

An Experimental Study of Diesel-Fuel Property Effects on Mixing-Controlled Combustion in a Heavy-Duty Optical CI Engine

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ABSTRACT

Natural luminosity (NL) and chemiluminescence (CL) imaging diagnostics are employed to investigate fuel-property effects on mixing-controlled combustion, using select research fuels—a #2 ultra-low sulfur emissions-certification diesel fuel (CF) and four of the Fuels for Advanced Combustion Engines (FACE) diesel fuels (F1, F2, F6, and F8)—that varied in cetane number (CN), distillation characteristics, and aromatic content. The experiments were performed in a single-cylinder heavy-duty optical compression-ignition (CI) engine at two injection pressures, three dilution levels, and constant start-of-combustion timing.

If the experimental results are analyzed only in the context of the FACE fuel design parameters, CN had the largest effect on emissions and efficiency. Low-CN fuels had higher indicated specific nitrogen oxides ($ISNO_x$) emissions, but up to 9 and 33 times lower smoke emissions, ~ 0.01 filter smoke number (FSN), at 80 MPa and 180 MPa injection pressure, respectively, independent of intake oxygen concentration, relative to the high-CN fuels. Low-CN fuels had lower combustion efficiency due to their higher hydrocarbon and carbon monoxide emissions, but there was no clear trend regarding fuel effects on fuel-conversion efficiency. Higher aromatic content appeared to have a secondary effect on NO_x and smoke emissions. There was no clear effect of 90% distillation temperature (T90) on emissions or efficiency at the operating conditions investigated in this work.

The results of the study indicate that neither emissions, efficiency nor operational parameters directly correlated with CN, aromatic content, or T90, independently at all operating conditions. On the other hand, the experimental results were better explained by the ignition delay differences between the fuels. The ignition delay correlated well with the lift-off length, H , at a constant injection pressure independent of the charge dilution. The corresponding equivalence ratio at the lift-off length, $\phi(H)$, affected the chemical reactions downstream of H and production of the fuel-rich partially reacted mixture inside the fuel jet. Additionally, the smoke emissions of the long-ignition-delay fuels provided further evidence that $\phi(H)$ below ~ 2 results in mixing-controlled combustion that does not produce soot.

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INTRODUCTION

Mixing-controlled combustion plays an important role in modern diesel engines, particularly in larger-displacement engines operating at moderate and higher loads. This combustion mode can produce high levels of particulate matter (PM) and/or nitrogen oxides (NO_x). Low-temperature premixed combustion strategies, such as Homogeneous Charge Compression Ignition (HCCI) and Premixed Charge Compression Ignition (PCCI), are capable of increasing fuel-conversion efficiency while minimizing NO_x and soot formation [1,2,3,4]. In these strategies, fuel is oxidized in a largely premixed combustion mode. Excessive pressure-rise rates and emissions can limit the applicability of premixed-combustion strategies at high loads, such that high-load conditions of a drive cycle are often still achieved through mixing-controlled combustion strategies.

Selective catalytic reduction (SCR), lean- NO_x trap (LNT), diesel particulate filter (DPF), and diesel oxidation catalyst (DOC) technologies are efficient at reducing tailpipe emissions. Hence, they are the exhaust-gas after-treatment technologies most commonly used to alleviate NO_x , soot, hydrocarbon (HC), and carbon monoxide (CO) emissions from modern diesel engines. The negative aspects of after-treatment technologies relate to increased fuel consumption, higher initial as well as operating costs, higher sensitivity to abnormal engine operation, and the need for fuel sulfur levels less than 15 ppm for adequate catalyst life. One alternative to after-treatment is in-cylinder emissions reduction, which includes the low-temperature combustion strategies mentioned above, as well as recent advances in engine design, turbochargers, high-pressure fuel-delivery systems, and exhaust-gas recirculation (EGR). In-cylinder emissions-reduction methods have thus far proven less effective in reducing both NO_x and soot emissions to current and future legislated levels, even though in-cylinder emissions-reduction methods are more cost effective. As a result, modern diesel engines currently use a combination of in-cylinder and after-treatment methods.

