

# Combustion Studies with FACE Diesel Fuels: A Literature Review

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## ABSTRACT

The CRC Fuels for Advanced Combustion Engines (FACE) Working Group has provided a matrix of experimental diesel fuels for use in studies on the effects of three parameters, Cetane number (CN), aromatics content, and 90 vol% distillation temperature (T90), on combustion and emissions characteristics of advanced combustion strategies. Various types of fuel analyses and engine experiments were performed in well-known research institutes. This paper reviews a collection of research findings obtained with these nine fuels.

An extensive collection of analyses were performed by members of the FACE working group on the FACE diesel fuels as a means of aiding in understanding the linkage between fuel properties and combustion and emissions performance. These analyses included non-traditional chemical techniques as well as established ASTM tests. In a few cases, both ASTM tests and advanced analyses agreed that some design variables differed from their target values when the fuels were produced.

This review summarizes six collective engine experimental studies performed with FACE fuels with various types of engines under a range of conditions. Engine experiments under various operating conditions were performed with a 0.517-liter HCCI single cylinder engine (SCE) and 4-cylinder 1.9-liter high-speed direct-injection (HSDI) diesel engine at Oak Ridge National Laboratory (ORNL), 0.744-liter DI diesel SCE at Navistar, and 2.44-liter DI diesel SCE and Cooperative Fuel Research (CFR) engine at National Research Council Canada (NRCC). The engine operating conditions of the six experimental programs can be categorized into one conventional diesel combustion (CDC), two homogeneous-charge compression ignition (HCCI), and three low-temperature combustion (LTC) modes. All six programs agreed that CN exhibited the strongest impacts on both combustion and emissions among the three design variables. As expected lower CN fuels exhibited longer ignition delay, which provided longer mixing periods. However, effects of aromatics were rather inconsistent in the engine experiments. In the HCCI studies higher aromatics fuels exhibited higher soot but little effect on NO<sub>x</sub>. In the two LTC studies higher aromatics and lower CN fuels exhibited higher NO<sub>x</sub>, whereas the aromatic impact on soot production was negligible. T90 effects were similar to those of CN, but at a lesser magnitude. Higher T90 fuels exhibited longer ignition delay in all experiments.

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## INTRODUCTION

Many investigations have been carried out in order to find effects of cetane number (CN), aromatics, and distillation temperature on emissions and performance of conventional diesel engines. CN effects are relatively well understood compared to the other two parameters. High CN fuels typically exhibit shorter ignition delay, which is beneficial under conventional diesel combustion (CDC). However, longer ignition delays associated with lower CN fuels may provide an advantage under premixed charge combustion mode by lengthening mixing times. Lower T90 fuels vaporize faster, but auto-ignite at higher temperature, which are known

to be beneficial traits in terms of mixing enhancement and soot reduction under Low Temperature Combustion (LTC) mode. Meanwhile, aromatics effects on advanced combustion techniques are still not well established.

Nakakita et al. found that aromatics exhibited higher soot/PM tendency under all speed and load conditions. It was also found in their study that cyclo-paraffins exhibited higher PM formation tendency than iso- or n-paraffins. [1] Nikolic et al. found that higher C/H ratio aromatics increased NO<sub>x</sub> and higher C/H ratio poly-aromatics further increased NO<sub>x</sub>. [2] Kee et al. found that fuels containing aromatics exhibited higher NO<sub>x</sub> formation tendency in their RCM and total-gas

sampling device experiments. [3] They explained the higher  $\text{NO}_x$  formation tendency originated from the fact that aromatics were decomposed to heavy saturate hydrocarbons during the initial combustion phase, which caused difficulty on further decomposition to  $\text{CH}_4$  during the following diffusion combustion phase. This gave longer  $\text{NO}_x$  formation duration with aromatic-containing fuels.

