

Conventional and Low Temperature Combustion Using Naphtha Fuels in a Multi-Cylinder Heavy-Duty Diesel Engine

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ABSTRACT

The regulatory requirements to lower both greenhouse gases and criteria pollutants from heavy duty engines are driving new perspectives on the interaction between fuels and engines. Fuels that lower the burden on engine manufacturers to reach these goals may be of particular interest. Naphtha, a fuel with a higher volatility than diesel, but with the ability to be burned under traditional mixing-controlled combustion conditions is one such fuel. The higher volatility promotes fuel-air mixing and when combined with its typically lower aromatic content, leads to reduced soot emissions when compared directly to diesel. Naphtha also has potential to be less energy-intensive at the refinery level, and its use in transportation applications can potentially reduce CO₂ emissions on a well-to-wheels basis.

This work investigates the combustion characteristics and emissions of two naphtha fuels (Naphtha 1: RON59; Naphtha 2: RON69) together with one ultra-low sulfur diesel (ULSD) in a model year (MY) 2013, six-cylinder, Cummins ISX15, heavy-duty truck engine. Engine geometric compression ratio (CR) was at 17.3 in the present study to promote partially premixed combustion.

Engine tests were focused on 1375 RPM, a medium speed, over a load sweep from 5 to 15 bar BMEP. At all tested operating conditions using the production hardware set, both naphtha fuels showed a substantial reduction in soot levels at an equivalent level of NO_x emissions and fuel efficiency. At 15 bar BMEP, cylinder pressure and temperature are sufficiently high to suppress the reactivity difference between ULSD and the naphtha fuels. Consequently, the three test fuels exhibited similar ignition delay times, but the naphtha fuels were still observed to produce less soot than ULSD. Under mixing-controlled combustion, this is likely due to their higher volatility, lower viscosity, and less aromatic content. At 10 bar BMEP with a less reactive thermal environment, naphtha fuels started to show longer ignition delays while retaining a soot benefit over ULSD. 3-D CFD combustion simulation at 10 bar BMEP suggests the higher volatility and lower viscosity of naphtha facilitate better air utilization and a reduced presence of fuel-rich regions in the combustion chamber. When further reducing engine load to 5 bar BMEP, the ignition delay difference between naphtha fuels and ULSD became more notable. As a result, compared to ULSD, the naphtha fuels exhibited markedly enhanced premixed combustion and substantially reduced soot emissions.

The benefits of the naphtha fuels allowed the engine to be recalibrated from 3-4 g/hp-hr NO_x (production base level) down to 1.5-2 g/hp-hr over the 12-mode non-idle SET steady-state test cycle while maintaining "soot-free" (smoke $\leq$ 0.2 FSN) operation and diesel-equivalent fuel efficiency.

In addition to conventional mixing-controlled combustion, partially premixed compression ignition (PPCI) low temperature combustion (LTC) operation was studied. Both early and late injection PPCI approaches were investigated. Through late injection coupled with high injection pressure, LTC operation was achieved up to 10 bar BMEP for Naphtha 1 and 11 bar BMEP for Naphtha 2. Under high EGR dilution, Naphtha 2, with its lower reactivity, had longer ignition delay times than Naphtha 1, thereby resulting in lower soot and a moderately improved LTC operation range.

CFD-guided combustion analysis identified two PPCI concepts at 10 bar BMEP: PPCI1 at 0.79 g/hp-hr NO_x and PPCI2 at 0.19 g/hp-hr NO_x. PPCI1 used single injection, while PPCI2 utilized two injections. For PPCI2, in addition to a main injection occurring at -9 °ATDC, a post injection with small fuel quantity was employed at 7 °ATDC. This effectively enhanced the late-stage air utilization and led to improved fuel efficiency over PPCI1.

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INTRODUCTION

Increasingly stringent regulations for criteria pollutants and greenhouse gas emissions have driven the development of high efficiency, clean compression ignition (CI) engines in the commercial transportation sector. To date combustion systems for on-road CI engines have been optimized primarily for diesel fuel. In the US market, diesel fuel typically has a cetane number (CN) between 40 and 45 and consists of hydrocarbons with 10-24 carbon atoms [1]. Due to the physical properties of diesel fuel, injection timing initiated auto-ignition can be controlled robustly over wide ranges of pressure, temperature, and equivalence ratio. However, diesel ignition quality is such that it typically does not allow for sufficient fuel-air mixing before the start of combustion. Therefore, diesel combustion is largely mixing-controlled due to the short ignition delay time and the nature of diffusion combustion leads to high NO_x and soot emissions.