Successful application of emissions-reduction technologies also depends on obtaining a better understanding of fuel-property effects on diesel combustion. Variability in diesel-fuel properties (e.g., cetane number (CN), volatility, and aromatic content) increases the difficulty of engine calibration for optimal performance and minimal engine-out emissions (i.e., fuel effects on injection quantity, air/fuel ratio, combustion phasing, EGR composition, and cold start). The open-loop control strategies of current diesel engines are not capable of adapting to major changes in fuel properties. It would be beneficial if future engines had automatic engine-calibration optimization for fuel variability. This capability would become more important as new alternative fuels with different properties are introduced into the market [5].

A large number of fuel-effects studies have been performed to provide answers, mostly addressing CN, aromatic-content, and distillation-temperature effects, but the correlations among fuel

properties make it difficult to identify the effects of changing a single fuel property at a time [6,7,8,9]. At the same time, the engine-research literature contains a number of studies describing contradictory fuel-property effects. Studies have shown that fuels with increased aromatic content have higher NO_x [6, 7, 9] and soot emissions [7, 9]. On the other hand, increased mono-aromatic content can lower the 90% distillation temperature (T90). As some studies have shown that lower T90 reduces NO_x [10] and soot emissions [9], if the fuel chemical composition is not properly accounted for it could imply that raising the aromatic content could be beneficial for lowering NO_x and PM emissions, a result that contradicts the previously mentioned studies. The main reason for the contradictory results is believed to be the large variety of fuels and engines used in these studies, which greatly increases the complexity of interactions between the engine hardware, operating conditions, combustion mode(s), and the chemical and physical properties of the fuels.

To help researchers study the effects of fuel CN, aromatic content, and volatility on diesel combustion, the Fuels for Advanced Combustion Engines (FACE) Working Group of the Coordinating Research Council (CRC) Advanced Vehicles, Fuels, and Lubricants (AVFL) Committee designed a matrix of nine reference diesel fuels [11]. The FACE diesel fuel matrix was designed so that eight of the nine fuels form the corners of a cubic space defined by variations in CN from 30 to 55, T90 from 270 to 340 °C, and aromatic content from 20 to 45 vol%, while the ninth fuel has property values near the center of the design space. The sulfur and olefin contents of the FACE fuels were capped at 15 ppm and 4 vol%, respectively. The CN, aromatic content, and T90 are not the only parameters that vary among the FACE fuels, but it is important to understand their effects on emissions and efficiency because the FACE design parameters are some of the same parameters used by energy companies and engine manufacturers to characterize fuel quality.

To date, the majority of studies employing the FACE fuels have been performed under low-temperature combustion conditions characterized by a large premixed-burn fraction [12,13,14,15,16]. While somewhat influenced by differences in mixture preparation (i.e., pre-vaporized versus directly injected fuel), these studies showed that low-CN and low-T90 fuels increased fuel-conversion efficiency and lowered PM, but raised NO_x , HC, and CO emissions when compared with the high-CN fuels, mostly through their effect on combustion phasing and duration. A higher T90 value increased HC and CO emissions, while a higher aromatic content increased NO_x emissions.

Only one other study found in the literature studied the FACE fuels under conventional diesel-combustion conditions, i.e., those characterized by mixing-controlled combustion. De Ojeda et al. [17] studied CN, aromatic-content, and T90 effects up to 14.6-bar gross indicated mean effective pressure (gIMEP) engine load in a 0.744 liter, single-cylinder, common-rail diesel engine. CA50 was kept constant at 12.5 crank angle

degrees (CAD) after top-dead-center (ATDC), while intake-oxygen content was swept for lower NO_x levels. Intake boost and injection pressure were load-adjusted to match production-engine values. Low-CN fuels presented NO_x and soot emissions benefits for all engine loads, but with no reference to fuel consumption it is difficult to assess their effect on fuel-conversion efficiency, especially at higher loads when their longer ignition delays can further decrease combustion efficiency. The combustion efficiency of low-CN fuels decreased at low loads due to larger HC and CO emissions. For similar CN and aromatic content, lower T90 was correlated with reduced soot emissions.