There are many implementations of advanced combustion including fuel injection and ignition control strategies and the design of the associated engine hardware. Gaining an understanding of the effects of fuel properties on this breadth of combustion strategies is complex. One pathway for gaining this information is through the use of a common matrix of research fuels in multiple combustion processes. The fuels for advanced combustion engines (FACE) working group was chartered as a Coordinating Research Council (CRC) working group, with the objective of putting forward designed matrices of fuels that could be used in combustion and emissions control programs. The FACE working group has provided a matrix of experimental diesel fuels for researchers to utilize in studies of the effects of three parameters, cetane number (CN), aromatics content, and distillation temperature (T90), on combustion and emissions characteristics of advanced combustion strategies. Detailed chemical analysis and advanced characterization techniques were performed by three national laboratories and a private research institute to characterize the nine FACE fuels. [4] ASTM Standard tests measured physical and chemical properties of the fuels. The ignition quality tester was additionally employed for ignition characterization. Various advanced characterization techniques, namely, gas chromatography-mass spectrometry (GC-MS), two-dimensional GC (2-D GC), GC-Field Ionization Mass Spectrometry (GC-FIMS), and Nuclear Magnetic Resonance (NMR), provided more detailed hydrocarbon categorization of the fuels. For instance, GC-MS revealed that isoparaffins were added into four of the fuels, presumably to lower their CN, whereas  $\text{C}_{10}$  monoaromatics were substituted into four of the fuels to increase aromatics content. Four of the fuels also exhibited higher concentration of  $\text{C}_{22}$  and  $\text{C}_{23}$  paraffins, which seemed to be added in order to raise their T90. Both ASTM tests and advanced analyses agreed that some design variables were somewhat off the target values.

To date, six collective engine experimental studies have been performed with FACE fuels by researchers working independently with various types of engines under various conditions. Engine experiments were performed with a 0.517-liter HCCI single cylinder engine (SCE) and a 4-cylinder 1.9-liter high-speed direct-injection (HSDI) diesel engine at Oak Ridge National Laboratory (ORNL), 0.744-liter DI diesel SCE at Navistar, and 2.44-liter DI diesel SCE and Cooperative Fuel Research (CFR) engine at National Research Council Canada (NRCC). [5, 6, 7, 8, 9, 10] The engine operating conditions of the six experimental studies

can be categorized as one conventional diesel combustion (CDC), two HCCI, and three LTC modes.

Several technical terms relating to the combustion process will be used in this paper to discuss and compare the results of the six engine studies. These terms are related to the location and duration of the combustion event with respect to the top-dead-center of the expansion stroke as measured by the rotational angle of the crankshaft. For example, the location of ignition is often defined as the point where the combustion event has consumed 5% of the injected fuel. This point is represented as CA05, meaning the crank angle location at which 5% of the fuel has burned, with the number representing the percentage of the fuel burned at that point. If the 5% burn point occurs exactly at top-dead-center, the CA05 result is zero. The CA05 point would be a negative number if it occurred prior to top dead-center, and a positive number if it occurred after top dead-center. Two other important timing parameters are CA50 and CA90, which represent the location at which 50% and 90% of the fuel has burned, respectively. Combustion duration is also an important process parameter, and is defined in terms of the number of degrees of crankshaft rotation between two combustion locations. For example, the duration between the 5% burn point and the 50% burn point is represented as CA05-50. Similarly, the duration of combustion from 50% to 90% fuel burnout is represented as CA50-90.

## EXPERIMENTAL SETUPS

Engine specifications and operating conditions for the several studies are listed in [Table 1](#). One case was classified as CDC mode, whereas two cases were as HCCI mode and three as LTC mode. Note that the only case with a multi-cylinder engine (MCE) among the six studies that are introduced in this review is LTC (MCE 1.9L). Experimental engines of the three LTC cases were equipped with common-rail high pressure injection system, whereas the one of the CDC case employed the unit-injector system, which was the standard fuel injection system of the engine, a Hatz 1D50Z. The engine employed in the HCCI (SCE 0.5L) study was equipped with an air-blast assist port-fuel injector and vaporizer in the intake system. Although the CDC (SCE 0.5L), HCCI (SCE 0.5L), and LTC (SCE 0.744L) studies investigated under various load conditions, only the low load cases were included in the present review in order to examine comparable conditions from the other combustion studies. It should be noted that in the LTC (SCE 0.744L) study injection timing was varied in order to achieve CA50 at 12.5° ATDC at all load conditions. The last three cases shown in [Table 1](#) were classified as LTC because all three studies used direct-injection and fuel injection locations that were too near firing TDC to produce a truly homogeneous fuel/air mixture.

