

A Comparison of Combustion and Emissions of Diesel Fuels and Oxygenated Fuels in a Modern DI Diesel Engine

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ABSTRACT

Two oxygenated fuels were evaluated on a single-cylinder diesel engine and compared to three hydrocarbon diesel fuels. The oxygenated fuels included canola biodiesel (canola methyl esters, CME) and CME blended with dibutyl succinate (DBS), both of which are or have the potential to be bio-derived. DBS was added to improve the cold flow properties, but also reduced the cetane number and net heating value of the resulting blend. A 60-40 blend of the two (60% vol CME and 40% vol DBS) provided desirable cold flow benefits while staying above the U.S. minimum cetane number requirement. Contrary to prior vehicle test results and numerous literature reports, single-cylinder engine testing of both CME and the 60-40 blend showed no statistically discernable change in NO_x emissions relative to diesel fuel, but only when constant intake oxygen was maintained. The increased NO_x emissions typically reported for oxygenated fuels are believed to be largely due to two factors: 1) the method used to control Exhaust Gas Recirculation (EGR), which is typically based on air mass or EGR rate rather than intake oxygen concentration, and 2) the shift in calibration set points (e.g., EGR, boost pressure, etc.) that result from the increased pedal demand needed to achieve the same torque with oxygenated fuels, due to their lower energy content. When compared at constant intake oxygen, results for NO_x emissions, combustion noise and thermal efficiency were similar between the diesel fuels and the oxygenated fuels tested. A substantial reduction in particulate matter (PM) emissions was observed with both oxygenated fuels (91% reduction with CME and 97% reduction with 60-40 blend on average over various operating conditions), which was attributed to the respective oxygen content of those two fuels and its effect on the average oxygen equivalence ratio at the lift-off length. Elevated hydrocarbon emissions were initially observed with the 60-40 blend and were attributed to poor pilot burn caused by the combination of that fuel's low cetane number and low energy content. When the injection quantities of both the pilot and main injections were adjusted to compensate for energy content, the hydrocarbon emissions were reduced to a level similar to that of the other fuels tested. Under Low Temperature Combustion (LTC), fuel-related effects appeared to track with the cetane number and were relatively insensitive to fuel oxygen content.

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INTRODUCTION

1.1. Biodiesel

Increasing concerns about global climate change have prompted a strong desire to reduce carbon dioxide (CO₂) emissions from vehicles and other sources. One method for reducing CO₂ emissions is the use of renewable fuels such as biodiesel. Biofuels can be produced domestically and thus additionally provide a means to move in the direction of energy independence. Biofuels also support domestic agriculture by increasing demand for the crops that serve as biofuel feedstocks.

For compression ignition engines, biodiesel is the most widely available biofuel. Biodiesel consists of plant oils or

animal fats that have been transesterified with an alcohol, typically methanol. This process converts the triacylglyceride fatty acids into fatty acid methyl esters (FAME). The side chains of these fatty acids typically contain 16 or 18 carbon atoms with 0, 1, 2, or 3 carbon-carbon double bonds. Many plant oils and animal fats contain combinations of these fatty acid structures and sizes. Animal fats and tropical plant oils tend to be high in saturated fatty acids. Oils from plants grown in colder climates such as soybean oil tend to be higher in mono- and poly-unsaturated fatty acids. [1]

In comparison to petroleum diesel, biodiesel has several attractive features, but also some drawbacks. As discussed above, biodiesel is produced from renewable resources and is estimated to provide an approximately 60% reduction in

greenhouse gas emission (including fossil CO_2) on a full lifecycle basis, though there is considerable uncertainty and variation depending on assumptions [2]. Biodiesel is an oxygenated fuel and has been shown to greatly reduce engine-out emissions of particulate matter (PM), with lesser reductions for carbon monoxide (CO) and hydrocarbons (HC) [3]. Literature reports regarding nitrogen oxide (NO_x) emissions are mixed, with most reports indicating a modest increase in NO_x while some report no change [3,4,5]. Biodiesel also increases lubricity when added to ultra-low sulfur diesel at relatively low concentrations [6].

