FUEL PROPERTY IMPACT ON A PREMIXED DIESEL COMBUSTION MODE

by

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LIST OF ACRONYMS

2-EHN	2-EthylHexyl Nitrate
AR	Activated Radicals
ASOI	After Start of Injection
ATAC	Active Thermo-Atmosphere Combustion
ATDC	After Top Dead Center
BMEP	Brake Mean Effective Pressure
BTDC	Before Top Dead Center
CA50	Location of 50% Mass Fraction Burned
CAI	Controlled Auto-Ignition
CARB	California Air Resources Board
CFR	Cooperative Fuels Research
CIHC	Compression Ignited Homogeneous Charge
CN	Cetane Number
DCN	Derived Cetane Number
DPF	Diesel Particulate Filter
DHCCI	Diesel Homogeneous Charge Compression Ignition
DOC	Diesel Oxidation Catalyst
ECM	Engine Control Module
EGT	Exhaust Gas Temperature
EHN	2-EthylHexyl Nitrate
EPA	Environmental Protection Agency
EU	European Union
FDCCP	Fluid Dynamically Controlled Combustion Process
FID	Flame Ionization Detector
FSN	Filter Smoke Number
GTL	Gas-To-Liquid
HC	Hydrocarbons
HCCI	Homogeneous Charge Compression Ignition
HCDC	Homogeneous Charge Diesel Combustion
HCN	High Cetane Number diesel fuel
HCTI	Homogeneous Charge Thermal Ignition
HiMICS	Homogeneous charge intelligent Multiple Injection Combustion System
ID_{CF}	Ignition Delay – Cool Flame
ID_{MHR}	Ignition Delay – Main Heat Release
IMEP	Indicated Mean Effective Pressure
ION	Iso-Octyl Nitrate
LCN	Low Cetane Number diesel fuel

LHV	Lower Heating Value
LPDC	Low-Temperature Premixed Diesel Combustion
LTC	Low Temperature Combustion
LTDC	Low Temperature Diesel Combustion
LTHR	Low Temperature Heat Release
MAP	Manifold Absolute Pressure
MCN	Mid Cetane Number diesel fuel
MFB	Mass Fraction Burned
MHR	Main Heat Release
MK	Modulated Kinetics
MK1	Swedish Environmental Class 1 diesel fuel
NDIR	Non-Dispersive Infrared
NEDC	New European Driving Cycle
NMOG	Non-Methane Organic Gases
NO_x	NO and NO_2 (combined)
NTC	Negative Temperature Coefficient
NVH	Noise, Vibration, Harshness
PAH	Polyaromatic Hydrocarbons
PCCI	Premixed Charge Compression Ignition
PCI	Premixed Compression Ignition
PCV	Positive Crankcase Ventillation
PM	Particulate Matter
PPCI	Partially Premixed Compression Ignition
PREDIC	PREmixed lean DIesel Combustion
PWM	Pulse Width Modulated
RAC	Radical Activated Combustion
RI	Radical Ignition
RMS	Root Mean Squared
RoHR	Rate of Heat Release
RSS	Root Sum Squared
SCRI	Stratified Charge Radical Ignition
SOF	Soluble Organic Fraction
SoHTHR	Start of High Temperature Heat Release
TDC	Top Dead Center
T50	Distillation temperature representing 50% recovery (mid boiling)
T90	Distillation temperature representing 90% recovery
TI	Thermal Ignition
TS	Toyota-Soken
TTO	Turbine Outlet Temperature
ULSD	Ultra Low Sulfur Diesel fuel
UNIBUS	UNIform BUlky combustion System
VGT	Variable Geometry Turbine

ABSTRACT

New premixed diesel combustion strategies, with their low engine-out PM and NO_x emissions, are highly attractive for production implementation given increasingly strict emissions regulations. Accordingly, premixed diesel combustion strategies must operate effectively on commercially available diesel fuel, whose critical properties vary substantially. It is therefore critical to understand how premixed diesel combustion strategies respond to variations in fuel properties, especially cetane number, the primary quantification of ignition behavior.

This research study sought to understand the connection between diesel fuel properties, in particular cetane number, and the combustion and emissions behavior of premixed diesel combustion. Four primary test fuels with cetane numbers varying over the range expected in the field (42-53) were used, along with a secondary matrix of fuels to characterize the behavior of a nitrate cetane improver. Fuel effects were quantified across a range of EGR levels, injection pressures, and engine loads to identify secondary parameter interactions.

Gaseous emissions, particularly NO_x emissions, were found to be dependent solely on combustion phasing and EGR for the primary petroleum test fuels at the studied condition. Fuel cetane number shifts the combustion phasing (increasing cetane number advances phasing) but is only one of many different parameters which shift combustion. The effect of varying cetane number can be counteracted by varying injection timing to yield matched combustion phasing.

The presence of 2-ethylhexyl nitrate (2-EHN) cetane improver within the fuel introduces a new fuel-borne NO_x formation mechanism to the combustion process, which significantly increases NO_x emissions in a premixed diesel combustion mode. The increase in NO_x emissions stems from NO_x formed by the decomposition of the 2-EHN additive.

The trends and magnitudes of soot, CO, and HC emissions remain constant for all tested fuels across a range of engine loads. The high load limit of the tested premixed diesel combustion mode is primarily limited by equivalence ratio, with excessive soot, CO, and HC emissions resulting as the overall equivalence ratio approaches stoichiometric. The light load limit is limited by high CO and HC emissions and the ability of a diesel oxidation catalyst to reduce these emissions to acceptable levels.

CHAPTER 1

INTRODUCTION AND MOTIVATION

1.1 Engine Research and Development

The motivation for engine research and development has long been a balance between legislated requirements and market forces. Since the introduction of the Clean Air Act in 1970, ensuring that engines pass legislated emissions standards has been a prime focus of research and development. However, the focus of engine research is also directed by consumer requirements. Of interest to consumers is total lifetime vehicle cost, which is comprised of several elements including initial equipment cost and usage costs including the fuel and repair costs. Increasing the life of the equipment and reducing the repair costs are prime goals of production development groups, and not particularly the focus of research groups. However, fuel costs and initial costs are certainly elements that affect engine research goals. Overall, the end desire is to minimize consumer cost by minimizing the cost of the powertrain system, maximizing engine efficiency for high fuel economy, while ensuring that the engine emissions are lower than the mandated maximum levels.

1.2 Exhaust Emission Regulatory Legislation

Maximum allowable emissions from engines in vehicles used in the United States are controlled by two standards: all vehicles must meet the levels prescribed by the Environmental Protection Agency (EPA), but vehicles registered in California, and other states that adopted the California emissions standards, must also meet the standards set by the California Air Resources Board (CARB).

Tier 2 emissions requirements set by the EPA for U.S. passenger vehicles specify the same maximum level of emissions from vehicles with compression ignition diesel engines and spark ignition gasoline engines. For vehicles made in 2007 and beyond, whether gasoline or diesel, the new (bin 5) standards require the fleet average particulate matter (PM) emissions be less than 0.01 g/mile, and the fleet average NO_x ($NO + NO_2$) emissions be less than 0.07 g/mile (CFR, 86.1811-04). This is a change from the Tier 1 emissions standards, which came into effect in 1994. Under the older standard, PM emissions was limited to 0.08 g/mile, eight times the level mandated under the new 2007 Tier 2 (bin 5) standards (CFR, 86.708-94). Furthermore, the Tier 1 emission standard only required NO_x emissions from a diesel engine be less than 1.0 g/mile, which is more lax than the 0.04 g/mile that gasoline engines were required to achieve (CFR, 86.708-94).

Starting in 2005, vehicles sold and registered in California must meet the CARB LEV-II emissions standards. Additionally, four other states (Maine, Massachusetts, New York, and Vermont) have also adopted CARB's LEV-II emissions standards. Five more states are slated to adopt the LEV-II standards by 2009. LEV-II (ULEV) mandates PM emission not exceed 0.01 g/mile, and NO_x emissions not exceed 0.05 g/mile (CCR, 1961). The PM emission level required currently by the LEV-II standard is the same as the Tier 2 (bin 5) US standard, but the required NO_x level is even lower than Tier 2 (bin 5).

New emissions standards have also been set for European vehicles. Euro 4 emissions standards implemented in 2005 mandate maximum PM emissions be less than 0.025 g/km (0.04 g/mile), and NO_x emissions be less than 0.25 g/km (0.40 g/mile) (EPC, 98/69/EC). Euro 5 legislation that comes into effect for new cars in 2009 and existing models in 2011, reduces these limits substantially, to 0.005 g/km (0.008 g/mile) for PM emissions and 0.18 g/km (0.29 g/mile) for NO_x emissions (EPC, 715/2007). Euro 6 regulations further reduces these limits for diesel passenger cars starting in 2014 for new platforms and 2015 for existing vehicles. The Euro 6 emissions limits are 0.080 g/km (0.13 g/mile) of NO_x, and 0.003 g/km (0.005 g/mile) of particulates, with a new limit on the number of particles added as well (EPC, 715/2007).

Standard	Enters into Effect	Maximum NO_x	Maximum PM
U.S. Tier 1	1994	1.0	0.08
U.S. Tier 2 (bin 5)	2007	0.07	0.01
CARB LEV-II (ULEV)	2005	0.05	0.01
Euro 4	2005	0.40	0.040
Euro 5	2009, 2011	0.29	0.008
Euro 6	2014, 2015	0.13	0.005
		g/mile	g/mile

Table 1: Current and future NO_x and PM emission standards. Standards are applicable to the United States and European Countries. European standards have two entrance dates, the first for new platforms, and the second for existing vehicle models.

It should be noted that the driving cycles used in the emissions tests are different between the United States and Europe. The United States uses the combination of three different driving cycles: the classic UDDS (FTP-75) cycle, the SFTP US06 cycle – a more aggressive test with harder accelerations and higher speeds, and SFTP SC03 cycle – a test with air conditioner load (CFR, 86.115, 86.159, 86.160). The overall specified emissions level is the result of a weighted combination of the emissions from all three driving cycles (CFR, 86.164). European nations are certified on the New European Driving Cycle, NEDC (EPC, 98/69/EC). It is generally known that emissions yields are similar between the UDDS and NEDC cycles, but the SFTP US06 test yields significantly higher emissions because of the increased loads and speeds. The differences suggest direct comparison of regulated emission levels is not perfect, but a reasonable estimate.

PM and NO_x are not the only regulated emissions in the United States and European countries. EPA Tier 2 and CARB LEV-II standards regulate emissions of CO and non-methane organic gases, NMOG, which is comprised of non-methane hydrocarbons and oxygenated hydrocarbons (CFR, 86.1811-04; CCR, 1961). Additionally, the Tier 2 standards establish a maximum acceptable level of formaldehyde, HCHO, emissions (CFR, 86.1811-04). European emissions standards regulate emissions of CO and the sum of HC and NO_x emissions (EPC, 98/69/EC). However, these other emissions do not pose a great problem for conventional diesel engines. Diesel engines produce very low CO emissions as a result of operating with lean air-fuel ratios, and hydrocarbon emissions are reduced to the specified level on current engines with a diesel oxidation catalyst (DOC). It is expected that current research on DOCs will result in a catalyst capable of achieving the lower NMOG emissions levels. However, achieving the low PM and NO_x requirements require substantial development in both diesel combustion and aftertreatment systems. As such, NO_x and PM are critical emissions for diesel engine development. However, it is acknowledged and foreshadowed that combustion development modes required to meet NO_x and PM emissions levels may place increasing CO and HC burden on the aftertreatment systems. Accordingly, CO and HC emissions remain important.