To meet the US EPA 2010 heavy-duty NO_x (0.2 g/hp-hr) and particulate matter (0.01 g/hp-hr) emissions regulation, it has become necessary to implement urea-based selective catalytic reduction (SCR) and diesel particulate filter (DPF) devices for on-highway diesel engines. Consequently, the cost and complexity of the engine system have appreciably increased over time. The continuing pursuit of improved fuel efficiency (i.e., lower greenhouse gas emissions) under mixing-controlled combustion is likely to keep putting more stress on the aftertreatment system and may increase engine total fluid consumption. Innovative clean combustion modes that can lead to significantly reduced engine-out emissions while maintaining high fuel efficiency may play an increasingly important role for future engine system development.

In recent years, research efforts have been dedicated to developing a partially premixed compression ignition (PPCI) combustion concept [2, 34], aimed to simultaneously reduce engine-out NO_x and soot emissions by attaining sufficiently premixed, low-temperature combustion. Compared to homogeneous charge compression ignition (HCCI), PPCI tailors the fuel injection strategy to generate advantageous levels of fuel stratification across the engine cylinder, thereby providing an effective means to control the progression of combustion heat release.

In essence, to harness the PPCI combustion concept, the engine thermal environment needs to be carefully designed to work together with the fuel's reactivity. This typically involves high levels of EGR dilution and boosted air pressure and is sometimes combined with variable valve actuation (VVA) [4] to limit effective compression ratio. Due to its high reactivity, diesel fuel operating under PPCI becomes particularly demanding and therefore can be achieved only at light loads without significantly sacrificing fuel efficiency.

To facilitate a wide range of PPCI operation, Kalghatgi and coauthors [5, 6, 7] proposed and conducted extensive studies on using low reactivity gasolines and similar fuels. Ignition delay times were substantially lengthened when using these low reactivity fuels. This not only facilitated sufficient fuel-air mixing, but also allowed for improved control over combustion phasing and maximum pressure rise rate (MPRR). As a result, high-load, fuel-efficient PPCI operation has been demonstrated in single-cylinder heavy-duty CI engines [8]. However, cold-start and low-load operation become challenging for such high octane gasoline fuels. Unstable combustion and

deteriorated combustion efficiency have been reported [9, 10] and the resulting high HC and CO emissions pose a significant challenge to the exhaust oxidation catalyst when encountering the low exhaust temperatures generated through low-load PPCI operation.

Recently, low octane fuels in the gasoline boiling range have shown good potential for widening PPCI's operating range. Johansson and co-authors [8, 11] investigated gasoline fuels with a variety of octane ratings and sensitivities for PPCI operation in a heavy-duty single cylinder engine. Under highly diluted and boosted conditions, PPCI operation was achieved from idle (600 rpm, 2.5 bar IMEPg) to a maximum load of 26 bar IMEPg at 1250 rpm using a RON70 gasoline when relaxing the MPRR limit to 15-20 bar/CAD at medium-to-high loads [11].

Naphtha fuels with lower octane and cetane have also drawn increasing attention for PPCI operation. Without significant modifications to engine hardware, researchers from different groups have demonstrated naphtha PPCI combustion with low engine-out NO_x and soot emissions [12, 13, 14, 15, 16, 17]. These low cetane naphtha fuels can potentially be sourced from gasoline production streams and require less processing at the refinery level. Consequently, the production of naphtha fuels has potential to be less energy intensive and using them in the commercial transportation sector could help reduce well-to-wheel CO₂ production while mitigating the projected increase in future transportation demand for diesel fuels [18].

Thus far, most heavy-duty naphtha combustion studies have been conducted using single cylinder research engines under PPCI operation. It is worth noting that air system boundary conditions in single cylinder engines are not as constrained as in production engines and are often times adjusted beyond the capability of production hardware to deliver sufficiently-premixed, low temperature combustion conditions.

To help bring naphtha combustion concepts into reality, this study investigates the combustion characteristics of two naphtha fuels: Naphtha 1:RON59, and Naphtha 2: RON69, in a Model Year (MY) 2013 Cummins ISX15 heavy-duty diesel engine at 17.3:1 compression ratio. One objective of the study is to better understand the practical implications of using naphtha fuels under the modern, high efficiency, mixing-controlled combustion operating conditions that are widely used by heavy-duty engine manufacturers. To that end, engine testing was conducted over a wide range of engine-out NO_x levels over a load sweep and covered the non-idle, steady-state, SET (Supplemental Emissions Test) 12-mode test points. A second objective is the exploration of the injection strategy requirement, performance, and limitations for naphtha PPCI low temperature combustion when using a production engine air system.