The objective of this paper is to increase the understanding of fuel-property changes on mixing-controlled combustion using a subset of the FACE diesel fuels. This is accomplished by employing high-speed optical imaging of combustion natural luminosity and OH^* -radical chemiluminescence, combined with measurements of in-cylinder pressure, engine-out emissions, combustion and fuel-conversion efficiencies, and injection rate. The experiments were performed using a common-rail fuel injector with a 2-hole tip to minimize the effects of interactions between adjacent jet flames, thereby making the results less hardware-dependent. Although engine loads were low due to the use of the 2-hole tip, the fuel-injection rate per orifice and the duration of injection used were representative of moderate-load operation with an 8-hole tip. The start of injection (SOI) and injection duration were selected to obtain predominantly mixing-controlled combustion (i.e., a premixed-burn fraction $< \sim 20\%$) for all tested fuels at constant start of combustion (SOC) timing and engine load. This approach was selected to minimize the secondary effects that different in-cylinder pressures and temperatures during combustion may have on combustion characteristics and engine-out emissions. The experimental results are presented in the context of the FACE fuel-design parameters with the understanding that there are significant property differences among the FACE fuels in addition to their CN, aromatic content, and T90 levels.

EXPERIMENTAL SETUP

Engine and Fuel System

The experiments were performed in a single-cylinder version of a Caterpillar heavy-duty engine modified to provide optical access to the combustion chamber. A schematic and the primary specifications of this optical engine are provided in Figure 1 and Table 1, respectively. The major differences between the optical engine and a comparable production engine relate to the piston bowl, which has a flat bottom, vertical walls, and a larger land above the top compression ring. The larger top-ring land allows optical access through a notch in the bowl-rim and prevents the rings from riding over the cylinder-wall windows. The above differences lead to a lower geometric compression ratio (CR) of 12.3:1 for the optical engine versus ~ 16 :1 for a comparable production engine. To compensate for the lower CR, the intake

temperature and pressure are elevated to closely match the conditions in the production engine over the crank-angle range during which combustion occurs [18].

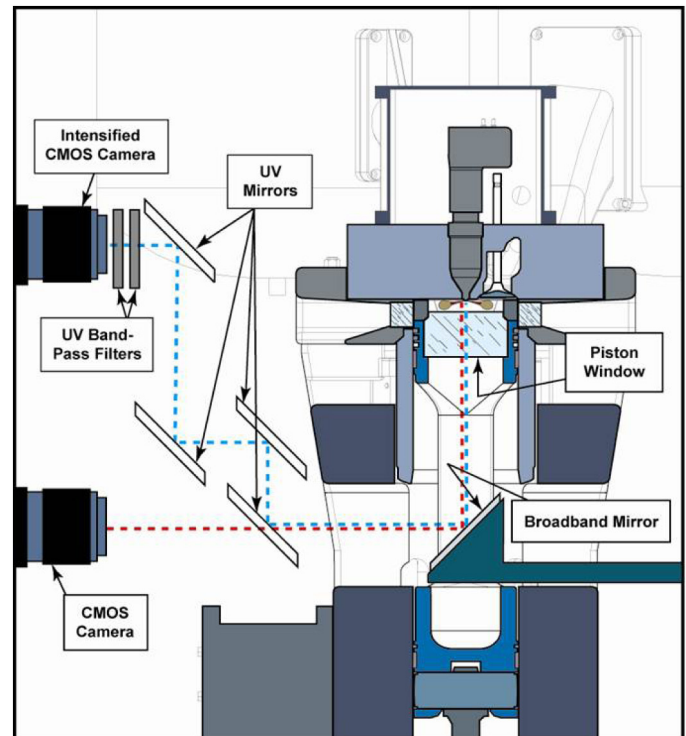


Figure 1. Optical engine schematic. Top and bottom cameras are used for chemiluminescence and natural luminosity imaging, respectively.

The optical engine was skip-fired with only one injection event every 5 engine cycles in these experiments. This approach was used to lower the magnitude of the thermal transient that results from switching between motored and fired operation, and the risk of window failure due to the corresponding thermal and mechanical stresses [19]. Because skip-firing affects the exhaust-gas composition, real EGR was not used. Instead, EGR was simulated by adding N_2 and CO_2 to the dry intake air. The resulting dry-air/ N_2 / CO_2 composition was designed to match the intake- O_2 mole fraction and specific heat at constant pressure of the charge-gas mixture at -10 CAD ATDC in a metal engine with comparable displacement and mass of fuel injected per orifice operating at 17.5% EGR (baseline). Using this approach, the residual exhaust-gas that remains trapped in the combustion chamber after a fired cycle is replaced with fresh intake charge (i.e., air, N_2 , and CO_2 for simulated EGR) during the subsequent motored cycles. The heat rejection from the combustion chamber to the coolant is lower due to the skip-fired operation and short run-times, which requires the optical engine to use a heater to maintain a realistic and constant coolant temperature.