1.3 Addressing New Emissions Standards

Creating diesel engines that meet the forthcoming emissions standards requires substantial development of the diesel engine system. While development is necessary on catalytic after-treatment systems, improving combustion is also required and is highly beneficial. Decreasing the level of engine-out emissions reduces demand on the aftertreatment system. Further, improving an engine by altering the combustion strategy and retaining existing components can more cost-effective - overall engine performance increases without a substantial increase in engine hardware cost. However, methods of reducing the engine emissions must not sacrifice fuel economy too significantly as this will increase end user fuel costs, making the engine less desirable to consumers.

1.3.1 Advanced Combustion Strategies

In response to the new restrictions on exhaust gas emissions, particularly PM and NO_x, new strategies for diesel combustion have been developed. Many different researchers have developed slightly different strategies, and most created their own moniker for their strategy. Acronyms including PCI, PCCI, PPCI, TS, UNIBUS, MK, PREDIC, DHCCI, CIHC, AR, CAI, FDCCP, HiMICS, ATAC, RI, SCRI, TI, HCTI, RAC, LPDC, HCDC, LTDC, and LSC all represent individual strategies, though they all share both similar objectives and general characteristics.

To achieve a simultaneous reduction in PM and NO_x emissions, these novel combustion strategies seek to exhibit two seemingly contradictory properties: a well mixed cylinder charge prior to ignition and relatively low combustion temperatures. The fuel and air in the cylinder must be well mixed to avoid regions with unfavorable carbon-oxygen ratios that lead to PM formation. The temperature in the combustion process must remain low to prevent NO_x from forming in significant quantities, and prevent the formation of soot precursors. Many different researchers have formulated strategies that simultaneously achieve the two stated requirements for low PM, low NO_x combustion. Characteristics of these strategies include heavy use of cooled exhaust gas recirculation (EGR), where a portion of the exhaust gas is cooled and drafted back into the intake system, and altered injection timings. Strategies have been established using both advanced and retarded injection timings to achieve the desired combustion.

While charge conditions with premixed diesel combustion are considered ‘well mixed’, this does not indicate that they are homogeneous. There is significant variation in mixture conditions (including local equivalence ratio) within the cylinder charge, owing to the combination of highly turbulent nature of the gas flows within the cylinder (heavily influenced by the combustion chamber shape and swirl of the intake flow), injection method (a direct injection usually near firing TDC), and the fuel used (diesel fuel has a relatively low volatility and slow evaporation and mixing rates). The cylinder conditions are considered well mixed compared to conventional diesel combustion, where a significant portion of the combustion is mixing-limited diffusion burning, but are not as uniform as the conditions within a homogeneous charge compression ignition (HCCI) engine. Conditions for HCCI combustion have a narrow range of local equivalence ratios compared to premixed diesel combustion. The ignition behavior also differs between HCCI and premixed diesel combustion. There is usually a strong link between the injection and ignition timing with premixed diesel combustion, but not for HCCI combustion, where the mixture is set very early in the cycle and then compressed until cylinder conditions reach a point where chemical kinetics initiate combustion. So, while control of HCCI ignition is a complex problem with thermal management highly critical to successful implementation, premixed diesel combustion offers more predictive control with the injection. This is indicative of premixed diesel combustion being an evolution of HCCI, an ‘HCCI-ish’ strategy, which yields some of the emissions benefits of HCCI over a narrow load range but with more manageable control over ignition timing. Thus, the main differences between premixed diesel combustion and HCCI are encapsulated:

(1) premixed diesel combustion, while well mixed relative to conventional diesel combustion, has less uniform cylinder conditions than HCCI, and (2) ignition control is linked to the injection timing with premixed diesel combustion, whereas it is highly dependent on thermal management and predictive control over cylinder conditions with HCCI. As a result of the inhomogeneity of the mixture with premixed diesel combustion relative to HCCI, emissions at higher equivalence ratios are increased, and subsequent emissions-based equivalence ratio limits are lower.

1.3.2 Implementation in Production Engines

More than ten years of development time have been invested in studying and developing these strategies for implementation in future vehicles. With new emissions regulations set to take effect in upcoming years, implementation of these strategies in production vehicles is becoming increasingly imminent. The principal implementation concern is whether these strategies work outside the research laboratory where variables are not as well controlled. Part of this concern is how these strategies will behave when exposed to the wide range of diesel fuel that is publicly available.

Diesel fuel properties are rather loosely regulated: the primary diesel fuel properties currently controlled by legislation are maximum sulfur content, maximum aromatic content, and minimum cetane number or index. Diesel fuels in the US and Europe are largely free of sulfur (US limit of 15 ppm, EU limit of 50 ppm but mandate complete availability of sulfur-free diesel fuel) (CFR, 80.520; EPC, 98/70; EPC, 2003/17). Diesel fuels in the United States must have a cetane index of at least 40 or a maximum aromatics concentration of 35%, while European fuels must have a cetane number of 51 or greater (CFR, 80.29; EPC, 98/70). The range of cetane number, however, is substantial. In the United States, the cetane number of diesel fuels available at filling stations can range anywhere from 38 to the mid 50s, with an average value of around 46 (NAFS, 2003; Peckham, 2003). A 15-point variation in cetane number represents a very significant variation in fuel ignition behavior.

With the wide cetane number range of diesel fuels available to consumers, understanding how the newly developed advanced diesel combustion strategies respond to changes in cetane number is critical for production implementation. Additionally, optimizing an engine for one fuel specification likely will not give optimum performance when the fuel is altered. It is then important to understand both the effects of running an engine on a different fuel with similar conditions, and what can be done to improve the engine's performance if a fuel causes sub-optimal behavior.

1.4 Project Objective and Motivation

This research study sought to understand the connection between diesel fuel properties and the combustion and emissions behavior of premixed diesel combustion. At the start of this project, very few researchers had studied the effect of fuel properties on premixed diesel combustion and all focused on specially blended fuels (which were substantially different than common diesel fuel) to enable the combustion mode. A desired to understand how changes in fuel affected the combustion process and resulting emissions provided motivation for this work. Since implementation of these combustion modes in future vehicles is highly probable, understanding issues which could complicate their introduction is of great utility. Thus, the objective was to understand which diesel fuel properties are critical to premixed diesel combustion modes, how they impact the combustion process and resulting emissions, why they cause these effects, and how to correct for or eliminate undesired behavior stemming from fuel changes.

1.5 Expansion of Published Research

This work extends beyond the existing published research on the effect of fuel properties on advanced combustion strategies by focusing on a direct-injection premixed diesel combustion mode, narrowing the range of test fuels, and conducting more detailed sweeps of main engine operating parameters.

A sizeable portion of the existing research in this field focuses on HCCI combustion (Risberg et al., 2005; Szybist et al., 2005; Bunting et al., 2007-1; Bunting et al., 2007-2). Due to the differences between HCCI and premixed diesel combustion (level of mixture homogeneity, temperature dependencies, combustion phasing, operating load level), HCCI combustion results often do not directly translate to premixed diesel combustion modes. It features more homogeneous mixtures than premixed diesel combustion reflecting different fuel induction methods (port injection, heated vaporizers). Also, HCCI ignition is dictated by chemical kinetics and therefore strongly dependent on cylinder thermal conditions: initial cylinder conditions, especially the intake charge temperature, are critical to HCCI control. Intake temperature becomes a primary variable within HCCI studies, while being of little interest in premixed diesel combustion studies where ignition timing is controlled by injection timing. There are further differences as well: several principal HCCI fuel studies (Szybist et al., 2005; Bunting et al., 2007-1; Bunting et al., 2007-2) feature combustion which has lower heat release rates, is phased earlier than, and produces lower engine loads than the premixed diesel combustion mode tested within this study.

The previously noted HCCI combustion studies, along with the principal studies of premixed diesel combustion fuel effects (Kitano et al., 2003; Sugano et al., 2005; Li et al., 2006), use test fuels which vary substantially from standard diesel fuel. The test fuels cover a wide range of cetane number (17-90) and include gasoline-type fuels and primary reference fuels (two component hydrocarbon fuels). Changes of combustion behavior across a wide range of cetane number, as reported in the prior literature, do not reflect the effects found with test fuels featuring a more narrowly specified range of cetane number.

While the work of Risberg et al. (2005) features both port injected HCCI and a late-injection, high-EGR combustion mode comparable to premixed diesel combustion, no corrections were made to account for differences in resulting combustion phasing between test fuels. Several of the studies on fuel effects with premixed diesel combustion also use singular test conditions with fixed injection timing (Li et al., 2006) or fixed ignition timing (Kitano et al., 2003). As discussed within this work (Chapter 4), differences in combustion phasing resulting from fixed injection timing with varied cetane number give rise to apparent cetane number effects. A portion of the present work clarifies this perceived effect.

Extending beyond these prior studies, the present work demonstrates the effect of fuel properties on a premixed diesel combustion mode. The test fuels are specified to cover a narrower range of fuels which is consistent with commercially available diesel fuel. Further, the fuel matrix is expanded to detail the effects of using a nitrate cetane number improver. Finally, principal control parameters including EGR, injection timing, injection pressure, and operating load are swept to quantify the significance of the fuel-caused combustion effects and understand their interdependence on other engine parameters.

1.6 Overview of Dissertation

Chapter 2 provides background material relating to premixed diesel combustion, fuel properties and specifications, and the effect of critical fuel properties on diesel combustion, both conventional and premixed. Chapter 3 provides details about the experimental setup, testing methods, and operating conditions used within this study. Chapters 4-6 cover results and observations of three distinct areas of study related to fuel effects on premixed diesel combustion. Chapter 4 covers the effect of cetane number on combustion and emissions behavior along with injection timing limits. A secondary study demonstrating the impact of using a nitrate cetane improver, 2-ethylhexyl nitrate, on operating behavior and emissions is contained in Chapter 5. A characterization of the tested combustion mode's usable load range, including the effect of varied cetane number, is demonstrated in Chapter 6. The final chapter, Chapter 7, provides an overall summary of the work, a highlight of the important conclusions, and recommendations for future studies.

CHAPTER 2

BACKGROUND

2.1 Summary

There are two elements inherent to an investigation into fuel effects on premixed diesel combustion: (1) premixed diesel combustion, and (2) fuels. Accordingly, this chapter seeks to provide appropriate background about those two subjects. Initially, a background into premixed diesel combustion strategies will be given, followed by a three-part discussion of fuels. The fuels discussion begins with background information about diesel fuels, followed by their effects on conventional diesel combustion (important because of the wealth of information and its ability to explain phenomena within premixed diesel combustion), and finally discussion of recent research results focusing on fuel effects on premixed diesel combustion modes.

2.2 Premixed Diesel Combustion – Historical Perspective

Conventional diesel combustion has long struggled with the tradeoff that exists between particulate matter (PM) and NO_x emissions. Generally, methods of reducing PM lead to increases in NO_x emissions and vice-versa. NO_x emissions are highly dependent on the combustion temperature: higher combustion temperatures yield higher NO_x emissions. In conventional diesel combustion, combustion temperature is largely dependent on the amount of energy released during the early stages of combustion, the bulk of which is premixed combustion. Increasing the ignition delay (the time between the start of fuel injection and the start of combustion) allows for improved fuel-air mixing, resulting in a more substantial premixed burn. This yields higher peak cylinder temperatures and NO_x emissions. However, the enhanced mixing allowed by a greater ignition delay also results in fewer zones within the cylinder possessing unfavorable (rich) carbon-oxygen ratios, zones that are known to form PM. As a result, when mixing time is increased or mixing is enhanced, PM emissions decrease while NO_x emissions increase. The perennial desire of a diesel combustion engineer is to avoid this tradeoff, causing simultaneous reductions in both PM and NO_x emissions, while not incurring a large increase in other gaseous emissions or a significant decrease in engine efficiency.

