporation of the fuel is affected so that the gas phase mixture becomes too lean to auto-ignite. However, at partially premixed combustion (PPC) conditions, all test fuels required almost same intake air temperature to match up with the combustion phasing of baseline naphtha. From the rate of heat release and combustion images, it was found that naphtha and PRF60 showed improved premixed combustion when compared dieseline mixtures. The stratification analysis shows that combustion is more stratified for dieseline whereas it is premixed for naphtha and PRF60. The level of stratification linked with soot emission showed that soot concentration is higher at stratified CI combustion whereas near zero soot emissions were noted at PPC mode.

1. Introduction

Partially premixed combustion (PPC) is extensively studied for various reasons: better combustion control over homogenized charge compression ignition (HCCI), reduced $\mathrm{NO_X}$ and soot emissions without any compromise in efficiency and improved combustion stratification [1–6]. In PPC, combustion phasing can be controlled by start of injection (SOI), intake air temperature, exhaust gas recirculation (EGR) and compression ratio (CR) [7–9]. Recently, the transition in combustion homogeneity is studied by advancing SOI from CI (compression ignition) to HCCI condition via PPC [10,11]. The combustion phasing is dependent on SOI at CI mode whereas it is dependent on only the intake air temperature at HCCI mode. PPC is intermediate between CI and HCCI condition in that the combustion phasing depends both on SOI and intake air temperature. Thus, it is reasonable to study the transition in combustion homogeneity from CI to HCCI condition via PPC for gasoline like fuels.

When SOI is advanced to early fuel injection timings (HCCI

condition), mixture becomes homogenous with the combustion being governed mainly by mixture kinetics. A recent study achieved PPC and HCCI by varying the intake air temperature and SOI [12]. Combustion was reported to be HCCI like for SOI from -130 to -80 CAD (aTDC) and transition region was noticed between -80 and -45 CAD (aTDC). After -45 CAD (ATDC), fuel is directed into piston and typical CI combustion is realized closer to TDC. In another study, effect of dilution on transition in combustion regime from HCCI to PPC was investigated when SOI is varied from -180 CAD (aTDC) towards TDC [13]. During this experimentation, combustion phasing was kept constant and intake air temperature is varied at each SOI. The study reported that combustion phasing is sensitive to SOI and intake air temperature, while it predominantly depends only on intake air temperature with EGR. While combustion homogeneity was studied for various fuels from HCCI mode to CI mode in metal engines, optical studies to evaluate combustion homogeneity were also performed [14,15]. In these studies, stratification analysis was performed based on the intensity of combustion images and the level of stratification was reportedly reduced as SOI is

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advanced to early injection timings.

Though PPC is achievable with diesel, combustion efficiency is deteriorated at high load conditions due to excess EGR [16]. Later on, gasoline like fuels that are resistant to auto ignition were used in CI engine to achieve PPC [17,18]. Gasoline like fuels are desirable for PPC as it creates a suitable ignition delay period for air fuel mixing process. This decreases the fuel to air equivalence ratio and in-cylinder temperature to simultaneously reduce NO_X and soot emissions [19-21]. It was identified that high research octane number (RON) fuels are not suitable for PPC study at low load condition as auto ignition under lean condition is difficult [22,23]. Given low RON fuels (RON ~ 70), not commercially available in market, is ideal for PPC at all loading conditions, researchers developed dieseline (diesel + gasoline) mixtures [24]. A study demonstrated destabilization of combustion at low load condition as the proportion of gasoline in dieseline mixture is increased [25]. Thus, the percentage of gasoline and diesel in the mixture should be appropriate to have a RON better suited for PPC mode operation. In another study, an extension in operating window of HCCI engines was achieved to demonstrate increased engine stability and reduced peak pressure [26]. The suitable mixture proportion of diesel and gasoline avoided the dependence of trapping exhaust gases or intake air heating at low load condition as opposed to high RON gasoline fuels.

While the idea of utilizing dieseline in PPC mode was proposed few years ago, there is an increasing attention in the use of naphtha (RON $\sim 70)$ in CI engine due to the benefits of less well to wheel CO_2 emissions, reduced fuel consumption and performance [27–29]. Moreover, naphtha with suitable RON and gasoline like fuel properties could emerge as a suitable replacement for dieseline. With higher resistance to auto-ignition, naphtha simultaneously reduces NO_X and soot emission with reduced fuel consumption [30–33]. A recent study investigated the combustion stratification in transition from CI to PPC combustion for naphtha in an optical engine. The analysis revealed increased premixing effect at PPC condition with the reduction of NO_X and soot simultaneously.