In addition, 3-D computational fluid dynamics (CFD) combustion simulation was conducted to gain insight into the spray and combustion behavior of naphtha fuels. The models were also used to help identify engine thermal boundary conditions and design injection strategies for high efficiency, clean PPCI operation at 17.3 compression ratio.

EXPERIMENTAL SETUP

Engine and Instrumentation

Aramco purchased a MY2013, six-cylinder, Cummins ISX15 heavy-duty diesel engine for this study due to its widespread use in North American heavy truck fleets. It is equipped with a common-rail fuel injection system capable of 2500 bar fuel injection pressure. The air system consists of a single-stage variable geometry turbocharger (VGT), a cooled high pressure EGR loop, and a charge air cooler (CAC). The engine compression ratio (CR) used in this study is 17.3. Detailed engine specifications can be found in [Table 1](#) and a schematic of the engine air system layout is detailed in [Figure 1](#). The cooling system and air system restrictions were tuned to be representative of those encountered in production vehicles.

Table 1. Engine Specifications

Displacement Volume	14.9 L
Number of Cylinders	6
Bore	137 mm
Stroke	169 mm
Compression Ratio	17.3
Diesel Fuel System	2500 bar common-rail
Air System	single-stage VGT high pressure EGR loop with cooling charge air cooler
Engine Ratings	336 kW @ 1800 rpm 2375 N-m @ 1000 rpm

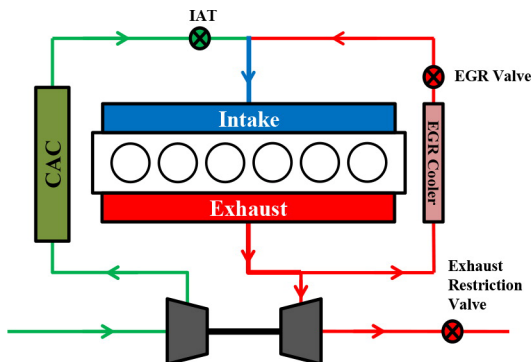


Figure 1. Engine air system schematic

Crank angle (CA) resolved cylinder pressure measurements were acquired using Kistler 6067C water-cooled pressure transducers in all six engine cylinders. Fuel flow was measured using a Coriolis flow meter. To prevent the boiling of naphtha fuels in the fuel return lines, extra cooling of the return line was implemented. A laminar flow element was used to measure the intake air flow. Gaseous exhaust emissions of THC, CO, CO₂ and O₂ were measured using FID (0-3500 ppm for THC), NDIR (0-2500 ppm for CO; 0-20% for CO₂), and Paramagnetic (0-25% for O₂) analyzers manufactured by California Analytical Inc (CAI). Intake CO₂ concentration was also measured for the calculation of EGR rate. NO_x emissions were measured using a chemiluminescent detector (CLD) manufactured by Eco Physics while soot emissions were measured in terms of filter smoke number (FSN) via an AVL 415SE Smoke Meter with a measurement range of 0-10 FSN and a detection limit of 0.002 FSN.

Fuels

The fuels tested in this study include one ultra-low sulfur diesel (ULSD) and two naphtha fuels. Naphtha 1 has a RON of 58.8 (CN33.7) and is a straight-run naphtha, meaning that it is derived directly from crude oil through distillation without any further processing. The selection of Naphtha 1 is intended to represent a large percentage of naphtha fuels produced from refineries worldwide. Naphtha 2 was formulated to target a RON of 70 (CN30), which has been shown in the literature to offer a wide PPCI operation range with a good balance between MPRR control at high load and combustion stability at low load [11].

To alleviate potential fuel system wear when using the low lubricity naphtha fuels, a lubricity additive was blended into each naphtha fuel at a dosage rate of 200 ppm. This concentration was determined through a screening test that applied the high-frequency reciprocating rig test with a wear scar pattern limit equal to US market diesel fuel. Detailed properties of the three test fuels are provided in [Table 2](#).

Test Conditions

NO_x sweeps were conducted at a medium engine speed, 1375 rpm, over a load range from 5 to 15 bar BMEP. 10 bar BMEP at 1375 rpm is representative of typical highway cruising conditions for this heavy-duty engine. During the NO_x sweeps, injection timing and fuel pressure were kept constant and the EGR valve was fully open to reduce the flow restriction across the EGR system. The desired NO_x targets were attained by carefully controlling the EGR rate through manipulation of the turbocharger VGT position.