Fuel delivery was accomplished using a high-pressure common-rail fuel-injection system, the principal components of which include a diaphragm pump (Newport Scientific, Model 46-16060) and a near-production Caterpillar electronically actuated solenoid-operated fuel injector. The fuel-wetted

internals of the pump are fabricated from stainless steel, Kalrez, or Teflon, making the system suitable for handling a wide range of conventional and unconventional fuels having high corrosivities, low viscosities, or other properties that can cause conventional piston-type pumps to fail.

Table 1. Optical-engine specifications.

Research engine type	Single-cylinder
Cycle	4-stroke CIDI
Valves per cylinder	4
Bore	125 mm
Stroke	140 mm
Intake valve open ^a	32° BTDC exhaust
Intake valve close ^a	153° BTDC comp.
Exhaust valve open ^a	116° ATDC comp.
Exhaust valve closed ^a	11° ATDC exhaust
Connecting-rod length	225 mm
Piston-pin offset	None
Piston-bowl diameter	90 mm
Piston-bowl depth	16.4 mm
Squish height	1.5 mm
Swirl ratio ^b	0.59
Displacement	1.72 liters
Compression ratio (geometric)	12.3:1

^aAll valve timings are for 0.03 mm lift

^bMeasured at the Caterpillar Technical Center using an AVL swirl meter

Table 2. Common-rail fuel-injector specifications.

Injector type	Cat CR350
Injector tip style	Mini-sac
Number of injector orifices	2
Orifice diameter (nom.)	110 μ m
Orifice length-to-diameter ratio	8
Hydro-erosion	20 $\pm$ 2%
Included spray angle	140°

Fuel-injector specifications are provided in Table 2. X-ray tomography was used to confirm the orifice diameter, length-to-diameter ratio, and included spray angle listed in Table 2. Figure 2 presents typical injection-rate profiles for the 2-hole tip at injection pressures of 80 MPa and 180 MPa, as measured using a momentum-based rate-of-injection meter developed at Sandia [20].

A flush-mounted, water-cooled pressure transducer (AVL Model QC32C) was used to measure cylinder-pressure every 0.5 CAD. Gas analyzers (California Analytical Instruments, Series 600) measured CO, CO₂, O₂, NO_x, and HC emissions. Engine-out particulate emissions were measured using both a smoke meter (AVL Model 415S) and a prototype laser-induced incandescence instrument (see Figure 5 of [21] and [22]). Reference [23] describes in detail the procedures used for cylinder-pressure data acquisition and how the skip-fired exhaust-gas measurements were converted to values similar

to those that would be obtained if the engine was operated in a continuous-fired mode. References [18, 19] provide further details of the experimental setup and procedures.

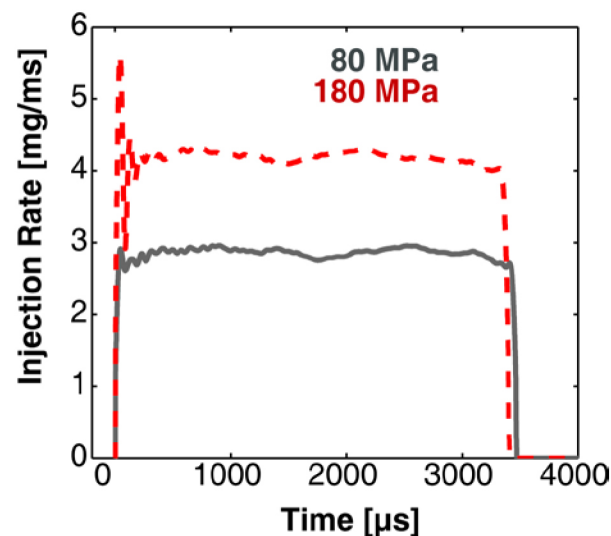


Figure 2. Injection-rate profiles (per injector hole).