The selection of ideal fuel for PPC traversed from gasoline to dieseline to naphtha, given fuels with mid octane ratings (60-70) is conducive to create the desired premixing effect at all operating conditions. While several studies focused on dieseline and naphtha operation in metal engines, this study attempts to investigate them in an optical engine. Dieseline with DCN closer to naphtha (DCN = 36) is prepared to have the same octane rating as that of naphtha. In this study, two different dieseline mixtures with same DCN considered are US dieseline (50% US diesel + 50% RON 91 gasoline) and EU dieseline (45% EU diesel + 55% RON 97 gasoline). Besides naphtha and dieseline, PRF60 (surrogate fuel) is also tested and combustion stratification is analyzed for all these fuels based on the combustion images. Furthermore, this work tries to answer the research questions: 1) Will naphtha, dieseline and PRF60 with same octane rating behave the same during the transition from HCCI to CI via PPC? 2) Naphtha has shorter boiling range, while dieseline has a wider boiling range. How would fuels with different boiling range, physical properties and composition behave at different combustion modes?

2. Methodology

2.1. Test fuels - Composition and properties

The fuels with same DCN = 36 considered in this study are naphtha, US dieseline (50% US diesel + 50% RON 91 gasoline), EU dieseline (45% EU diesel + 55% RON 97 gasoline) and PRF60. While Haltermann supplies naphtha and RON 91 gasoline, US diesel (DCN = 48), EU diesel (DCN = 54) and RON 97 gasoline are supplied by Coryton. The mixture proportion for both the dieseline is selected based on the experimentation in ignition quality tester (IQT). IQT is a constant volume combustion vessel, which accounts for both physical and chemical ignition delay based on ASTM D6890. Fuel is injected

Table 1
Compositional details of all test fuels.

	US Diesel	RON 91 gasoline	EU diesel	RON 97 gasoline	Naphtha
n-paraffins (%)	71.3	13.4	74.1	10	32.4
iso-paraffins (%)		33.7		38.5	36.5
Olefins (%)		6.7		10	2.2
Naphthenes (%)		15.2		5.1	17.4
Aromatics (%)	28.7	22.7	25.9	32.4	11.3
Oxygenates (%)	0	8.2	0	4	0

through a pintle hole nozzle – injector system into heated air. The chamber pressure and temperature are fixed at standard operating conditions (P = 21 bar and T = 853 K). The other specification and details on IQT experimental set up can be found in [34,35]. The ignition delay time (τ_i id) is estimated according to the gradient method proposed in [36]. For τ_i id in the range of 3.1–6.5 ms, DCN is calculated using Eq. (1a) and for values outside this range, it is calculated using Eq. (1b):

$$DCN = 4.46 + (186.6/\tau id)$$
 (1a)

$$DCN = 83.99[(\tau id - 1.512) \land (-0.658)] + 3.547$$
 (1b)

In order to match the DCN with naphtha, IQT test results identifies that 50% RON 91 gasoline and 55% RON 97 gasoline are required to be blended with US diesel and EU diesel, respectively. While DCN is kept constant for all fuels, the composition of fuel changes amongst different fuels. The compositional details of US diesel, EU diesel, RON 91 gasoline and RON 97 gasoline are compared with naphtha and shown in Table 1. While aromatics in naphtha amounts to 11%, the proportions of paraffin's and isoparaffins are higher. Based on the composition of diesel and gasoline fuels, the percentage of aromatics in US dieseline and EU dieseline are found to be 25.6% and 28.5%, respectively. In addition to investigating the effect of physical properties, it is rational to compare the effect of aromatics on combustion and emission test results for fuels with same octane rating. While diesel and naphtha have no oxygen in the fuel composition, the proportion of oxygen in RON 91 gasoline ($O_2 = 8.2\%$) and RON 97 gasoline ($O_2 = 4\%$) is expected to improve the combustion process.

The physical and other properties of naphtha, RON 91 gasoline, RON 97 gasoline, US diesel and EU diesel are listed in Table 2. The H/C ratio for diesel and gasoline fuels is comparable, while it is higher for naphtha. Though diesel is viscous, addition of gasoline with it decreases the viscosity of resultant dieseline mixtures. The boiling range of naphtha falls in gasoline boiling range, while diesel has higher boiling range. In order to improve the lubrication properties of naphtha and PRF60, 500 ppm of lubricating additive is added, while diesel in dieseline mixture provides lubrication. The distillation plot (Fig. 1) show a flat boiling range for dieseline up to 50% recovery, while naphtha has a steady rise in boiling range. When diesel and gasoline are blended, the boiling ranges of US and EU dieseline become wider. After 50% of volume recovered, the dieseline mixture shows an increasing trend in boiling range. With same octane rating, dieseline and naphtha have different boiling range and this is likely to influence the fuel evaporation characteristics. PRF60 show a flat boiling range at most part of the

Table 2
Thermo-physical properties of all test fuels.

	US Dieseline	EU Dieseline	Naphtha	PRF60
Density (kg/m³)	795	787	705	687
Viscosity (mm ² /s)	2.27	2.4	0.6	0.5
Final boiling point (°C)	263	271	152	110
Heating value (kJ/kg)	42,430	42,771	43,360	44,482
H/C ratio	1.86	1.78	2.32	2.26
Cetane number	36	36	36	36

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