## FUEL MATRIX

The FACE diesel fuel matrix included 9 fuels, ideally arranged about a cubic design space with two levels for each

**Table 1. Engine specifications and operating conditions.**

| Case                    | Displacement (L/cylinder) | CR    | Fuel Delivery | Nozzle   | Speed (RPM) | MEP (Bar) | EGR (%) | Intake O <sub>2</sub> (Vol%) | Variable          |
|-------------------------|---------------------------|-------|---------------|----------|-------------|-----------|---------|------------------------------|-------------------|
| <b>CDC (SCE 0.5L)</b>   | 0.517                     | 10.5  | Unit Injector | --       | 1800        | 2~6       | 0       | --                           | M <sub>fuel</sub> |
| <b>HCCI (SCE 0.5L)</b>  | 0.517                     | 10.5  | Atomizer      | --       | 1800        | 2~4       | 0       | --                           | T <sub>int</sub>  |
| <b>HCCI (SCE CFR)</b>   | 0.612                     | 9~15  | Air-Assist    | --       | 900         | 4         | 60      | --                           | CR                |
| <b>LTC (MCE 1.9L)</b>   | 0.477                     | 17.5  | CRDI          | 7-H 148° | 1500        | 2.6*      | 41      | --                           | SOI <sub>C</sub>  |
| <b>LTC (SCE 2.44L)</b>  | 2.44                      | 16.25 | CRDI          | --       | 900         | 3.5*      | 60      | --                           | SOI <sub>C</sub>  |
| <b>LTC (SCE 0.744L)</b> | 0.744                     | 16.2  | CRDI          | 6-H 156° | 1671        | 5.5~14.6  | --      | 13~17                        | EGR               |

\*MEP values for these studies are brake values; the remaining studies used indicated values.

design variable, plus a center fuel that was similar to marketplace diesel fuel in the US. When the fuels were blended, some design targets could not be met, causing some discrepancies between the target and as-blended values. These discrepancies between target and actual values of the three variables are listed in [Table 3](#). The most noteworthy differences are the aromatics of FACE #1, and CN of FACE #7 and #8. Individual control variables' effects were evaluated based on the two selected pairs that can isolate the other two control variables. The two pairs of each control variable are listed in [Table 4](#).

**Table 2. FACE diesel fuel property targets and actual values.**

| FACE Fuel # | Cetane Number |        | Aromatics (%) |        | T90 (°C) |        |
|-------------|---------------|--------|---------------|--------|----------|--------|
|             | Target        | Actual | Target        | Actual | Target   | Actual |
| 1           | 30            | 29.9   | 20            | 26.1   | 270      | 284    |
| 2           | 30            | 28.0   | 20            | 23.1   | 340      | 346    |
| 3           | 30            | 32.0   | 45            | 50     | 270      | 274    |
| 4           | 30            | 28.4   | 45            | 40.7   | 340      | 338    |
| 5           | 55            | 54.2   | 20            | 22.2   | 270      | 274    |
| 6           | 55            | 53.3   | 20            | 21.2   | 340      | 339    |
| 7           | 55            | 44.3   | 45            | 46.2   | 270      | 267    |
| 8           | 55            | 50.0   | 45            | 43.5   | 340      | 342    |
| 9           | 43            | 45.0   | 33            | 37     | 320      | 319    |

**Table 3. Selected pairs of FACE fuels by control variable.**

| Variable  | Parameters of Effects               | Pair# | Face# |   |
|-----------|-------------------------------------|-------|-------|---|
| CN        | Ignition Delay                      | 1     | 1     | 5 |
|           | Combustion Duration                 | 2     | 2     | 6 |
| Aromatics | Soot                                | 3     | 2     | 4 |
|           | NOx                                 | 4     | 6     | 8 |
| T90       | Ignition Delay, combustion duration | 5     | 1     | 2 |
|           | Soot, CO                            | 6     | 5     | 6 |

## CONVENTIONAL DIESEL COMBUSTION (CDC) MODE

In the one CDC study that was identified, the commanded start of injection (SOI<sub>C</sub>) was fixed at -8°ATDC for all test cases. Fueling rate was gradually increased in order to increase IMEP from approximately 2 to 6 bars. The three different CN groups exhibited quite different trends in CA50 as shown in [Figure 1](#). At a given IMEP, the low CN fuels exhibited a later CA50 than the high-CN fuels, as expected. As the IMEP was increased by increasing fueling rate, the

overall burn duration increased for the high CN fuels, causing the CA50 location to shift further after TDC. The CA50 timing for this engine exhibited a lower sensitivity to CN effects as load increased, and hence, the difference in CA50 timing between low- and high-CN fuels decreased as the IMEP increased.