Fuels

The present study investigated four of the nine diesel fuels designed by the CRC FACE Working Group, together with a 2007 ultra-low-sulfur #2 diesel certification fuel having properties that are more representative of diesel fuels currently in the US market. The non-yellow-colored fuels (1, 2, 6, 8 and CF) in Figure 3 were used in this study. All of these fuels were produced by the Chevron Phillips Chemical Company (CPCChem). All FACE fuels used in this study came from the first batch of fuels produced by CPCChem. In this paper, the FACE fuels will be denoted Fx, where x is the numerical designation of the fuel (e.g., FACE Diesel #1 is denoted F1). The emissions-certification fuel is denoted CF.

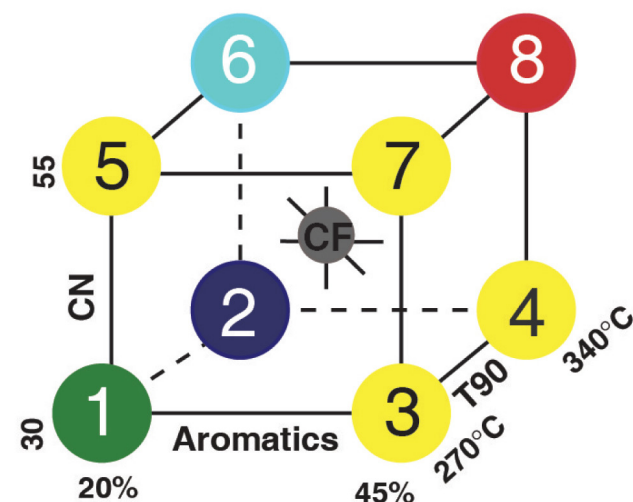


Figure 3. The positions of the 2007 #2 ULSD certification fuel (CF) and FACE diesel fuels studied in this work (F1, F2, F6, and F8) within the FACE diesel fuel property matrix.

Table 3. Tested fuel properties. FACE and certification diesel-fuel properties are from [11] and [24], respectively.

Parameter	ASTM method	Cert fuel ULSD #2	FACE fuel no.			
			1	2	6	8
Specific gravity [g/ml]	D4052	0.848	0.8084	0.8037	0.8411	0.8688
Cetane number	D613	43.3	30.3	28.4	53.7	49.5
Distillation temperature [°C]	D86					
T10		211	184	181	223	248
T50		253	200	193	275	273
T90		310	284	346	339	342
Carbon [mass %]	D5291	87.04	85.74	85.71	86.25	87.40
Hydrogen [mass %]	D5291	13.03	13.82	13.94	13.62	12.42
Molar C/H ratio		0.561	0.521	0.516	0.532	0.591
Sulfur [ppm]	D5453	14.4	1.8	0.4	8.2	1.7
Aromatics (by SFC)	D5186					
1-ring [mass %]		20.7	24.6	22	17.1	21.8
2 or more rings [mass %]		9.0	2	1.3	4.4	22.6
Total [mass %]		29.7	26.6	23.3	21.5	44.4
Net heat of combustion [MJ/kg]	D240	42.9	42.8	43.2	42.8	42.2
Kinematic viscosity @ 40°C [cSt]	D445	2.3	1.7	1.8	3.1	3.2

Table 4. FACE fuel pairings, where ↗ indicates a difference in fuel design parameter, while “High” and “Low” indicate a similarity in design parameter between pairs of fuels.

FACE Fuel pair	CN	Aromatic %	T90
F1 vs. F2	Low	Low	↗
F2 vs. F6	↗	Low	High
F6 vs. F8	High	↗	High
F1 vs. F8	↗	↗	↗

The selection of F1, F2, F6, and F8 enabled the study of the effects of T90 at low CN and aromatic content (F1 vs. F2), CN at low aromatic content and high T90 (F2 vs. F6), aromatic content at high CN and high T90 (F6 vs. F8), and all variables at their low and high values (F1 vs. F8). Tables 3 and 4 present the measured property values for these fuels and the FACE fuel pairings, respectively. Table 3 also shows that even though only one design parameter changes between each fuel pair, other fuel characteristics also are different between two fuels in a pair. For example, some FACE diesel fuels had specific gravity and kinematic viscosity outside the range of the specification for U.S. #2 diesel fuel (0.840-0.855 g/ml and 2.0-3.0 cSt, respectively). High-aromatic fuels had higher specific gravities, while the high-CN and high-T90 fuels had the highest kinematic viscosities. Chemical composition also affected fuel lubricity. With the exception of F8, no FACE diesel fuel met the U.S. #2 diesel lubricity specification.