Biodiesel has generally poorer cold flow properties and oxidation stability as compared to petroleum diesel. Both properties depend on the biodiesel feedstock (which determines the predominant types of FAMES in the biodiesel). Current biodiesel fuels are sometimes not robust to cold climates due to poor cold flow properties, resulting in fuel precipitation and/or gelling which can clog fuel filters. Saturated FAMES are more problematic than unsaturated FAMES in this respect [7]. Oxidative stability, however, correlates very strongly with the amount of poly-unsaturated FAMES in the biodiesel, with di- and tri-unsaturated FAMES being considerably more reactive than mono-unsaturated FAMES [8].

In the US, soybean oil is the most common biodiesel feedstock material due to its relatively low cost and wider availability as compared to other plant oils. However, without anti-oxidant additives, soy biodiesel exhibits poor oxidation stability due the prevalence of polyunsaturated FAMES. It also has relatively poor cold temperature properties due to significant amounts of saturated FAMES and possibly due to partially reacted feedstock (monoacylglycerols) or other trace organic compounds present in the plant oil [9,10].

A variety of new biofuels were investigated that improve cold flow properties. Canola oil was identified as a preferred conventional biodiesel feedstock due to its comparatively low content of poly-unsaturated fatty acids and saturated fatty acids, with the majority being oleic acid (a mono-unsaturated fatty acid) [7]. This composition should provide better oxidative stability and cold temperature properties than soy biodiesel [10]. In addition to methyl esters, ethyl, propyl, and butyl esters were evaluated. Dibutyl succinate (DBS), which could also be produced from renewable feedstocks, [11,12] was identified as one promising fuel for blending with canola oil FAME.

1.2. Low-Temperature Combustion (LTC)

Since the use of biodiesel fuels may increase in the future, new combustion systems and combustion modes must be robust to its use. While the effect of biodiesel on combustion and emissions has been studied, it is not well understood how possible alternative biodiesel fuels (such as blends of biodiesel and DBS) behave. In addition, not much is known about how advanced modes of combustion such as LTC behave with oxygenated fuels, such as biodiesel, particularly

when the engine is calibrated to operate with a typical diesel fuel. LTC is a series of combustion modes including MK combustion [13, 14, 15], smokeless rich combustion [16], and partially premixed compression ignition (PPCI or PCCI) [17,], all of which have been shown to significantly reduce engine-out NO_x and soot emissions. The formation of soot and NO_x in a diesel engine can be visualized on the Φ -T diagram shown in Figure 1, a version of which was first introduced by Akihama *et al.* [16]. Conventional diesel combustion produces local equivalence ratios and temperatures giving rise to both soot and NO_x . In LTC, the start of combustion is delayed to provide time for fuel-air mixing prior to combustion, which reduces the hot-rich zones in the combustion chamber to substantially avoid the soot formation area. Elevated levels of exhaust-gas recirculation (EGR) are also used both to suppress peak flame temperatures, thereby substantially avoiding the thermal NO_x formation region, and to control the rate of combustion. Fuel oxygenation is likely to alter in-cylinder equivalence ratios, thus it may impact the behavior of the engine in LTC. While there have been some study combining LTC and biofuels [18, 19, 20, 21], further study is warranted to understand how this combustion mode behaves with both FAMES and other oxygenated fuels.

1.3. Study Objectives

The intent of the current study was to identify potential bio-derived diesel fuels with better cold flow properties and to understand the performance of those fuels in an engine relative to both diesel fuel and conventional biodiesel. In addition, testing was aimed at understanding the effect of oxygenated fuels on combustion, emissions, and fuel consumption in both conventional diesel combustion and LTC with particular emphasis on the robustness in the latter mode of combustion.