Following the NO_x sweeps, the non-idle, Supplemental Emissions Test (SET) defined steady-state points were measured with the naphtha fuels at a calibrated level of 1.5-2 g/hp-hr NO_x.

Finally, PPCI low temperature combustion (LTC) operation was studied for the two naphtha fuels by conducting start of injection (SOI) sweeps over a load range from 5 to 11 bar BMEP using the production engine air system hardware. Detailed engine operating conditions are listed in [Table 3](#).

Table 2. Properties of test fuels

		ULSD	Naphtha 1	Naphtha 2
IBP	°C	176	32	38
T10	°C	206	58	70
T50	°C	249	94	101
T90	°C	303	124	132
FBP	°C	337	140	163
Dry Vapor Pressure	psi	-	8.83	6.07
Density at 15.56 °C	g/mL	0.841	0.705	0.726
Kinematic viscosity	cSt	2.25	0.58	0.59
Aromatics	vol%	29.7	9.1	16.3
Olefins	vol%	4.3	0.4	0.5
Saturates	vol%	66.0	90.5	83.2
Sulfur	ppm	11.9	19.3	20.8
H/C ratio	mol/mol	1.834	2.124	1.998
Cetane Number (CN)		43.7	33.7	30
RON	-	30.1*	58.8	68.7
MON	-	-	57.9	65.8
AKI	-	-	58.4	67.2
Lower heating value	MJ/kg	42.818	43.363	43.493

* Calculated from the equation $CN = RON * (-0.39) + 55.5$ in Ref. [19]

Table 3. Engine operating conditions

Speed [rpm]	1375				
Load [bar BMEP]	10	15	5	5...11	5...20
Tests	NOx (EGR) Sweep			LTC	SET
BSNOx [g/hp-hr]	1...3	1...3.5	0.5...3	0.2	2
Fuels	ULSD Naphtha 1 Naphtha 2			Naphtha 1 Naphtha 2	Naphtha 1
Injection Strategy	Single Injection				
SOI [°ATDC]	-9	-7	-6	-15...9	
Fuel Pressure [bar]	1450	1900	1300	1300...2500	
EGR Rate [%]	19...28	15...23	24...41	33...47	
IMP [bar, abs]	1.82...1.85	2.39...2.66	1.19...1.33	1.30...2.35	

COMPUTATIONAL MODEL

3-D CFD, closed-cycle (i.e., from intake valve closing to exhaust valve opening), sector combustion simulation was conducted in the current study to gain insight into the spray-charge air mixing, combustion and emissions characteristics for naphtha. Viable PPCI low temperature combustion strategies were also explored and evaluated at 1375 rpm and 10 bar BMEP. All combustion simulations were performed at a compression ratio of 17.3. The pistons used in this study retained the same spray targeting as the MY2013 production CR18.9 pistons. Geometric features of these pistons were slightly modified from the MY2013 production pistons to facilitate better air utilization at a reduced CR of 17.3

Model Description

A commercial CFD software package, CONVERGE, was used for the 3-D in-cylinder combustion simulation with detailed chemical kinetic calculations. The base grid size was 1mm, while the smallest grid was at 0.25 mm with fixed nozzle embedding and adaptive mesh refinement (AMR) on velocity and temperature. Table 4 lists the primary CONVERGE sub-models used in this study.

Table 4. Primary CONVERGE sub-models [21]

Spray Models	
Injection	Blob
Evaporation	Frossling
Collision	NTC
Break-up	KH-RT
Combustion and Emissions	
Solver	SAGE
Fuel Surrogate	<i>n</i> -Heptane for <i>ULSD</i>
	Primary Reference Fuels (PRF) for <i>Naphtha</i>
Chemical Kinetic Mechanism	Chalmers <i>n</i> -Heptane mechanism [22] for <i>ULSD</i>
	Liu et al. PRF mechanism [23] for <i>Naphtha</i>
NOx	4 species and 13 reactions [23, 24]
Soot	Hiroyasu-NSC
Turbulence	RNG <i>k</i> - ϵ
Wall Heat Transfer	O'Rourke & Amsden
Grid Size	
Base	1 mm
Smallest	0.25 mm

In this CFD study, *n*-heptane was used as a surrogate for ULSD, while primary reference fuels (i.e., *n*-heptane and *iso*-octane) were selected to represent naphtha fuels. The reduced *n*-heptane mechanism developed at Chalmers University of Technology contains 42 species and 283 reactions [22]. For the reduced PRF mechanism developed by Liu et al. [23], there are 44 species and 139

reactions. NOx emissions were predicted using a reduced mechanism that contains 4 species and 13 reactions [24]. The two-step Hiroyasu-NSC (Nagle and Strickland-Constable) approach was used to simulate soot formation and oxidation. Acetylene was used as the inception species in the soot model.