The compositions of the FACE fuels had to be adjusted from typical market diesel fuels to obtain the desired property values. The rest of this paragraph contains a summary of fuel

characteristics from [11]. Analysis in [11] suggests that branched alkanes were added to F1 and F2 to lower their CNs. F1 and F2 also contain more than 20 wt% C₈-C₁₀ mono-aromatics (see Figs. 6.6 and 6.7 in [11]), which is different from typical market diesel fuels. F1 exhibits an n-alkane profile that is skewed toward C₁₁, but continues to C₂₀ (see Fig. 4.12 of [11]). F2 has a bi-modal distribution of hydrocarbons, being mostly made up of very volatile mono-aromatics and iso-alkanes plus some alkanes (C₂₂ and C₂₃) with boiling points in the range of 345-375 °C (see Fig. 4.13 of [11]). Contrary to typical diesel fuel, it contains no hydrocarbons distilling in the range from 230 to 340 °C. F6 contains a large fraction of n- and iso-alkanes distributed from ~ C₈ to > C₂₂, with the higher-molecular-weight alkanes contributing to the high-T90 of this fuel (see Fig. 4.21 of [11]). F8 was blended from a narrow selection of normal and branched alkanes from C₁₃ to C₁₇ with high concentrations of diphenyl compounds (see Fig. 4.25 of [11]), which are 2-ring aromatics that are not very representative of the types of aromatics found in refinery diesel fuels. Mono-aromatics make up the majority of the first 10% of the distillation. Similar to F2 and F6, higher-molecular-weight alkanes (C₂₁ to C₂₃) make up the last 10% of the distillation.

In addition to the information found in [11], Figure 4 shows updated compositional data from recent two-dimensional gas chromatography analyses done at CanmetENERGY [25]. Figure 4 indicates that, similar to commercial diesel fuels, the FACE diesel fuels are predominantly composed of normal and branched alkanes, cycloalkanes, and aromatics, with near-zero alkene content [26]. In terms of aromatic content, Figure 4 indicates that, except for F8, the fuels used in the current study primarily contain mono-aromatics. F8 was the only FACE

diesel fuel whose di- plus tri-aromatic content was greater than its mono-aromatics. A heavy aromatic fraction labeled “diphenylalkanes” in [11] was used in F8 and to a lesser extent in F6 to enhance aromatic content. The higher aromatic content of F8 also could have increased the deviation between the target and actual CN (i.e., F8 has a CN ~50 instead of 55) because aromatic compounds typically have lower CNs. References [11] and [25] provide many further details about the compositions of the fuels used in this study.

A detailed look at the CF and FACE fuel properties and compositions revealed that a number of important fuel properties were correlated with each other or with fuel composition. For example, using data from Figure 4 and [11], Figure 5 indicates that CN has some degree of correlation with normal and iso-alkanes, >2-ring cycloalkanes, and 1-ring aromatics.