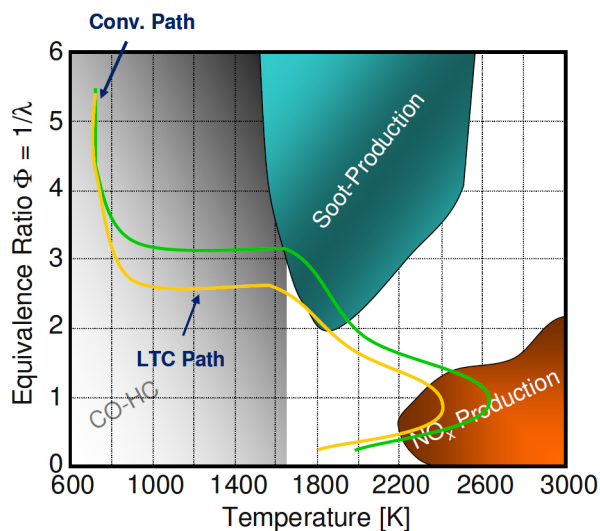


Figure 1. Visualization of LTC and conventional combustion in Φ -T space.

EXPERIMENTAL METHODOLOGY

2.0. Oxygenated Fuels Selection

Canola biodiesel (canola methyl ester, CME) was produced from canola oil, while DBS could be produced from succinic acid and 1-butanol derived from biological feedstocks. DBS was one of several potential compounds screened as part of a DOE-funded research project which had an emphasis on improving cold flow properties using new fuel compounds that could be produced from renewable feedstocks. For example, DBS has a relatively low freezing point (-29°C). CME was blended with DBS over a range of blend ratios, ranging from 100% CME to 100% DBS and the cold flow properties were characterized. Cold flow properties were measured using standard test methods for automated cloud point (CP; ASTM D2500-05 [22]) and automated cold filter plugging point (CFPP; ASTM 6371-05 [23]).

Samples of CME and blends of CME and DBS were analyzed for fuel properties including cetane number (CN), net heating value (NHV), density, and carbon, hydrogen, and oxygen content. Key results are summarized in Table 1.

The cold flow properties of CME are improved by blending with DBS. The CFPP and CP were measured for CME-DBS blends in ratios ranging from 100% CME to 100% DBS (Figure 2). The CP (-6°C) and the CFPP (-10°C) of CME were much higher than the CP (-29°C) and CFPP (-41°C) of DBS. The addition of increasing amounts of DBS to CME produced blends with improved cold flow properties as compared to the pure CME. The cold flow properties were most improved at the highest blend ratios of DBS.

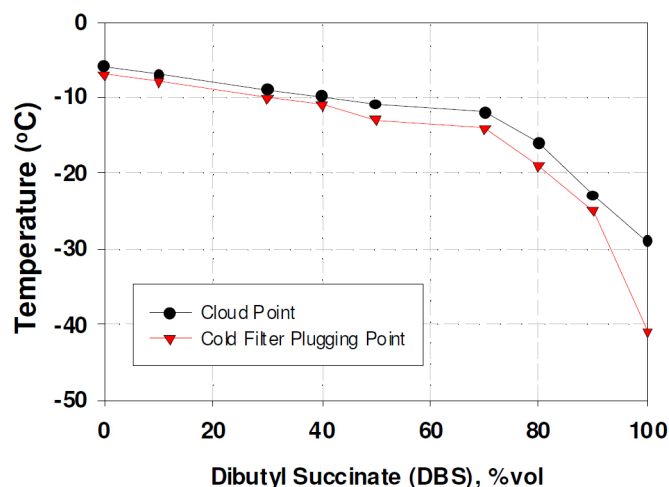


Figure 2. Cloud point and cold filter plugging point for blends of DBS in CME.

However, the cetane number of blends containing high DBS concentration were found to be unacceptably low, as shown in Figure 3. Based on linear extrapolation of these results, pure DBS is estimated to have a CN of approximately 20, considerably lower than the measured CN of the CME (51-55) and minimal CN requirement for U.S. diesel fuel (40)

in ASTM D975 [24]. Increasing DBS content also resulted in a decrease in NHV, the result of its greater oxygen content. Based on these results and as shown in Figure 3, a blend containing 60% CME and 40% DBS by volume was selected for further engine testing. This blend achieves the minimum CN of 40 while still providing significant cold flow improvement (approximately 9°C) over conventional soy biodiesel.