2.2.1 Required Combustion Properties

To achieve a simultaneous reduction in PM and NO_x emissions, the combustion process must exhibit two seemingly contradictory properties: it must be well premixed and result in low temperatures. The fuel and air in the cylinder must be mixed well enough to avoid regions with unfavorable carbon-oxygen ratios, but the mixture must also be able to sustain combustion to prevent misfires. Second, the temperatures in the combustion process must remain low enough so NO_x is not formed in significant quantities.

2.2.2 Achieving Low Temperature Combustion

Many different researchers have formulated strategies that attempt to simultaneously achieve the two requirements stated above for low PM, low NO_x combustion. Most of the strategies use cooled exhaust gas recirculation, EGR, where a portion of the exhaust gas is cooled and drafted back into the intake system. Cooled EGR reduces NO_x formation through several mechanisms. The first results from EGR dilution of the intake mixture (Ladommatos et al., 1996-1). Additionally the water concentration and CO_2 in the recirculated exhaust gas acts as a thermal sink, absorbing energy released by the combustion process and decreasing the combustion temperature (Ladommatos et al., 1997-1). Finally, the CO_2 in the recirculated exhaust gas slows the production rate of soot precursors (Lida and Sato, 1988). The high levels of EGR used in premixed combustion modes decrease the combustion temperatures enough that the dissociation effect of the CO_2 noted by Ladommatos et al. (1996-2) will be minimal.

2.2.3 Achieving Premixed Combustion

Achieving the desired premixed combustion requires increasing the mixing of the fuel and air prior to ignition. The goal of having the entire combustion event be premixed combustion with no diffusion portion following requires a high degree of fuel-air mixing prior to ignition. However, it is imperative to prevent the fuel and air from becoming mixed to the point where it is too lean to sustain combustion (overleaning). To accomplish this, most new combustion strategies focus on achieving a well-mixed zone. The contents of the zone are well mixed and between the lean and rich limits, but regions outside the mixed zone do not contain any fuel. Therefore, the combustion chamber is locally homogeneous and stratified overall.

Several of the strategies seek to create these well mixed regions by injecting the fuel very early in the engine cycle. The extreme case is early attempts at diesel HCCI (Homogeneous Charge Compression Ignition) where diesel fuel was mixed with the intake air in the intake manifold prior to being inducted into the cylinder (Gray and Ryan, 1997). The low volatility of diesel fuel requires preheating the intake air, and the difficulty of combustion control creates limits on operating conditions. These two factors make this method impractical for implementation anywhere but in a laboratory research engine.

To eliminate the need for intake heating systems, most methods inject the fuel directly into the cylinder, using part of the compression stroke to heat the air in the cylinder to a temperature that will cause the injected fuel to vaporize. In-cylinder direct injection occurring early in the compression stroke is the centerpiece of several methods. Fuel is injected very early in the cycle to give the fuel a long period of time to vaporize and mix, resulting in solely premixed combustion.

To prevent the fuel from mixing over too wide a region, which would result in too-lean mixtures, or wetting the cylinder wall, which would lead to high PM and HC emissions, many of the very early injection timing strategies employ a specialized injector configuration. Toyota’s Uniform Bulky Combustion System, UNIBUS, uses a fuel injector with a pintle-type nozzle featuring a large hole and a bulbous protrusion to reduce penetration and keep the fuel mixture in the center of the cylinder away from the walls (Yanigahara et al., 1997). During different stages of New ACE Institute’s development of their Premixed Diesel Combustion strategy, PREDIC, they utilized two different injection methods to provide spray behavior such that the fuel was in the desired location. Two different injector configurations were used in the early portion of their work: a centrally mounted injector with a three stage (multiple cone angle) injector nozzle, and two opposing injectors such that the fuel sprays from each injector impinge at the center of the cylinder (Takeda et al., 1996). Both strategies create a nucleus of fuel at the center of the cylinder, away from all of the cylinder surfaces. A later strategy utilized the two injector format, but used pintle-type injector nozzles similar to those used by Toyota to reduce the spray penetration (Akagawa et al., 1999). Several studies used injector tips with narrow cone angles to target the spray at the combustion bowl even during advanced injection timings (Walter and Gatellier, 2002; Lechner, 2003; Wåhlin and Cronhjort, 2004; Okude et al., 2004).

One of the main problems with implementing any of the very early injection strategies in a production engine is the strategies are only applicable for a narrow range of operating conditions. Further, the nature of the special injectors used to implement these methods make it impossible to achieve clean conventional combustion at higher load conditions, where premixed combustion cannot be sustained and early injection timings yield poor combustion quality.

Other methods for achieving low soot, low NO_x premixed diesel combustion focus on injecting the fuel at more retarded locations than conventional. Nissan's Modulated Kinetics, MK, strategy injects fuel at retarded timings, even after top dead center (TDC) (Kimura, 2001). The methodology proposed by Jacobs utilizes a single injection occurring before TDC, but still retarded from conventional timings (Jacobs, 2005). These strategies use high levels of cooled EGR to help extend the ignition delay. For the strategies to work, the ignition delay must be extended until it is longer than the duration of the fuel injection and the time required for the fuel to mix effectively. They also utilize the high swirl and turbulence present when the piston is near TDC to enhance mixing, decreasing the time required to achieve the well mixed conditions required for low soot combustion.

The retarded injection timing strategies are more suitable for implementation in a production engine because implementation requires changes required to the engine control software, not to engine hardware. Since both conventional and these novel combustion strategies inject the fuel near TDC, the injection spray targeting is the same and the same injectors can be used during conventional or premixed operation.

2.3 Diesel Fuel

2.3.1 Diesel Fuel Chemical Composition

Diesel fuel is not a single component entity, but composed of numerous different hydrocarbons. The hydrocarbons are classified by their chemical structure into groups exhibiting similar chemical structure, properties, and behavior. Paraffins, also referred to as alkanes, are hydrocarbons with either straight or branched structures and with all single bonds between the atoms. The structure of the chemical is based off the layout of the carbon atoms: in a straight molecule, all of the carbon atoms are in a line, while a branched molecule has carbon atoms lying in multiple planes. Napthenes, also called cycloparaffins, feature a ring structure with single bonds between carbon atoms. Olefins, or alkenes, are similar to paraffins being straight chain or branched hydrocarbon structures, but have at least one double bond between the carbon atoms. Finally, aromatics are hydrocarbons based on one or more benzene rings. Monoaromatics are based around one benzene ring, and polyaromatics, commonly abbreviated PAH, are made up of multiple benzene rings.

The resulting properties of a diesel fuel depend on the concentrations of the different groups of hydrocarbons in the final fuel blend. Within each molecular structure classification, there are variances in properties due to exact number of atoms and structure of the hydrocarbon. Generally, larger hydrocarbons with more carbon atoms have higher density, higher boiling temperature, and lower heat of combustion than other members of their structural class. As classes, the paraffins, napthenes, and olefins all have similar densities, boiling points, and heating values, but olefins are much more reactive because of the presence of an unstable double bond between carbon atoms. Aromatics generally have a higher density and lower heat of combustion than paraffins, napthenes, or olefins, but are also much less reactive due to the stable nature of the benzene ring upon which they are based. The multiple benzene rings in a polyaromatic compound make it very unreactive, even in comparison to monoaromatics.

With the different properties of each hydrocarbon group contributing to the overall characteristics of a fuel, understanding the nature of a fuel is dependent on the hydrocarbon makeup. For example, a fuel with a high aromatic content will be less reactive (resulting in lower ignitability), denser, and have a higher boiling point (indicating a heavier distillate) than a comparable fuel with lower aromatic content. This shows how fuel properties become very interrelated: the final fuel characteristics are based off the properties of a set of groups with interrelated properties. Varying the concentration of one group will change multiple fuel properties simultaneously.

2.3.2 Principal Fuel Property - Ignitability

Cetane Number

Cetane number is a qualitative expression of the ignitability of a fuel. The concept of cetane number was presented by Boerlage and Broeze in a 1932 paper, where they compared the ignition quality of different blends of two reference fuels: cetane ($C_{16}H_{34}$) and mesitylene (C_9H_{12}). Cetane is an ignition-prone paraffin, while mesitylene is an aromatic hydrocarbon that would not combust in the test engine. They measured the ignition delay of the different blends of cetane and mesitylene to establish a chart relating measured ignition delay to cetane concentration in the fuel blend.

The current standard method for determining the cetane number of a fuel, detailed in ASTM International Standard D-613, compares the compression ratio required to achieve a specified ignition delay (ASTM, D613). The base reference fuels are n-cetane ($C_{16}H_{34}$) with a cetane number of 100, and heptamethylnonane ($C_{16}H_{34}$) with a cetane number of 15. Alphamethylnapthalene ($C_{11}H_{10}$), with a cetane number of zero, was used to establish the cetane scale. Current cetane number testing uses two secondary reference fuels: T, a reference fuel with a cetane number of approximately 74-77, and U, a reference fuel with a cetane number of 18-20 (Chevron, T-23, U-16). The test engine used is a Waukesha single-cylinder CFR (Cooperative Fuels Research) variable-compression-ratio prechamber diesel engine. With the CFR engine operating at 900 rpm, fuel is injected at 13 ºBTDC (Before Top Dead Center) and the compression ratio is varied by changing the volume of the prechamber until the fuel ignition point is at top dead center (TDC), giving an ignition delay of 13 crankshaft degrees. This same procedure is carried out with different blends of the T and U reference fuels until the compression ratio required to achieve the 13 degree ignition delay of two reference fuel blends bracket the required compression ratio of the test fuel. The test fuel's cetane number is a linear interpolation, based on the compression ratios, between the blend cetane numbers of the bracketing fuel blends.

Cetane Index

Cetane index is a parameter calculated from a fuel’s distillation characteristics and density, and is an alternative to the engine experimentally determined cetane number. Accepted methods for calculating cetane index are given by ASTM International Standards D976 and D4737, with the latter being the more recent, detailed, and common procedure (Totten et al., 2003). The difference between the two standards is that D976 relates cetane index to the fuel density and mid-boiling (50% recovery) temperature, while D4737 relates the cetane index to density, 10%, 50% and 90% distillation (recovery) temperatures (ASTM, D976, D4737). The cetane index parameter is an approximate prediction of cetane number based on easily measureable distillation parameters.

IQT Derived Cetane Number

The most recent method of quantifying a fuel’s ignitability characteristics is to use an Ignition Quality Tester (IQT™). ASTM International Standard D6890 covers the measurement procedure and correlation to derived cetane number (ASTM, D6890). This device injects fuel, using a representative diesel fuel injector, into a pressurized combustion bomb at controlled conditions. By monitoring the conditions within the bomb, the device measures the ignition delay between time of fuel injection and the start of combustion. This ignition delay itself can be compared across fuels to compare properties, or it can be converted into a derived cetane number, DCN, using a linear correlation.

Limitations of Cetane Number, Cetane Index, and Derived Cetane Number

Cetane number has one main limitation: it is an experimentally determined parameter. As such, the result is subject to experimental variations and uncertainty. Even though the operating conditions are carefully specified, a degree of variation in repeatability does still exist. ASTM International reports the repeatability (repeated tests of a single sample on one engine) of the D613 test at ± 1, and the reproducibility (tests of a fuel at different facilities and times) at ± 5 cetane numbers (ASTM, D613). Several studies into the data scatter associated with the D613 method of determining cetane number established the measurement uncertainty due to repeatability variation ranged from ± 1.6 cetane numbers to ± 5 cetane numbers (Totten, 2003). Furthermore, the cetane number established with the D613 test does not offer a clear prediction of ignition delay in a modern diesel engine, since the CFR engine used in the tests is not representative of most modern diesel engines (Totten, 2003).