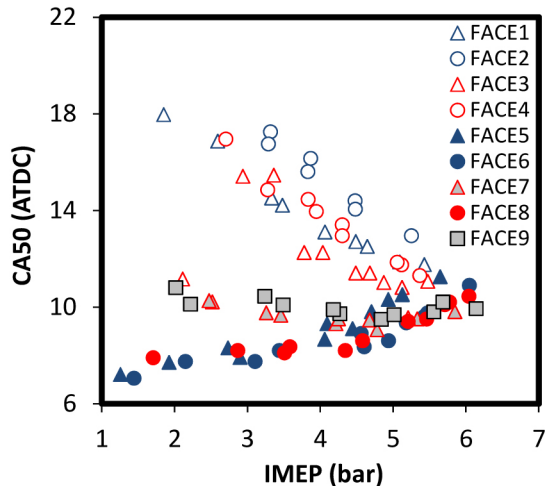


Figure 1. CA50 vs. IMEP for CDC in the SCE (0.5L) study

## CN and T90 Effects

Figure 2 and figure 4 show that CN exhibited substantial impacts on ignition delay and combustion duration in the CDC mode, as expected. The high- and low-CN level fuels exhibited distinctive traits in terms of ignition delay and combustion duration. Low-CN fuels exhibited higher sensitivity in ignition delay to increases in IMEP than high-CN fuels as seen in Figure (2). Figure (3) shows that IMEP increase elongated CA00-50 burn duration in high-CN fuels, but shortened CA00-50 in low-CN fuels. However, both high- and low-CN fuels exhibited similar combustion duration (CA00-90), while showing linear relationship with IMEP as seen in Figure (4).

The low-CN pairs exhibited greater T90 effects as shown in Figure 2. High-T90 fuel, FACE#2, exhibited substantially longer ignition delay than FACE#1. This ignition delay trend seems to indicate that at high-CN levels the cetane effect is dominant, however, as the CN level decreases fuel distillation characteristics increase in significance. The low-T90 fuels exhibited lower FSN levels compared with the high-CN fuels as shown in Figure 5.

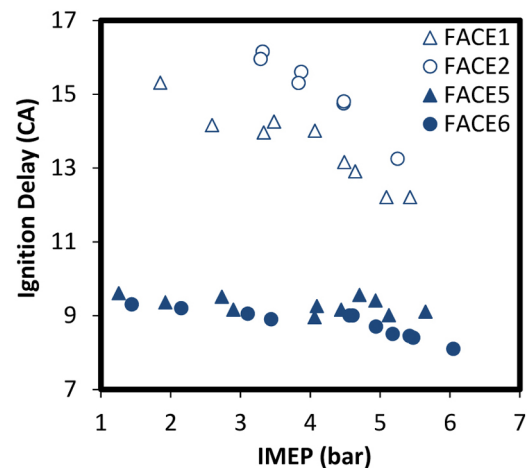


Figure 2. Ignition delay vs. IMEP for CDC in the SCE (0.5L) study.

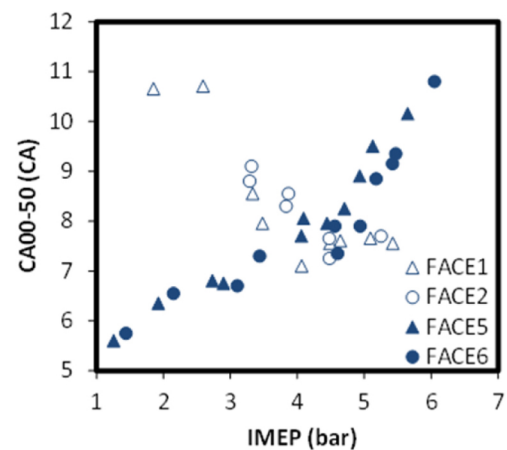


Figure 3. 50% burn duration vs. IMEP for CDC in the SCE (0.5L) study.

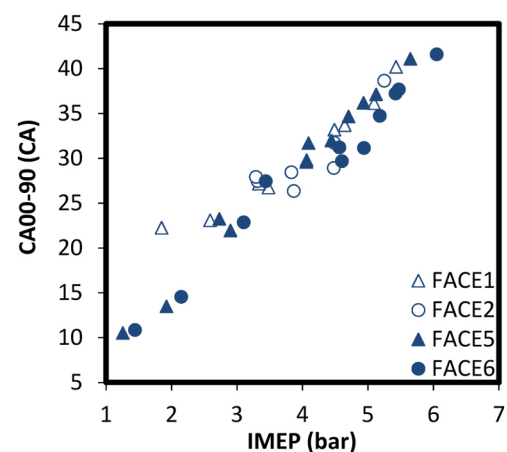


Figure 4. 90% burn duration vs. IMEP for CDC in the SCE (0.5L) study.