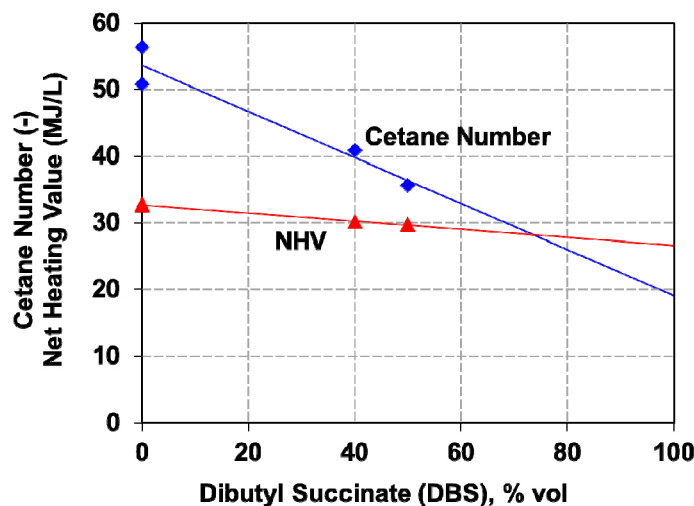


Figure 3. Cetane number and net heating value for blends of CME with DBS. Data points indicate measured values. Lines show best linear fits to the data.

3.0. Single-Cylinder Engine Testing

3.1. Test fuels

Both the 100% canola biodiesel (CME) and the 60%-40% vol CME-DBS blend (60-40) were evaluated on a single-cylinder engine to understand the impact of those fuels on combustion, emissions, NVH, fuel consumption and thermal efficiency. These two fuels were compared to a typical diesel fuel in North America (720). A summary of the properties of these fuels is shown in Table 1.

As shown in the table, the two biofuels (CME & 60-40) studied have significantly different cetane numbers from 720 diesel fuel as well as each other. Consequently, a low cetane diesel fuel (727) was included to match the low CN of the 60-40 blend, while a high cetane fuel (668) was added to match the CN of B100. The properties of the two additional fuels are also included in Table 1. It is worth noting that 668 fuel was composed of primarily saturates with very low aromatic hydrocarbon content.

Since the oxygen content of DBS is greater than that of the CME, the oxygen-carbon ratio of the 60-40 blend is higher than that of CME. Furthermore, the net heating value has a negative correlation with the oxygen content such that all three diesel fuels have similar energy content, while B100 is lower and 60-40 is the lowest.

Table 1. Summary of fuel properties

	720	727	668	CME	60-40
Full Name /Description	Typical Diesel	Low CN Diesel	High CN Diesel	100% CME	60% vol CME 40% vol DBS
Cetane No.	45.6	41.8	56.5	50.8	40.8
Molar H:C	1.81	1.78	1.95	1.88	1.86
Molar O:C	0	0	0	0.106	0.191
NHV (MJ/kg)	42.9	42.4	43.2	37.0	32.7
NHV (MJ/L)	36.8	36.2	35.9	32.6	30.1
Spec. Gravity*	0.848	0.853	0.830	0.883	0.923
Aromatics	28.6% vol	32.4% vol	<5% vol		
Olefins	1.3% vol	1.9% vol	0.1% vol		
Saturates	70.1% vol	65.7% vol	97.7% vol		
Esters				100%	100%

* 15.56°C/15.56°C

3.2. Single-cylinder engine test setup

The engine used for this study was a 0.83L single cylinder diesel engine. Details of the engine can be found in [Table 2](#). The engine was equipped with a piezo common rail fuel system capable of 2000 bar injection pressure. Further information about the engine and combustion system upon which the single-cylinder engine used in this study was based can be found in DeRaad et al. [25] and Styron *et al.* [26], respectively.

Table 2. Engine specifications.

Bore	99 mm
Stroke	108 mm
Connecting Rod Length	176 mm
Number of Valves	4
Compression ratio	16.2
Bowl design	Chamfered

The engine was lubricated by an externally driven oil pump that was set up to control oil pressure as a function of engine speed based on multi-cylinder engine data. Coolant was also externally supplied through a conditioned water system. Both oil temperature and coolant temperature were controlled to 90°C for all operating conditions.