Also, the working range of the cetane number test is limited to cetane numbers less than 74, because the T reference fuel (high CN) used in the D613 tests has a cetane number of 74-77. It is not possible to correctly bracket a fuel whose cetane number is outside the range of the secondary reference fuels. This is a limitation because many synthetic (Fischer-Tropsch) fuels have a cetane number exceeding 74.

Calculated cetane index is not applicable for many fuel comparisons, especially not with pure hydrocarbons, synthetic fuels, fuels with cetane-improving additives, or as a comparison between fuels with vastly different chemical compositions (Totten et al., 2003). The correlation was developed based on a limited set of petroleum fuels – fuels possessing properties substantially different than the original set may not follow the trend. As such, the experimentally derived parameter, cetane number, is preferred over the calculated parameter, cetane index.

Derived cetane number, measured by an IQT, was developed to address many of the issues and limitations of cetane number and cetane index. It has the ability to test fuels of a wide range of ignitability characteristics, can correctly quantify fuels with cetane improving additives, uses a combustion system comparable to current engines, and has respectable repeatability characteristics. However, the reproducibility characteristics are not especially improved (on paper at least) over the cetane number engine tests.

2.3.3 Legislated Diesel Fuel Properties

Maximum sulfur content, maximum aromatic content, and minimum cetane number are the primary diesel fuel properties currently controlled by legislation. Within the United States, there are two different fuel standards: one set out by the EPA applicable to all fifty states, and a separate standard established by CARB applicable only to California.

Established in 1993 as an extension to the Clean Air Act, the current EPA standard requires all diesel fuels sold in the US destined for vehicular use have a maximum sulfur content of 500 ppm, a maximum aromatic content of 35%, and a minimum cetane index of 40 (CFR, 80.29). The same legislation decreased the maximum sulfur level to 15 ppm in June 2006, with the maximum aromatic content and minimum cetane index remaining at 35% and 40 respectively (CFR, 80.520).

The fuel requirements established by CARB for diesel fuel used in all non-stationary engine applications in California set the maximum sulfur content at 500 ppm starting in 1993, but this was reduced to 15 ppm in June 2006 (CCR, 2281). There is not a specified minimum cetane number or index, but the federal minimum cetane index of 40 still applies. The maximum aromatic content is 10%, but with the exception that fuels can have an aromatic content up to 20% provided the fuel, when tested in a standardized engine, shows similar cold-start performance and emission levels as a certification fuel with an aromatic content of 10% (CCR, 2282).

European countries also legislate the properties of diesel fuel for vehicular use. The European Union has established an outer set of limits on fuel properties, but some countries have enacted stricter standards. European Union directives establish that, starting in 2005, all fuels destined for on-road use must have a maximum sulfur content less than 50 ppm (EPC, 98/70). Additionally, by 2009, there must be a complete Europe-wide availability of diesel fuels with zero sulfur content (EPC, 2003/17). The minimum cetane number of European diesel fuels is 51, and the maximum aromatic content is 11% (EPC, 98/70).

Along with the property controlling legislation, there are also other controlling standards for diesel fuels. In the United States, diesel fuels are classified according to ASTM International Standard D975 into three different grades: 1-D, 2-D, or 4-D (ASTM, D975). The lowest grade, 4-D, is for heavy distillations of diesel fuel that are solely used on stationary or marine engines, and therefore is not applicable to automobile bound fuel. The two lighter grades, 1-D and 2-D, are the two grades used in automotive applications. Diesel fuel classified as 1-D is a lighter distillation than 2-D diesel fuel, with a lower boiling temperature range. As a result, numerous other properties are different between the two different grades of diesel fuel. European diesel fuels are classified into 11 different grades by the EN590 standard (CEN, EN 590:2004). The classifications, like those set out by the ASTM D975 standard, relate to the distillation properties of the fuel, which are dictated by the climate the fuel is destined for. Both the D975, and EN 590 fuel standards set either a wide range of acceptable values or a limit value for the different fuel properties. As an example, the boiling range limits set by the D975 standard mandate the 1-D diesel fuel have a T90 (90% recovery temperature) less than 288 ºC and 2-D diesel have a T90 between 282 ºC and 338 ºC. Fuels can vary substantially and still be within these standards.

With these fairly loose fuel property requirements, there is wide variation in properties of the fuels produced for these markets. Fuels are also modified to give different properties depending on the climate and time of year. For example, a fuel destined for a colder geographic region in the winter will tend to be lighter and have a higher cetane number than a fuel for a warm climate to make it easier to start the vehicle's engine in cold weather.

Fuel properties are also not consistent across a single fuel company. The fuel distribution system (interstate transport – pipelines, rail, and trucking) in the United States is separate from the fuel companies (refineries, local transport, and fueling stations). A fuel company puts a certain quantity of fuel into the distribution system at the refinery, and then takes that quantity out of the distribution system at a different hub. However, the fuel they take from the system is not necessarily the same exact fuel they put into the system, but rather a blend of fuels with similar properties from different refineries. This is especially true when the fuel is transported in pipelines, as pipeline companies prefer to operate in fungible mode where they ship bulk quantities of material that meet a set of specifications, and the delivered product is not the product submitted for shipment (EIA, 2001). Fungible shipping through pipelines is the preferred method of regional transport for non-specialized fuels because of its low cost, short shipping time, and undemanding storage requirements (EIA, 2001). Because fuel companies decrease their transportation cost by using fungible shipping methods, the fuel they sell is a mix of fuels refined by different companies. The exact fuel makeup is normally slightly different from batch to batch, even though all the batches meet ASTM standards and are legal within EPA or CARB regulations.

2.4 Fuel Property Effect on Conventional Diesel Combustion

Copious research has been published which analyzes the effect of different fuel properties on engine performance and emissions. Primarily, this prior research focuses on running a carefully prescribed set of fuels in a production engine over either a transient driving cycle or multiple point steady state mode tests, and comparing the overall emissions produced. Unfortunately, the effects measured may not be universal effects, but more the effect on a specific set of engine hardware and controls. Several studies have noted that fuel property effects can be highly engine specific. A study which tested 30 fuels on five different engines found that each engine behaved differently, and that the differences could neither be attributed to the technological level of the engine, nor to the specifics of the test setup (Cowley et al., 1993). A literature review of diesel fuel tests, which included Cowley et al., also shows the same phenomenon across a wider range of engines and test programs (Lee et al., 1998). Additionally, another paper establishes that the engine response to a fuel property change is affected by the reaction of the Engine Control Module, ECM, to sensor feedback related to the fuel property change (Mann et al., 1998).

2.4.1 Influence on Mixing Process and Ignition Delay

Much of the impact fuel properties have on combustion relates to their impact on the mixing process and ignition delay. Therefore, understanding the effect of these changes on the combustion process is critical.

An improvement in the mixing process results in a greater quantity of fuel and air being premixed before ignition. When this larger fuel/air mixture combusts, it does so in a rapid and intense manner. An increase in the premixed portion of combustion causes a corresponding reduction in the diffusion portion of the combustion, leading to higher post-flame gas temperatures. The heat release rate for premixed combustion is substantially higher than that of diffusion combustion, and occurs prior to it. Accordingly, an increase in the premixed fraction results in more energy being released over a short time scale close to TDC with a nearly constant combustion chamber volume, resulting in higher gas temperatures. NO_x forms in the high post flame gas temperature conditions by the thermal mechanism (Zeldovich, 1946; Lavoie et al., 1970). However, these higher gas temperatures also lead to the increased oxidation of soot particles.

Additionally, soot formation is tied to the amount of diffusion combustion, so a decrease in diffusion combustion reduces the amount of soot formation. An improvement in the mixing process results in a decrease in soot formation due to the reduced diffusion burn and the increase in soot oxidation by the high gas temperatures. However, NO_x emissions are higher because of the high gas temperatures resulting from increased premixed burn.

Reducing the effectiveness of the mixing process results in a smaller quantity of fuel that is well mixed with the air by the time of ignition. This translates into a smaller premixed burn, resulting in a larger diffusion burn and lower combustion gas temperatures. The reduced gas temperatures lead to a decrease in NO_x formation, but also a decrease in soot oxidation. Additionally, the increase in diffusion burning leads to an increase in soot formation. The combination of these factors results in an overall increase in soot emissions.

2.4.2 Cetane Number Effect

The cetane number of a fuel is a general indication of ignition delay length, with higher cetane fuels exhibiting shorter ignition delays in a test engine (Boerlage and Broege, 1932). However, this is not necessarily a direct correlation. Wilson and Rose (1937), using an open chamber diesel engine showed that there was a fundamental minimum ignition delay for all fuels regardless of cetane. By maintaining a constant compression ratio and varying the ignition timing, they noted that when the injection occurred after a set timing, the ignition delay was constant for all fuels; earlier injection timing caused an increase in ignition delay, generally corresponding with cetane number. In a more modern engine, it was noted that ignition delay was correlated, albeit in a non-linear way, with cetane number (Wong and Steere, 1982).

With all other fuel properties constant, a fuel with a higher cetane number will generally have a shorter ignition delay, resulting in a smaller premixed burn portion of combustion. The shorter ignition delay allows less time for the fuel and air to mix properly, resulting in the smaller premixed burn. A longer ignition delay gives the fuel and air more time to mix, so a greater degree of fuel/air is mixed at the time of ignition, which results in a larger premixed burn. Too long an ignition delay results in mixture overleaning (mixture becomes too lean for ignition) causing a misfire.

The magnitude of emissions effects to variations in cetane number is dependent on the original level of emissions produced by the engine. In modern diesel engines producing a relatively low level of emissions, changing the cetane number of the test fuel often resulted in a negligible change in the output emission (Lee et al., 1998). The effect is more apparent on older higher polluting engines, or engines with older, less advanced, ECM software calibrations (Ullman et al., 1994).

Increasing the fuel cetane number improves HC and CO emissions in older, higher polluting engines, with negligible effect on modern engines (Ullman et al., 1994; Lee et al., 1998; Kidoguchi et al., 2000). CO and especially HC emissions are linked to injection behavior and especially to the interaction between fuel properties and the injection process. Fuel parameters which are frequently complimentary to cetane number (density, hydrocarbon composition, and individual hydrocarbon species levels) cause slight perturbations in fuel injection behavior which lead to significant shifts in CO and HC emissions production. The change in ignition behavior (as indicated by cetane number) is not responsible for the effect, but simply a reflection of the responsible properties. The high-pressure, multiple-injection strategies used by modern engines are less responsive to these effects than the single injection strategies used on older engines.

The impact of increasing cetane number on NO_x emissions is favorable, producing a slight reduction in most engines, including many modern engines, but the effect is still quite small. The reduction of NO_x with increasing cetane is due to the resulting shortened ignition delay causing less premixed burn and a greater diffusion controlled portion (Ullman et al., 1994; Lee et al., 1998; Kidoguchi et al., 2000). It is generally known that decreasing the amount of premixed burn reduces the peak pressures and temperatures in conventional diesel combustion causing a decrease in NO_x production (Heywood, 1988). Balancing this, a decrease in premixed burn with higher cetane fuels causes an extended diffusion burn, increasing combustion duration and resulting in increased PM emissions (Kidoguchi et al., 2000). Thus, a PM - NO_x tradeoff can exist between combustion of fuels with different cetane numbers.

Furthermore, cetane variations can cause load specific effects: at low engine loads, the ignition delay is long enough with low cetane number fuels that they tend to overmix, leading to lean mixtures incapable of supporting combustion (Kidoguchi et al., 2000). For engines with a single injection, this can lead to misfires and resulting high HC emissions. For engines with multiple injections (pilot + main), lack of pilot combustion can lead to an unintended large premixed combustion during the main injection, resulting in high NO_x emissions and loud combustion noise (diesel knock).