Model Validation

The ULSD and naphtha models were validated against experimental data from mixing-controlled combustion operation at 1375 rpm and 10 bar BMEP. For naphtha, the KH spray break-up model time constant was adjusted to match the level of premixed combustion observed from engine experimental results. As shown in Figures 2 and 3 as well as in Table 5, good agreement was attained between the experimental data and the model predictions in terms of cylinder pressure trace, NOx, and soot emissions.

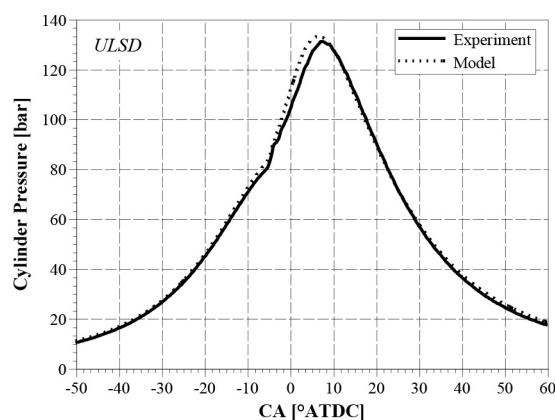


Figure 2. Comparison in-cylinder pressure trace for ULSD at SOI of -9 °ATDC

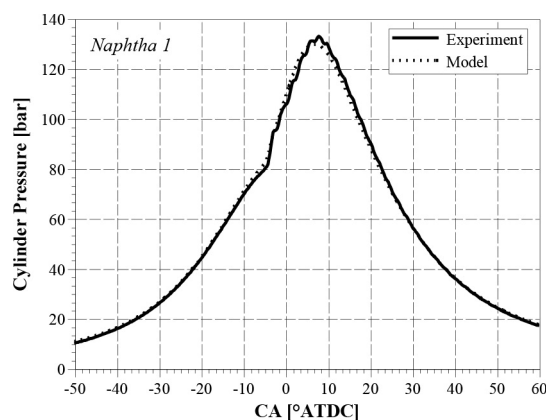


Figure 3. Comparison in-cylinder pressure trace for Naphtha 1 at SOI of -9 °ATDC

Table 5. Comparison in gross indicated NOx and soot emissions

	Emissions	Experiment	Model
ULSD	NOx [g/ihp-hr]	1.79	2.07
	Soot [g/ihp-hr]	0.05	0.06
Naphtha 1	NOx [g/ihp-hr]	1.67	1.88
	Soot [g/ihp-hr]	0.02	0.02

RESULTS AND DISCUSSION

NOx Sweep at 10 Bar BMEP

At 10 bar BMEP, engine-out NOx was swept from 1 to 3 g/hp-hr and the start of injection (SOI) was kept constant at -9 °ATDC with the fuel injection pressure set at 1450 bar.