A schematic of the single-cylinder engine test cell setup is shown in [Figure 4](#). Intake and exhaust pressure and temperature measurements were taken at various locations shown in the figure. The air path for the engine was set up to control the intake pressure, intake temperature and exhaust pressure to simulate turbocharging and to control the exhaust gas recirculation. Air was supplied from the critical air system, which provided dry air at up to 700 bar upstream of the critical flow orifice to provide sonic flow through the orifice under highly boosted conditions. Air pressure and critical flow orifice size were used to control the intake pressure measured in the intake manifold. A 15.5L intake

surge tank was used to dampen out pressure pulses caused by the pulsed flow of single-cylinder operation. Intake temperature measured in the intake runner was controlled using a Chamalox heater as well as band heaters strapped to the intake surge tank. To facilitate rapid transition from high intake temperature to lower temperature, a heater bypass was also used and the heated and unheated streams were blended with a three-way valve. Air flow was measured both with a critical flow orifice and, when the flow across the critical flow orifice was subsonic, a Micromotion CMF050 flow meter. This was typically only necessary when very high intake pressures were used, making it difficult to meet the sonic pressure ratio criteria across the critical flow orifice.

The exhaust system consisted of a specially designed exhaust runner to attenuate exhaust pressure wave reflection and a surge tank identical to the intake surge tank. These combined allowed the cylinder pressure to reasonably resemble that on a multi-cylinder engine during the intake and exhaust strokes. Exhaust pressure was controlled using two valves in parallel. The larger of those valves was controlled in an open loop manner, while the smaller was controlled closed loop based on exhaust surge tank pressure. EGR was extracted from the exhaust surge tank and was directed towards the engine through one of two paths, cooled or uncooled. The uncooled path had a single valve capable of being controlled closed loop based on EGR rate, while the cooled path had a two-valve control system similar to that used to control exhaust pressure. The uncooled path was used either to facilitate high intake temperature or to avoid overcooling and condensation in the cooled path at low load conditions. Additional temperature control was provided by an EGR cooler coolant flow control valve.

Exhaust NO_x, CO, HC, CO₂ and O₂ concentrations were measured with separate emissions benches, one sampling from the exhaust surge tank (MEXA-7400DTRLE) and the second sampling from the exhaust line downstream of the exhaust pressure control valves (MEXA-7100DEGR). No correction was made for FID response to oxygenated species

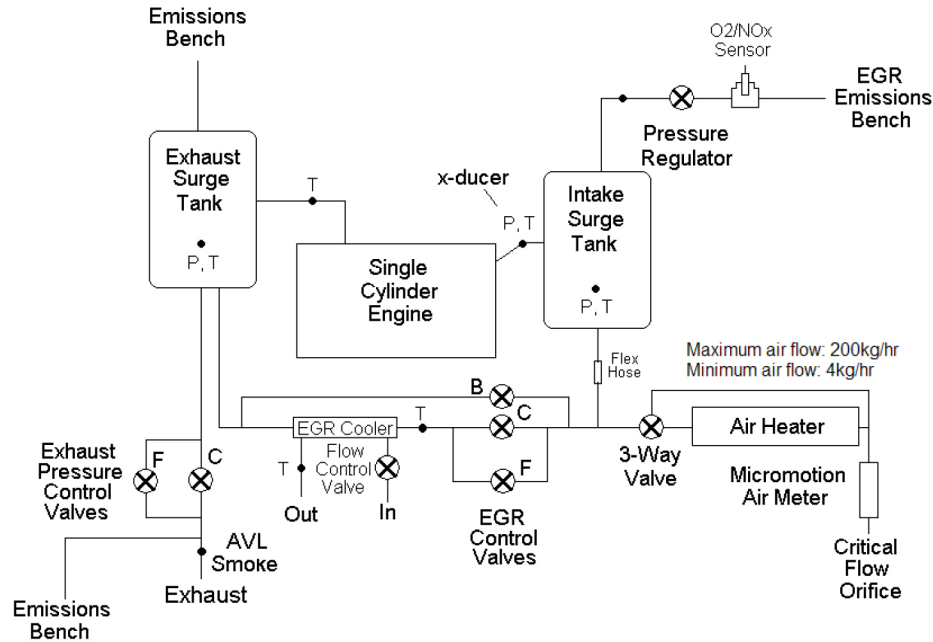


Figure 4. Schematic of the single-cylinder engine test cell setup.