2.4.3 Effect of Aromatics

Conclusions of prior research often disagree on the exact effect of aromatic content on combustion behavior and emission formation. Many of the changes appear to be due to engine specific responses and, perhaps more importantly, the method the researchers used to isolate the effect of aromatics. Many other fuel properties are strongly affected by aromatics concentration, and the specification of the fuels tested has a significant impact on the results of the work. Especially relevant is the connection between aromatic content and cetane number. Increasing the aromatic content of a fuel has been shown to decrease the fuel cetane number (Gülder et al., 1985). The implications of this are important, as cetane number is correlated to ignition delay, which will have an impact on the nature of the combustion (Wong and Steere, 1982).

A literature survey by Lee et al. (1998) reports that HC, CO, and PM emissions generally remain unchanged with variations in fuel total aromatic content. NO_x emissions from their tests are slightly reduced by decreasing the total aromatic content of a fuel. The impact of reducing polyaromatic hydrocarbon, PAH, concentration in the fuel is more consistent and beneficial. A reduction in PAHs yields a decrease in NO_x and HC emissions, and has no effect of PM or CO emissions. Decreasing aromatics slightly reduces the flame temperature, and reduces the number of oxygen radicals due to a more beneficial C/H ratio in the fuel. Both of these phenomena correspondingly reduce NO_x formation.

Ladommatos et al. (2000) completed a series of tests on a single-cylinder CFR engine that analyzed the impact of total aromatic, monoaromatic, and diaromatic content on diesel combustion. Starting with a GTL synthetic diesel fuel with zero measurable aromatic content, they doped the fuel with different levels of European low sulfur diesel (containing mono, di, and triaromatic compounds totaling 27%), toluene (a monoaromatic compound), and methylnaphthalene (a diaromatic compound) to create a series of fuels with varying aromatic content. Due to the similar base fuel stock, the resulting fuels had similar distillation characteristics and sulfur levels. Cetane numbers of the fuels varied according to aromatic content, and were generally higher than typical available diesel fuels (CN = 60-64). Results of engine tests based on the ASTM International D613 test show that ignition delay is directly related to total and monoaromatic content in a linear fashion. Replacing monoaromatic content with diaromatic content in two test fuels causes a small, but consistent, increase in ignition delay. Reflecting ignition delay effects, cetane number decreases in a linear fashion with total and monoaromatic content, illustrating a direct connection between changes in aromatic content and cetane number for their fuel blend.

The results of Ladommatos et al. show HC, NO_x, and smoke emissions generally trending upwards with an increase in total and monoaromatic content, with smoke being the most linear effect. However, inconsistencies within the emissions measurements indicate that engine specific details may be playing a role. It should be noted that the CFR engine used in cetane number tests is an indirect injection prechamber engine, which is drastically different from current production engines. The correlation showing HC and smoke emissions increase with monoaromatic content disagree with the conclusions of prior research work (Lee et al., 1998), further illustrating the impact of engine specific effects, and the interrelation of fuel properties.

A test where total aromatic content was varied while keeping cetane number constant by changing the ratio of normal and iso-paraffins demonstrates that aromatic content does not affect the combustion characteristics of an engine when cetane number is held constant (Kidoguchi et al., 2000). The primary impact of increasing the aromatic concentration is to increase soot and PM emissions, believed to be a result of incompletely oxidized aromatic compounds polymerizing directly into polycyclic hydrocarbons, PAHs. The benzene ring that an aromatic compound is based on is inherently stable, making oxidation difficult, and incomplete oxidation likely (Owen and Coley, 1995).

Kouremenos et al. (1999) sought to isolate the effect of mono, di, and triaromatics on combustion and emissions. The total aromatic content was kept constant across their test fuels, and the cetane numbers of the test fuels were adjusted to be as close as possible. The conclusion of their work is that for a given total aromatic content, the ratio of mono, di, and triaromatics does not have a significant effect on combustion behavior or emissions. This does not contradict the findings of Ladommatos et al., as the fuels in this test were doped so that the cetane number remained constant across all of the fuels. This adjustment of the cetane number insured that the ignition delay, which was the bulk of the Ladommatos et al. study, remained nearly constant.

2.5 Fuel Effect on Premixed Diesel Combustion – Existing Literature

At the beginning of this research project, there was very little published work regarding the effect of fuel properties on low-temperature premixed combustion strategies. Significant work had been conducted and published on fuel effects on conventional diesel combustion, but only one main group had published on premixed diesel combustion fuel effects.

Kitano et al. (2003) investigated the effect of distillation characteristics and cetane number on premixed diesel combustion, termed PCCI combustion in their work. Their work indicates lighter and more volatile fuels improve mixture formation. However, as a result of this improved mixture formation, the mixture becomes increasingly too well mixed, with larger areas that are too lean to support combustion, leading to increased HC emissions. Decreasing the fuel cetane number increases the ignition delay, allowing the injection timing to be advanced and premixed combustion sustained under higher load conditions, yielding a decrease in NO_x emissions at the high load conditions compared to conventional. However, at lower loads, the poor ignitability of the lower cetane number fuels requires a decrease in EGR rate to prevent misfires, which increases NO_x emissions compared to the higher cetane number fuels. Thus, they established that the optimum cetane number for PCCI combustion is dependent on the engine load: high load requires a low cetane fuel to have a long enough ignition delay, but low load requires a higher cetane number fuel to enable the EGR rate to be optimized for minimal emissions.

Since the study by Kitano et al., there have been further studies investigating the effects of various fuel properties on many of the various forms of premixed diesel combustion or diesel fueled HCCI combustion. The differences between these combustion strategies frequently make it difficult to apply the results of the different studies (e.g. late injection vs. early injection vs. port injection). The primary variable in most previous studies was cetane number, not surprising since cetane number is one of the foremost methods of quantifying diesel fuel.

Using experimental and modeling methods, prior studies investigated various aspects of novel diesel combustion with respect to cetane number. The general finding is that increasing the fuel cetane number results in a shorter ignition delay (Kitano et al., 2003; Sugano et al., 2004; Risberg et al., 2005; Li et al., 2006; Bunting et al., 2007-1, Bunting et al., 2007-2). This can be viewed as an expected result, since cetane number itself is essentially an experimental characterization of ignition delay in a standardized engine (ASTM, D613). However, it is noteworthy since small changes in cetane number have been reported to not have a strong effect on modern engines operating with conventional diesel combustion (Massa et al., 2007). Significant changes to fuel composition and cetane number have been shown to make a difference, however (Maly et al., 2007).

Also common are studies that investigated the operable load range as a function of cetane number. The general holding is that lower cetane number fuels yield larger operating ranges since their longer ignition delay allows for additional premixing, even as load and/or engine speed increases (Kitano et al., 2003; Li et al., 2006). Other studies detail changes in general combustion phenomenon with respect to fuel variances, including characterization of low temperature heat release (Bunting et al., 2007-2) and combustion as a whole (Kusaka et al., 2004).

Implications of cetane number on emissions show strong dependency on the combustion strategy, and particularly the analysis methods. One study reports NO_x increases with increasing cetane number in a late injection premixed diesel combustion mode (Kitano et al., 2003), while another shows NO_x decreasing with an increase in cetane number in a diesel HCCI engine (Szybist et al., 2005). Additionally, another indicates that NO_x emissions from heavy-duty diesel HCCI combustion can be minimized to similar values if the combustion was optimized for each fuel, with the exact method unspecified (Bessonnette et al., 2007). A further paper suggests that NO_x appears higher for higher cetane number fuels in a diesel HCCI engine, but is principally a function of the ignition delay, and if ignition delay is held constant, NO_x is independent of cetane number (Risberg et al., 2005). Additionally, it reports that CO emissions are tied to ignition delay, and HC emissions to combustion phasing, with both remaining relatively independent of cetane number (Risberg et al., 2005). However, in a different study, the hydrocarbon and carbon monoxide emissions are shown to be a function of cetane number, though they trend in a similar fashion as the previously noted study (Szybist et al., 2005).

CHAPTER 3

EXPERIMENTAL METHODS

3.1 Experimental Setup

The test engine used in this study is a single-cylinder version of a production diesel engine. The cylinder head and intake manifold system are kept as unmodified as possible so that the in-cylinder flow characteristics of the single-cylinder engine are similar to the production engine. However, unlike the production engine, all other engine systems are controlled individually to give the highest degree of freedom possible. For example, changes in boost on the parent production engine require changing the turbocharger VGT settings, which cause changes in other parameters such as backpressure and EGR rate. On the single-cylinder engine, these effects are decoupled: boost can be adjusted mainly independent of other parameters. Finally, the engine is well instrumented to provide detailed and accurate measurements of its behavior.

3.1.1 Engine System

The work of this research project was carried out on a single-cylinder version of a General Motors (GM) 1.7 liter high-speed direct-injection four-cylinder diesel engine. The engine is based on a Ricardo Hydra crankcase, but utilizes a specially built cylinder jug and liner. A cylinder head from a production GM 1.7 liter Circle-L engine is employed with the valve gear removed from the three unused cylinders. Figure 1 shows the test engine system, and Table 2 gives detailed specifications of the test engine geometry.

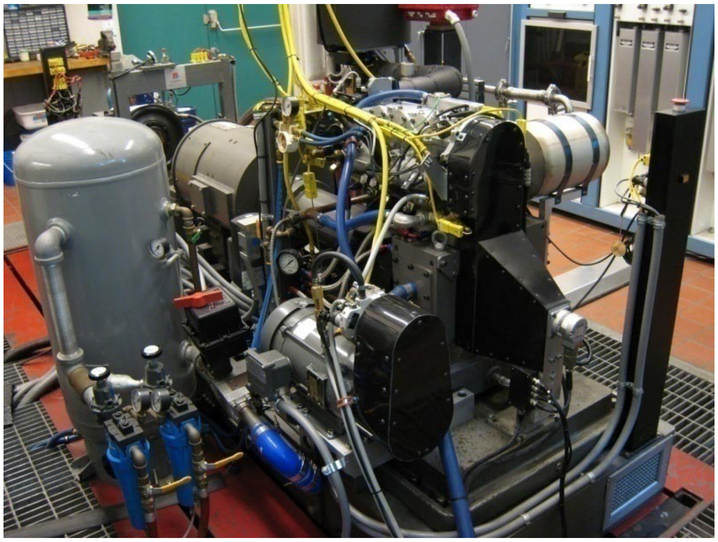


Figure 1: Single-cylinder GM Circle-L derivative diesel research engine.

Number of Cylinders	1
Displacement	425 cm^3
Bore	79.0 mm
Stroke	86.0 mm
Connecting Rod Length	160.0 mm
Wrist Pin Offset	0.6 mm
Compression Ratio	15:1
Valves per cylinder	4
Camshafts	2
Injector Nozzle Hole Number	6
Injector Nozzle Spray Angle	150 degrees
Injector Flowrate	320 cc/30s
Intake Valve Open (IVO)*	366 ºBTDC-c
Intake Valve Close (IVC)*	136 ºBTDC-c
Exhaust Valve Open (EVO)*	122 ºATDC-c
Exhaust Valve Close (EVC)*	366 ºATDC-c

Table 2: Basic specifications of the single-cylinder test engine.

* Valve timings are specified at 0.1 mm valve lift

One important difference from the production engine is the decreased compression ratio. In a related prior study, Lechner decreased the compression ratio of his test engine (multi-cylinder GM 1.7L) from 19:1 to 16:1 by employing a piston with a new, larger volume, piston bowl geometry (Lechner, 2003). The same piston geometry used in the prior work by Lechner (2003), Jacobs (2005), and Knafl (2007) is utilized in this single-cylinder test engine. However, engine specific differences (different valve cutout profiles in the piston, possible head gasket thickness) results in a lower, 15:1, compression ratio.