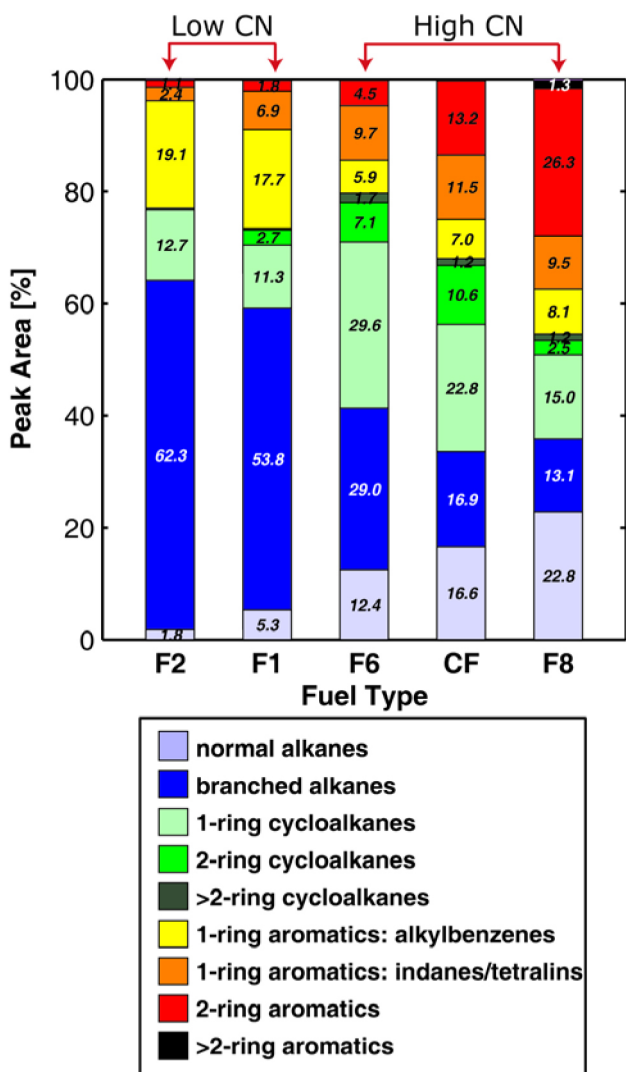


Figure 4. Fuel composition determined using reverse-column two-dimensional gas chromatography [25].

Figure 6 shows that T90 does not fully characterize the distillation curves for the FACE diesel fuels. F1 and F2 have similar distillation curves from T20 to T80, but different T90

values. A similar observation can be made for F2, F6, and F8, which have similar T90 values, but there is a difference of as much as 100 °C between the distillation curves for F2 and F6/F8 from the initial boiling point to T80.

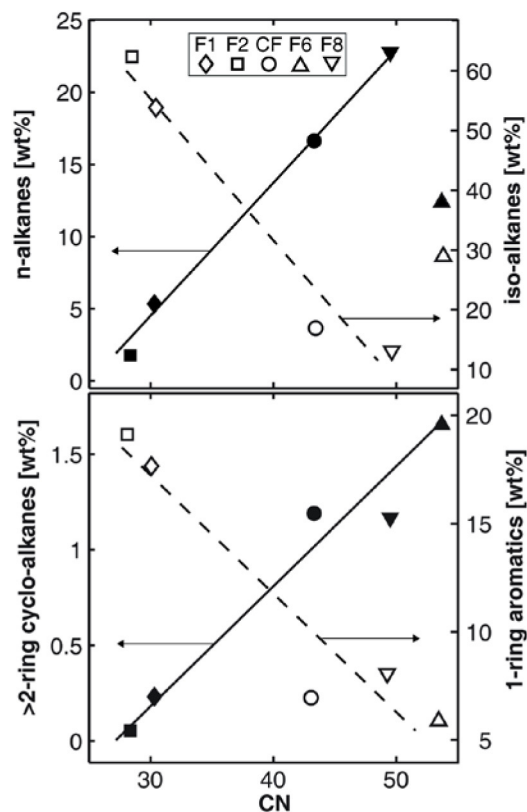


Figure 5. Suggested correlations between CN and fuel chemistry (data from [11] and [25]).

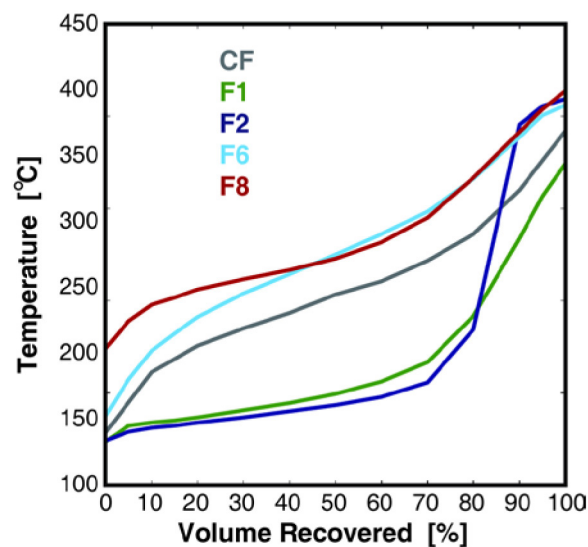


Figure 6. Distillation curves of studied fuels.

There are other significant differences between F1 and F2 in addition to the T90 differences that the FACE matrix was designed to study. These include (but are not limited to) differences in the levels of indanes/tetralins, total aromatics, and 2-ring cycloalkanes. F2 and F6, while chosen to show the