when the oxygenated fuels were used. Heated sample lines were used to maintain sample line temperature above the HC and water dew points and heated soot filters were used to protect the analyzers from contamination. The exhaust surge tank measurement was used whenever possible to minimize errors associated with water and hydrocarbon condensation, which could occur in the exhaust pipe as a result of heat transfer. A comparison of the result of the two analyzers showed that errors in HC and NOx emissions occurred primarily at the lowest speed and load conditions where the exhaust flow rate and temperature was very low. At high speed and load, the target exhaust surge tank pressure exceeded the analyzer limit of 150kPa. Consequently, the exhaust surge tank measurement was discontinued at those conditions to protect the analyzer and the downstream measurement was used as the primary measurement instead. Under those conditions, exhaust temperature and flow rate was sufficiently high and errors associated with condensation were negligible.

Intake CO₂ concentration was measured in the intake surge tank using the MEXA-7100DEGR analyzer to determine EGR rate when combined with the exhaust CO₂ measurement using Equation 1.

$$EGR = \frac{CO_{2,int} - CO_{2,bg}}{CO_{2,exh} - CO_{2,bg}} \cdot 100 \quad (1)$$

CO_{2,int} and CO_{2,exh} are the measured intake and exhaust CO₂ concentrations while CO_{2,bg} is the atmospheric CO₂, which was measured to be 0.03%. It is also useful to look at EGR in terms of intake oxygen concentration, a parameter

that fundamentally controls NOx emissions. Consequently, an oxygen sensor was used in the intake sample line to measure intake oxygen concentration directly. Furthermore, the burnt mass fraction (FMAN), a control parameter that is directly related to intake oxygen proposed by Roettger et al. [27] and calculated as shown in Equation 2, was used for analysis in this study.

$$FMAN = \left(\frac{EGR}{100} \right) \cdot \left(1 - \frac{O_{2,exh}}{20.95} \right) = 1 - \frac{O_{2,int}}{20.95} \quad (2)$$

Smoke was measured using an AVL 415S smoke meter located after the exhaust backpressure control valves. Filter smoke number (FSN) was then correlated to soot concentration (K_C) in mg/Sm³ at 20°C and 101.3 kPa using the MIRA correlation (see equations 3).

$$K_C = 0.982e^3 \cdot FSN \cdot 10^{(FSN \cdot 0.1272 - 1.66)} \quad (3)$$

Soot concentration was then converted to mass flow rate (G_{soot}) in g/hr using equation 4.

$$G_{soot} = K_C \cdot (m_{air} + m_{fuel}) \cdot \frac{0.001}{1.2048} \quad (4)$$

Where air and fuel flow are in kg/hr.

Fuel flow rate was measured with a Pierburg low flow fuel cart. Results from the direct measurement tended to be erratic. Consequently, fuel flow was verified using the critical flow orifice air flow measurement and the air-fuel ratio