3.1.2 Engine Swirl Control

Swirl can be controlled with a manually selectable valve that restricts flow entering through one of the intake ports. The two different intake ports cause different levels of swirl in the cylinder, with the overall swirl in the cylinder the balance of the high and low swirl from the two ports. Closing a throttle in the low-swirl port generates higher levels of swirl but with a corresponding increase in flow losses due to the reduction in port area. The production port throttle is used in the single-cylinder engine with 10 different positions, every 10 degrees from open to closed. The production port throttle does not fully block the low-swirl port, so the swirl ratio varies over a small range, from 2.8 to 3.2. This is a reflection of its intended use – calibration engineers use the swirl control to provide small tweaks to the final engine control calibration. Extending the port throttle plate to fully block the port would increase the range of swirl numbers up to 5.6. Testing revealed that changing the position of the swirl throttle between 2.8 and 3.2 did not enhance combustion, but rather merely lead to increased flow losses. Accordingly, all tests were operated with the swirl valve fully open, yielding the overall swirl number of 2.8.

3.1.3 Fuel Injection System

The single-cylinder test engine uses the Bosch 1400 bar common rail injection system from the production engine. The stock Bosch 1210 common rail injector is retained, along with the factory selected copper depth spacer which sets the injector at the depth optimized during factory assembly. The timing, duration, and number of injections are controlled with an engine controller made by GENOTEC Electronik. This unit allows for up to nine independent injection events per engine cycle. Injection timing is controlled to within ± 0.1 crankangle degrees, based off the minimum resolution of the encoder. Injection duration (pulsewidth) is adjusted in increments of 1 μs.

A Bosch CP3 high pressure pump, driven through a 4:3 reduction belt drive by a 3.7 kW (5 hp) electric motor, supplies high pressure fuel to the production fuel rail. The production supply line and injector for the number one cylinder are retained, with the three unused ports sealed off. Fuel rail (injection) pressure is modulated by a flow control valve on the CP3 pump, which restricts inlet fuel flow. Adjusting and maintaining fuel pressure requires balancing the controlled flow into the pump and the quantity of fuel injected into the cylinder. A Labview based Pulse Width Modulation (PWM) controller manufactured in-house provides PID control over the fuel control valve, and therefore rail pressure.

3.1.4 Intake System

The engine is operated on oil-free, dry compressed air. Entering the test cell at 6.2 bar (90 psi), the compressed air runs through two desiccant air dryers which reduce the humidity to a dew point temperature of -40 °C. The dry air is then filtered with grade three coalescing air filters to remove oil down to a concentration of 1 part per billion. A large surge tank is employed to damp out abrupt changes in supply pressure. Downstream of the supply surge tank is a two-stage set of electrically operated valves that provide pressure and flow control for the intake air. A process-controlled 3500 Watt electric heater is used to heat and maintain the intake air at 65 °C, measured in the intake manifold. A second smaller surge tank is used to damp out the pulsating intake flow into the single-cylinder engine to allow for accurate measurement of intake pressure. For accurate pressure measurements, the intake surge tank for a single-cylinder engine needs to be at least 50 times the displaced cylinder volume (Taylor and Taylor, 1962). The surge tank used for this test engine has a 22.4 liter volume, or 53 times the engine displacement. Following the surge tank, the intake air joins the production intake system. The production intake system is retained from the port throttle/EGR valve unit through the intake manifold. A three millimeter thick blanking plate blocks the flow from the manifold to the cylinder ports of the three unused cylinders.

3.1.5 Exhaust System

The production engine exhaust manifold and turbocharger are not used on the single-cylinder engine. Instead, a short exhaust runner attached to a 7.85 liter (18.5 times the engine displacement) exhaust surge tank. This, like the intake surge tank, dampens the pulsating flow that occurs from a single-cylinder engine. Mounted downstream of the surge tank is a manually adjusted ball valve used to control the exhaust backpressure (manifold pressure).

3.1.6 Exhaust Gas Recirculation

Exhaust gas recirculation (EGR) is heavily used on this test engine. Exhaust gas is drawn off the main exhaust pipe immediately after the surge tank. A needle valve provides control over the amount of EGR flowing into the intake system and a cooler is used to decrease the EGR temperature. Typical EGR coolers, including the cooler used on the production 4-cylinder version of this engine, cool the EGR by circulating engine coolant through a heat exchanger, but the EGR cooling setup on the single-cylinder engine uses a separate cooling system that is independent of the engine cooling loop. This allows for independent control over the temperature of the coolant, giving more flexibility in the EGR temperature. The cooling system is a simple single loop system similar in design to the oil and engine coolant systems, and the coolant is a 50:50 mixture of ethylene glycol and distilled water.

EGR is fed into the intake system directly before the intake surge tank to allow for proper mixing to take place in the tank before the intake air goes into the engine. The quantity of EGR inducted into the engine is computed by comparing the concentration of CO_2 in the intake stream to CO_2 concentration in the exhaust gas, with the calculations described further in the Section 3.2. The CO_2 in the intake stream is measured on a dry basis by a Siemens Ultramat 23 Infrared analyzer. This analyzer is mounted in a stand-alone sample cart with full gas conditioning including a sample pump, a filter to remove soot, and a chiller to remove the water from the sample gas. The sample port for the CO_2 measurement is located in the intake manifold, immediately after the intake throttle where EGR is normally introduced into the engine. By this point, the EGR and fresh intake air should be well mixed.

3.1.7 Engine Coolant System

The engine cooling system is a single loop system with a 0.18 kW pump, an immersion heating element, and a heat exchanger. The immersion heater is used for coolant preheating and remains on throughout engine operation. A process temperature controller monitors the coolant temperature and when coolant temperature exceeds the desired setpoint, opens an electrically actuated valve allowing city water to flow through the heat exchanger. The city water cools the engine coolant and then is drained into the trench. This system does not provide the same degree of stability as a two-loop simulated radiator system, but is smaller and less complex. The coolant is a 50:50 mixture of ethylene glycol and distilled water.

3.1.8 Lubrication System

A five quart wet sump oiling system provides lubrication and, with the piston oiljet, piston cooling to the test engine. Oil pressure is set at 4.2 bar (60 psi) with the oil at 85 °C for all engine test conditions. Temperature control of the lubricating oil is achieved using a cooling system similar to the system used for the engine coolant system. The production Positive Crankcase Ventilation (PCV) system is not used. Instead, breather hoses to provide crankcase and valve cover ventilation are tied together and vented to atmosphere near the test cell's ventilation system exit.

3.1.9 Fuel System

Fuel is measured and supplied by a Max 710-100 Fuel Flow Measuring System. Fuel supply comes from either the Autolab main fuel tanks or from a 5 gallon can. In either case, the fuel passes through a 10 micron and then a 2 micron fuel filter before entering the fuel measurement and supply unit, which consists of a variable pressure transfer pump, fuel cooler, and flowmeter. A second 2 micron fuel filter is mounted downstream of the fuel supply unit before the high pressure pump. The fuel unit supplies the fuel to the high pressure pump on the engine at 1.05 bar (15 psi). Fuel flowrate is measured by a MAX model 213 positive displacement piston flowmeter.

3.1.10 Exhaust Emissions Measurement

Gaseous engine emissions are measured with a Horiba 200 Series emissions bench. This machine gives steady state measurement of carbon dioxide (CO_2), oxygen (O_2), carbon monoxide (CO), and NO_x ($NO + NO_2$). Hydrocarbon (HC) emissions are measured with a separate Horiba emissions bench.

The NO_x analyzer is a Horiba CLA-22A chemiluminescent analyzer. Both the carbon monoxide and carbon dioxide analyzers are Horiba AIA-23 Non Disruptive Infrared (NDIR) analyzers. The oxygen analyzer is a Horiba MPA-21A paramagnetic analyzer. A

Horiba FIA-34A-2 heated flame ionization detector (FID) measures the total hydrocarbon emissions.

Two separate ports for the emissions benches are located downstream of the variable exhaust backpressure valve. Heated remote sample filters remove particulates from the gaseous emissions samples before the gaseous exhaust sample flows to the emissions benches through heated lines operating at 190 ºC.

Particulate emissions are measured with an AVL 415S particulate smokemeter. This instrument compares the reflectivity of clean filter paper to filter paper where 3000 mL of exhaust have flowed through it. The system outputs Filter Smoke Number on an AVL 4210 Instrument Controller and the data is logged manually. Filter Smoke Number (FSN) is defined as the function of post flow reflectivities for a set flow quantity through the filter paper (ISO, 10054). Four smokemeter samples are taken at each operating condition and their results averaged.

3.1.11 Data Acquisition

Cylinder pressure is measured in the engine with a water-cooled Kistler 6041 piezoelectric pressure transducer. Filtered city water at 3.4 bar (50 psi) is used to cool the transducer. The signal from the pressure transducer is sent to a DSP Technologies 1104CA charge amplifier, and then to the DSP technologies high-speed data acquisition system. Within the DSP Technologies charge amplifier, a low-pass filter with a cutoff frequency of 12.5 kHz removed noise from the cylinder pressure signal. The pressure transducer was calibrated before the engine tests using a dead-weight pressure calibration at six different pressures, with each point repeated three times for consistency.

The high speed data acquisition system is a DSP Technologies CAMAC crate based system. A 100 kHz model 2812 digitizer provided a sampling rate that, along with a BEI 1800 pulse per revolution optical encoder, gives measurements every 0.2 crankangle degree up to the maximum engine speed of 2000 rpm. Three 4325 TRAQ RTP real time processing units provide real time calculation of pressure based parameters including Indicated Mean Effective Pressure (IMEP), the parameter used to monitor engine load.

The high speed data acquisition system software was DSP Red Line ACAP 5.0d. Since the piezoelectric cylinder pressure transducer measures gauge pressure fluctuations only, not absolute pressure, the pressure must be referenced (pegged) to a point in the cycle. During all tests, the software averages the cylinder pressure for the five degrees after bottom dead center of the intake stroke. The absolute pressure at this point in the engine cycle is pegged to the pressure in the intake manifold, as measured by the manifold absolute pressure (MAP) sensor.

Other signals measured by the high-speed data acquisition system include manifold pressure (used for pegging the cylinder pressure transducer), fuel injection line pressure, and injector current. Fuel injection line pressure and the injector signal are monitored to provide details of actual injector and injection behavior in the absence of a needle lift sensor which would directly measure the opening and closing of the injector needle. Needle lift sensors are not available for the Bosch injector used in the test engine. Fuel line pressure is measured with a Kistler model 4329A2000 piezoresistive transducer. Injector signal current is monitored with a Pearson model 411 current sensor with the wire wrapped through twice to give improved measurement resolution. The GENOTEC controller also provides a secondary current measurement which closely matches the one from the external current monitor.

Combustion noise is measured using an AVL 450 Combustion Noise Meter. This instrument uses correlations based off a filtered version of the cylinder pressure to output an estimated engine noise level in decibels.

Low speed data acquisition of engine and emissions parameters is conducted using a 32 channel Measurement Computing A-D converter board, with logging and display handled by in-house developed Labview program. The data sample rate is 10 Hz, and 10-cycle averages were logged for 200 seconds. The sample time is long to eliminate cyclic variations in emissions and fuel measurements.

3.2 Principal Operating Condition Development

The primary operating condition is a light load condition based off a condition from related prior research on the parent multi-cylinder GM engine. This prior research specifies a condition with a speed of 1500 rpm and a brake mean effecting pressure, BMEP, of 375 kPa (Jacobs, 2005; Knafl, 2007). An equivalent of this point, redefined for the single-cylinder engine, is used as the primary operating condition.