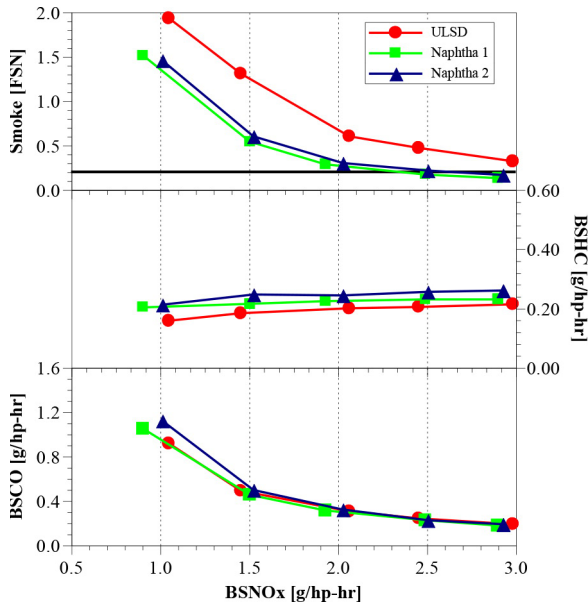


Figure 4. Engine emissions for ULSD and naphtha fuels at 10 bar BMEP

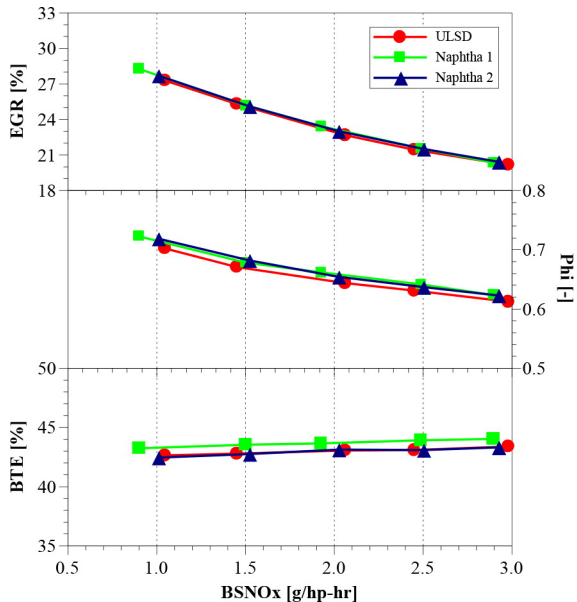


Figure 5. Engine air system boundary conditions and fuel efficiency for ULSD and naphtha fuels at 10 bar BMEP

As seen in Figure 4, the naphtha fuels produced notably less soot compared to ULSD. In particular, the naphtha fuels were able to achieve “soot-free” operation (smoke ≤ 0.2 FSN) at an engine-out NOx of 2.5 g/hp-hr, a target that could not be attained by ULSD at a 3 g/hp-hr NOx range. This emissions benefit is of practical significance in terms of reducing aftertreatment fluid consumption,

protecting the longevity of the aftertreatment devices, and meeting the increasingly stringent future emissions regulations. The key factors that may contribute to the soot benefit of naphtha fuels will be discussed in detail later.

Figure 4 also shows that the naphtha fuels and ULSD had similar levels of hydrocarbon (HC) and CO emissions, indicating combustion loss is not a concern when using naphtha fuels in this engine at medium to high loads. In Figure 5, it can be observed that the air system operating boundary conditions and fuel efficiency are fairly comparable between naphtha fuels and ULSD.

Figure 6 provides a look into the combustion characteristics of naphtha fuels compared to ULSD at 17.3 compression ratio. As can be seen for all three fuels, combustion was initiated through fuel premixing after a short ignition delay and then proceeded predominantly via mixing-controlled combustion. In this study, the ignition delay (ID) is defined as the period from the start of injection to the crank angle at 2% of cumulative heat release (CA02), while combustion duration (CD) is defined as the period (CAD) between 2-90% of cumulative heat release. As seen in Figure 6, naphtha fuels had slightly longer ignition delay times and exhibited more pronounced premixed combustion when compared to ULSD. The enhanced premixed combustion for naphtha fuels could be attributed to both the longer ignition delay times and the high volatility of the fuel. Naphtha 2 has the most pronounced premixed combustion with the longest ignition delay, while Naphtha 1 exhibited the earliest CA50 and the shortest combustion duration due to possessing the highest volatility among the three test fuels.

The longer ignition delay times for naphtha fuels are mainly due to their lower reactivity since they have cetane ratings 10-13.7 lower than ULSD. Note that in modern diesel engines, fuel ignition quality (or cetane number) affects ignition delay largely in the negative temperature coefficient (NTC) region, where low temperature chain-branching reactions compete with chain propagation channels. This leads to differences in cool flame behavior and consequently affects the temperature progression [25]. It is well-established that reaction system pressure has a significant impact on NTC behavior and ignition delay [26]. With an increase of pressure, the low-to-intermediate temperature fuel oxidation chemistry is accelerated, resulting in a faster transition across temperature regimes and consequently leading to diminished NTC behavior. Therefore, the impact of fuel ignition quality on ignition delay can be expected to become increasingly weaker with the increase of pressure. This has in fact been observed and reported in shock tube and rapid compression machine experiments at pressures up to 50 atm [27, 28].

In light of the rather large cetane number difference between naphtha fuels and ULSD, the slight increase of ignition delay times for naphtha fuels indicates that the pressures and temperatures encountered at medium-to-high load conditions in modern diesel engines are sufficiently high to suppress the difference in fuel reactivity among the test fuels. Note that at 10 bar BMEP, the pressure at SOI is around 72 bar, while the corresponding temperature is around 1000 K.