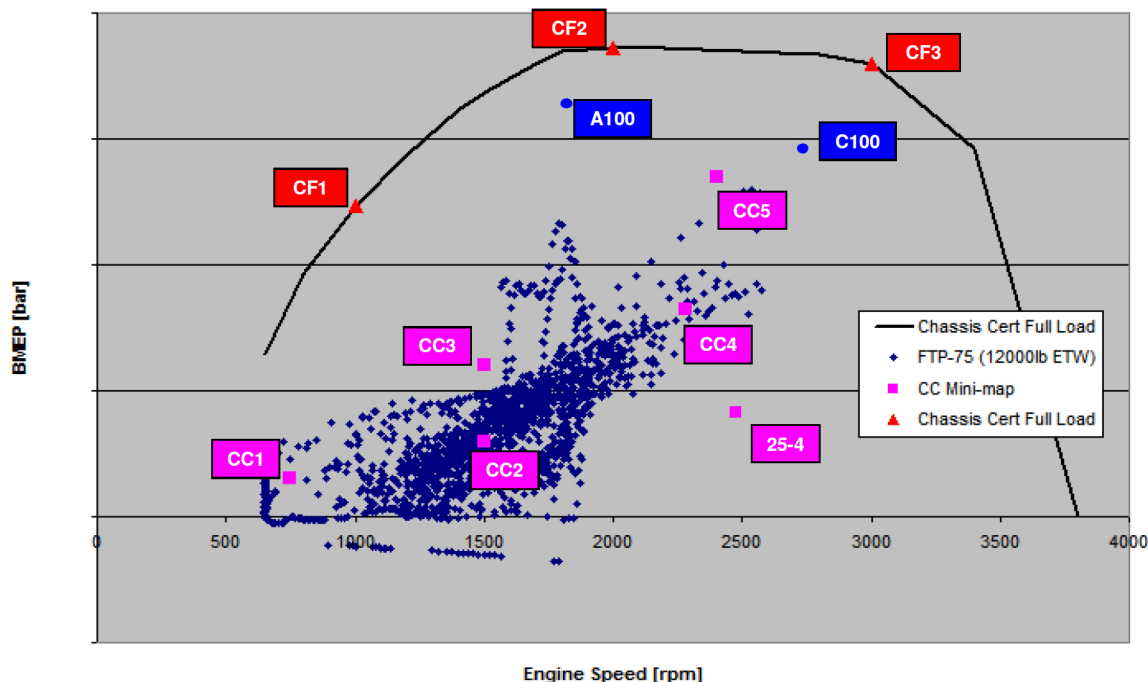


Figure 5. Single-cylinder engine test conditions.

determined by the emissions bench using the Spindt method [29]. The result of this calculation tended to be more consistent than the low flow fuel cart measurement, so it was used in calculations of emissions and fuel consumption.

Cylinder pressure was measured with an AVL GH12D flush mount pressure transducer. Data was recorded at a 0.05 CAD resolution. Analysis of the measured cylinder pressure trace was used both for heat release analysis, a first law analysis to determine the rate at which the fuel is burned in-cylinder, and noise analysis, an analysis that determines the frequency content of the cylinder pressure trace, attenuates it appropriately and converts the result to an engine radiated noise level of dB attributable to combustion. The cylinder pressure measurement was also used to determine the projected multi-cylinder BMEP, which was used to correct single-cylinder brake specific emissions and fuel consumption into projected multi-cylinder brake values. This projected BMEP was based on the Net Mean Effective Pressure (NMEP) determined from the cylinder pressure trace and a projected multi-cylinder friction (FMEP). The projected FMEP was calculated as a function of engine speed (or mean piston speed) and peak firing pressure. This transfer function was developed from 6.7L multi-cylinder engine data over a full engine map.

3.3. Test conditions

Tests were conducted at the 11 engine speed and projected BMEP test conditions shown in Figure 5. Five of these conditions (CC1-CC5) were established to represent the FTP city cycle. Three of these test points (CC1-CC3) and one additional condition (25-4), were tested in low temperature

combustion mode. It is worth noting that the two lower load conditions (CC1 and CC2) utilized a PCCI strategy, while an MK-like strategy was employed for the two higher speed-load LTC test conditions (CC3 and 25-4). Two additional operating conditions (A100, C100) were used as an indicator of heavy-duty FTP performance. The remaining three test points (CF1, CF2, CF3) were used to assess potential light-duty full load performance.

The intake pressure, intake temperature and exhaust pressure boundary conditions for each of these test points was established based on prior multi-cylinder engine data. At CC2, which had very high intake temperature on the multi-cylinder engine due to the use of the EGR cooler bypass, the intake temperature was lowered for LTC tests to increase ignition delay, thus enabling LTC. The calibration, while similar to the multi-cylinder engine, was optimized for the single-cylinder engine with the baseline fuel. The injection strategy employed depended on the operating condition. CC1-CC5 as well as CF1 employed a single pilot and a main injection. The other test conditions employed a single main injection. The injection strategy in LTC was also a single injection. The phasing of that injection was near TDC for the MK-like test conditions, but 10-2 degrees before top dead center at PCCI test conditions.

3.4. Test Procedure

3.4.1. Conventional combustion

A series of tests were established to evaluate the fuels as though tested at the same engine speed and pedal position on a multi-cylinder engine. The intent of this approach was to emulate the behavior of an engine control unit (ECU), in