3.2.1 Derivation of Single-Cylinder Equivalent Condition

While the operating condition on the multi-cylinder engine used in prior research was based off BMEP, a brake based parameter, using this same definition for a single-cylinder engine is not appropriate. There are distinct differences between the single and multi cylinder versions of the engine when it comes to brake (torque) measurements. For example, the single cylinder engine will likely have higher friction loads because the crankshaft and bearings are different and the engine is running a full length set of camshafts for only one cylinder. At the same time, the single cylinder engine does not have any of the accessory loads, such as the coolant, oil, and high pressure fuel pumps. Combining all of these differences, it is clear that comparing parameters based on overall engine torque output is not representative.

Examination of data taken on the multi-cylinder version of the GM engine showed that both the average IMEP and the IMEP of the number one cylinder (the one used on the single-cylinder engine) centered around 500 kPa (5 bar), with individual point variations of ± 30 kPa, as shown in Figure 2.

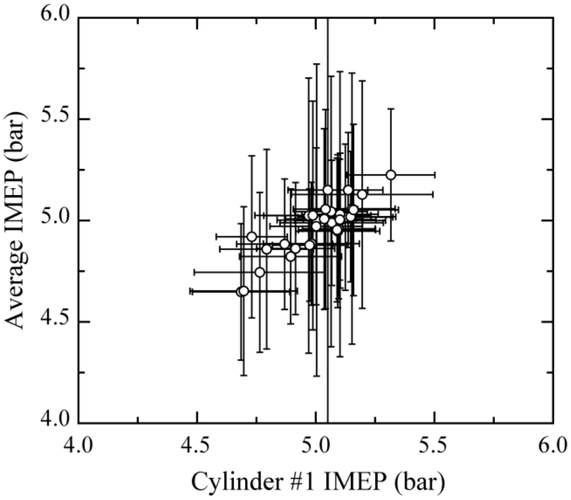


Figure 2: Average versus cylinder 1 IMEP for operating condition on multi-cylinder engine. Tests at 3.75 bar IMEP with varied injection timing and injection pressure. Both average and cylinder one IMEP center around 5 bar IMEP. Data courtesy of Alex Knafl.

There is a particularly strong degree of similarity between the cylinder one and average IMEP. Cylinder one is, more so than the other cylinders, very representative of the average IMEP. Based off these results, the engine load for the corresponding condition on the single-cylinder engine was defined as an IMEP of 500 kPa (5 bar). During the single-cylinder tests, fueling was controlled to maintain 200-cycle average IMEP within ± 2 kPa, with no single cycle exceeding ± 20 kPa from the specified 500 kPa operating point.

3.2.2 Operating Condition Parameters

Additionally, other important control parameters are based upon measurements from the multi-cylinder version of the engine. Manifold pressures can have significant impact on combustion. The absolute intake manifold pressure was fixed at 100 ± 0.2 kPa, to match the intake manifold pressure measured on the multi-cylinder engine during PCI operation at the specified condition. Exhaust manifold pressure was not measured on the multi-cylinder engine, so it could not be matched. Instead, a constant 10 kPa differential between the intake and exhaust manifolds was specified, fixing the absolute exhaust manifold pressure at 110 ± 0.5 kPa. There is a slight dependency of exhaust manifold pressure on injection timing: retarded injection timings phase combustion later, yielding slightly higher cylinder pressure at exhaust valve opening, which results in a slightly higher exhaust manifold pressure. The exhaust backpressure valve did not give sufficient control resolution to eliminate this effect, which is why the exhaust manifold pressure specification has a slightly higher level of accepted uncertainty than the intake manifold pressure. Its overall effect on combustion is also less than the intake manifold pressure, and hence the larger tolerance is acceptable. Both oil and coolant temperatures were maintained at 85 °C.

3.3 Measurements

3.3.1 Gaseous Emissions Indexes

The gaseous emissions CO_2, CO, NO_x, and HC are reported as a per-mass-fuel emissions index. While CO_2, CO and NO_x are all measured on a dry basis due to the constraints of the emissions bench analyzers, they are converted to wet basis and reported as such. The emissions index for a given gaseous emission is the form of Equation 1 (Stivender, 1971).

$$EI - EMM = [EMM]\left(\frac{MW_{EMM}}{MW_f([CO] + [CO_2] + 3[C_3H_{3\alpha}])}\right) \tag{1}$$

Where:

EI-EMM :	Emissions index (g/kg-fuel) of species EMM, wet
MW_{EMM} :	Molecular weight of species EMM
MW_f :	Molecular weight of fuel per carbon atom
[ ]:	Exhaust species concentration, wet
$C_3H_{3\alpha}$:	Hydrocarbon emissions, on C_3 basis, wet

For HC emissions: MW_{EMM} is set at 83.25 to reflect the EPA definition of a hydrocarbon, and the overall expression is halved to account for the EPA definition of HC emissions on a C_6 basis.

3.3.2 EGR Rate

The flowrate of EGR is calculated by comparing the concentrations of CO_2 in the intake and exhaust gas streams. The individual concentrations are converted to a wet-basis, and then used to calculate EGR flow rate on a mass flow based percent, using Equations 2 and 3 (Stivender, 1971).

$$EGR = \frac{100}{1 + \frac{MW_a}{MW_e}\left(1 + \frac{1}{AF_{avg}}\right)\left(\frac{100}{m} - 1\right)} \tag{2}$$

With:

$$m = 100\,\frac{(100 + [H_2O]) * [CO_2]_{intake}}{[H_2O] * [CO_2]_{intake} + 100[CO_2]_{exhaust}} \tag{3}$$

Where:

EGR:	EGR mass percentage, wet
MW_a:	Molecular weight of air (28.96)
MW_e:	Molecular weight of EGR (29.06)
AF_{avg}:	Average of carbon and oxygen based air fuel ratios
[ ]:	Exhaust species concentration
$[H_20]$:	Calculated water concentration in exhaust, dry
$[CO_2]_{intake}$:	CO_2 concentration measured in intake system, dry
$[CO_2]_{exhaust}$:	CO_2 concentration measured in exhaust system, dry

3.3.3 Particulate Emissions

The logged values of filter smoke number, FSN, given by the AVL smokemeter are reported for the particulate measurements. Smoke measurements, a measurement of the blackening of filter paper, are not *particulate* measurements, a measurement of the weight of material deposited on a filter and also the method used to certify vehicle emissions. Smoke measurements measure the dry soot component of the particulates but do not fully account for the soluble organic fraction (SOF). There are methods to correlate between smoke numbers (given as a filter smoke number, FSN), and a particulates measurement (reported as a mass per volume, or mass per fuel flow index) such as the MIRA correlation and others (Dodd and Holubecki, 1965; Christian et al., 1993). However, the accuracy and utility of these correlations is highly questionable at the smoke and particulate levels seen with PCI combustion. Accordingly, smoke measurements are simply reported in terms of filter smoke number.

3.3.4 Equivalence Ratio

Equivalence ratio, the ratio of the stoichiometric air-fuel ratio to the actual air fuel ratio, is computer from the exhaust emissions. The stoichiometric air-fuel ratio is computed from fuel properties including carbon and hydrogen ratio and molecular weight. The actual air-fuel ratio used is the average of two different air-fuel ratios, one computed based on a carbon balance and the other on an oxygen balance. Equations 4 and 5 show the computation of actual air-fuel ratio based on the oxygen and carbon balances, respectively (Stivender, 1971). Dividing the calculated stoichiometric air-fuel ratio for the fuel with the average air-fuel ratio from these two equations yields the equivalence ratio.

$$AF_O = 4.744\left(\frac{MW_{air}}{MW_{fuel}}\right)\left(\frac{[CO_2] + [O_2] + 0.5([H_2O] + [NO] + [CO])}{[CO] + [CO_2] + 3[HC]}\right) \tag{4}$$

$$AF_C = \left(\frac{MW_{air}}{MW_{fuel}}\right)\left(\frac{100 + 1.5[H_2O] + (1.5y - 1)[HC] - 0.5[CO]}{[CO] + [CO_2] + 3[HC]} - \frac{y}{2}\right) \tag{5}$$

Where:

AF_O: Air-fuel ratio, calculated with oxygen balance
MW_{air}: Molecular weight of air (28.96)
MW_{fuel}: Molecular weight of the fuel per carbon atom
y: H/C ratio of the fuel
[ ]: Exhaust species concentration
$[CO_2]$: Carbon dioxide concentration in exhaust, wet
$[O_2]$: Oxygen concentration in exhaust, wet
[H2O]: Water concentration in exhaust, wet
[NO]: NO concentration in exhaust, wet
[HC]: Hydrocarbon concentration in exhaust, wet, C_3 basis

3.3.5 Intake Oxygen Concentration

Absent a direct measurement, the oxygen concentration in the intake air is calculated from measurements of oxygen in the exhaust gas and the volumetric ratio of EGR flow. The intake oxygen concentration is reported on a wet, volumetric basis, accounting for combustion sourced water content in the EGR gas. The concentration is calculated from the ratio of the intake flow which is EGR versus fresh air. The oxygen content in the fresh air of the intake is a standard value, while the oxygen concentration in the EGR flow is the same as in the exhaust gas, which is measured with the emissions bench. Accordingly, the intake oxygen concentration can be calculated using Equation 6.

$$[O_2]_{intake} = (EGR_{VOL})[O_2]_{exhaust} + (1 - EGR_{VOL})[O_2]_{air} \tag{6}$$

Where:

[ ]: Exhaust species concentration
$[O_2]_{intake}$: Intake oxygen concentration, wet
EGR_{VOL}: EGR volume percentage, wet
$[O_2]_{exhaust}$: Oxygen concentration in exhaust, wet
$[O_2]_{air}$: Oxygen concentration in air, 20.9% (standard)

3.3.6 Combustion Efficiency

Accordingly, the combustion efficiency is calculated using Equation 7.

$$\eta_{comb} = 100 - \left(\frac{100}{[CO] + [CO_2] + 3[HC]}\right)\left(\frac{254[CO] + 217.1[H_2]}{(h_{fuel})(MW_{fuel})} + 3[HC]\right) \tag{7}$$

Where:

η_{comb}: Combustion efficiency
[ ]: Exhaust species concentration
[CO]: Carbon monoxide concentration in exhaust, wet
$[CO_2]$: Carbon dioxide concentration in exhaust, wet
[HC]: Hydrocarbon concentration in exhaust, wet, C_3 basis
$[H_2]$: Hydrogen concentration in exhaust, wet (Equation 8)
h_{fuel}: Lower heating value of the fuel (MJ/kg)
MW_{fuel}: Molecular weight of the fuel per carbon atom

$$[H_2] = \frac{y}{2}([CO] + [CO_2] - [H_2O]) \tag{8}$$

Where:

$[H_2]$: Hydrogen concentration in exhaust, wet
y: H:C ratio of fuel
[CO]: Carbon monoxide concentration in exhaust, wet
$[CO_2]$: Carbon dioxide concentration in exhaust, wet
$[H_2O]$: Water concentration in exhaust, wet

3.3.7 Noise

An AVL 450S Combustion Noisemeter is used to estimate the sound level of combustion. This device applies two filters to the cylinder pressure data, one to simulate the structural attenuation of a typical engine block and another to meter a subjective loudness criteria of a human ear, passes the data through a root mean square (RMS) converter and displays the result in decibels (AVL, 450). The intent is to estimate the sound level heard from outside the engine during operation.

3.4 Heat Release Analysis Based Parameters

3.4.1 Heat Release Details

Central to much of the analysis following in this dissertation is the use of parameters calculated by heat release analysis of the cylinder pressure data. Using cylinder pressure data taken on a crank angle basis, the heat release tracks the progression of combustion through the cycle. The heat release code used here was a General Motors internal code, and uses a single-zone, ideal-gas model of the combustion process of the form published by Gatowski et al. (1984).

The quantity of residual gases in the cylinder impacts the ability of heat release calculations to reasonably represent the combustion process. An accurate model for calculating the residual content is therefore highly important. Mass of residuals is calculated using the expression published by Yun and Mirsky (1974). The final blowdown conditions are specified in the same manner of the original publication: cylinder pressure and volume at exhaust valve closing

To account for the heat transfer out of the cylinder, the apparent heat losses are calculated using a simple pipe flow convective heat transfer correlation. The wall temperature is assumed to be the same as the bulk gas temperature of the cylinder charge at intake valve closing. The Hohenberg expression for determining the convection heat transfer coefficient, the standard for use with compression ignition engines, is used here as well (Hohenberg, 1979). Once calculated, the heat losses are scaled so that the sum of the apparent heat released and the calculated heat losses is equal to the total energy expected from the fuel, based on the fuel flow measurement and lower heating value.

Heat release analysis was independently conducted on each of the 200 recorded engine cycles. The resulting calculated parameters are averaged across all the cycles for the final result.

3.4.2 Ignition Delay

The ignition delay is the duration between when fuel is initially injected into the cylinder and when combustion begins. One of the defining characteristics of PCI combustion is the notable and pronounced cool-flame combustion region, appearing as a low intensity heat release prior to the large main combustion heat release. The timing of each event is important, so an ignition delay is separately defined for the cool-flame region and the main combustion event. While the beginning of the delay period is identically defined, there are different criteria for start of combustion.

Start of Injection

As noted previously, a current sensor on the injector signal wire measures the signal sent to the injector. The location of 70% rise (12.5 A) on the leading edge of the opening current spike is used as the location of the start of injection. This is well correlated to the measured drop in injector line pressure which occurs during injection, as demonstrated in Figure 3. The location of 70% current rise occurs one degree ahead of the characteristic drop in injector line pressure. This is identical behavior to the stock injector used on the production multi-cylinder engine.

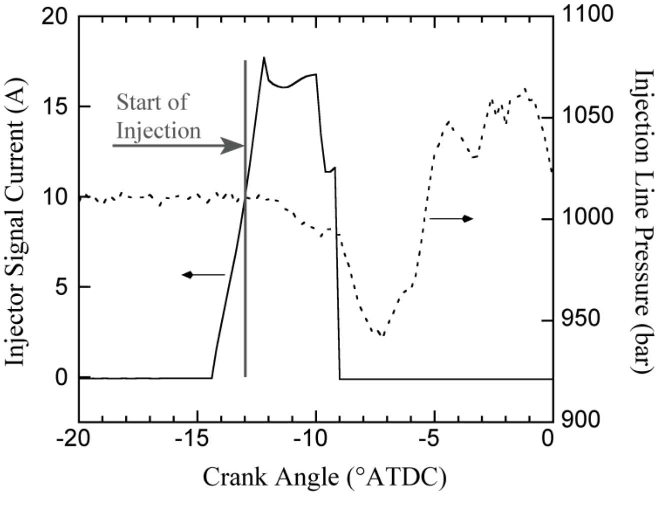


Figure 3: Start of injection location, defined as the location where injector current signal reaches 70% of opening value. 13 °BTDC injection timing shown.

The current signal leads the lifting of the injector needle (the needle will not lift until when signal reaches near its opening peak current), and the drop in injection line pressure trails the needle lift (fuel is compressible at the injection pressures used and there is a physical distance between the injector tip and the line pressure sensor, so there will be some lag). This establishes that the physical start of injection occurs between the location of the current signal and the drop in line pressure. Monitoring the injector signal current is easier and more repeatable, so it used as the parameter to monitor start of injection.

Start of Cool-Flame Combustion

As the cool-flame combustion is the first heat release, the start of combustion for the cool-flame region is defined as the location where rate of heat release (RoHR) returns to zero after the negative period. This is a refinement of a commonly cited method of determining ignition as the location of initially measurable heat release. Following injection the bulk cylinder gas temperature decreases due to fuel evaporation, showing an apparent negative rate of heat release. At the point where the rate of heat released by combustion equals the rate of heat loss, the overall heat release returns to zero. This point is established as the start of combustion for the cool-flame (Kuniyoshi et al., 1980) and is illustrated in Figure 4.

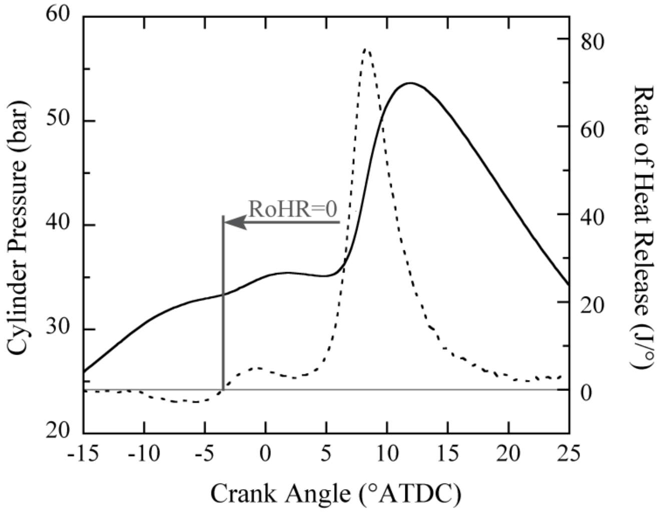


Figure 4: Start of combustion location for cool-flame region, defined as the location where rate of heat release returns to zero after fuel evaporation endotherm. Condition is 40% EGR, 14 °BTDC injection timing, with US mid-cetane fuel.

Start of Main Combustion – 10% Mass Fraction Burned

The location of 10% mass fraction burned (MFB) has been widely used as the indicator of the start of combustion for conventional diesel combustion, in particular by prior researchers in this project (Jacobs, 2005). With premixed combustion, the location of 10% MFB is a reasonable indicator of the start of main combustion. This measure of 10% MFB does not include the energy required to overcome the fuel evaporation endotherm, but does include all energy released after the heat release returns positive including the cool flame heat release. Slightly less than 10% of the heat release occurs in the cool-flame region. While a somewhat arbitrary point, and not necessarily perfectly describing the exact start of combustion, it does provide a reasonable indicator to measure changes between different conditions. This location with respect to a sample point is shown in Figure 5.

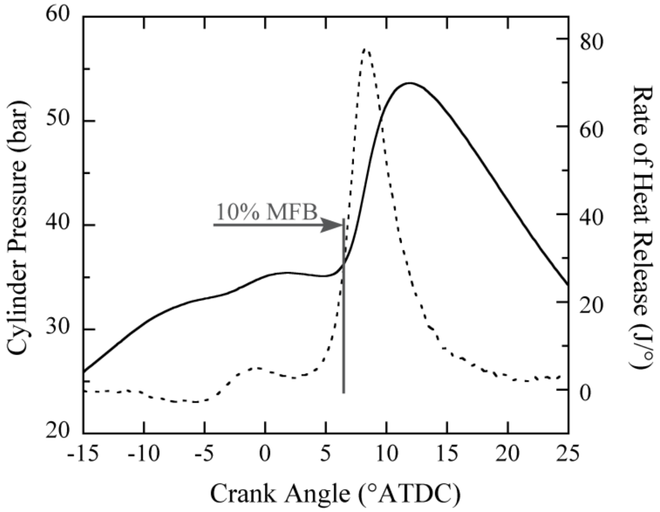
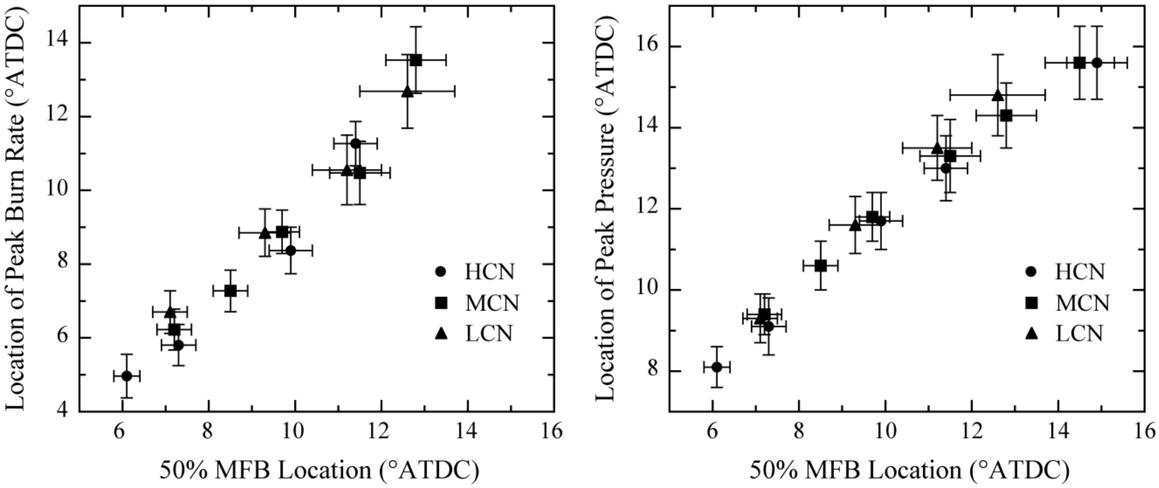


Figure 5: Start of combustion location for main combustion, defined as the location of 10% mass fraction burned. Condition is 40% EGR, 14 °BTDC injection timing, with US mid-cetane fuel.

3.4.3 Combustion Phasing

The location of 50% mass fraction burned, CA50, is used as the standard indication of combustion phasing, the relative position of combustion within the cycle. With premixed diesel combustion, the main combustion heat release is a single sharp event, with the heat release peak, pressure peak, and 50% burn location all very well correlated, as shown in Figure 6.



a. b.

Figure 6: Interrelation of combustion phasing metrics, including location of peak burn rate (a) and location of peak pressure (b) versus location of 50% mass fraction burned. Timing sweeps at 40% EGR with varied US fuels.

3.5 Determination of Experimental Uncertainty

Experimental measurements are inherently not exact, but rather contain a degree of uncertainty. This uncertainty of raw measurements is broken into three main components: instrument uncertainty, measurement variation, and condition variation.

Instrument uncertainty reflects the capability of the instrument (including its measurement method) to accurately measure the physical phenomenon. They are fundamental to the measurement device, and minimizing them can only be done by the selection of measurement method and instrument.

Measurement variation, the variation in recorded values across a test, can be viewed as a measure of the relative stability of the test system and operating condition. Measurement uncertainty is presented in this work at 95% confidence levels, representing two standard deviations (2σ) of the measurement variation.

It is near impossible to quantify certain uncertainties, such as bias errors and true repeatability. Both of these are addressed by developing rigorous test procedures. Calibration methods and plans were used to minimize the possibility of bias errors in the measurements. Also, by using the same test method and equipment, it is hoped that any bias errors apply to all points equally. The inability to truly repeat an exact condition leads to condition variation. Carefully following a detailed and strict experimental procedure for the tests of each fuel helps to minimize condition variation within the results. These types of uncertainty are not reported, but everything possible has been done to eliminate these errors.

3.5.1 Combining Uncertainties and Uncertainty Propagation

As noted before, the overall uncertainty of a given measured result is the combination of measurement uncertainty and the instrument uncertainty. The Root Sum Squares (RSS) method is used to combine these two separate uncertainty parameters into one overall uncertainty (Figliola and Beasley, 2000). The formula is as follows in Equation 9.

$$U_x = \sqrt{\sum_{1}^{n} (e_x)^2} \tag{9}$$

Where:

U_x: overall combined uncertainty
e_x: elemental uncertainties

Some reported parameters, in particular the emissions indexes, are calculated using several individual measurements. Each of the different measurements has unique uncertainty associated with it. The uncertainty of the end parameter is computed by sequential perturbation, where the uncertainty of each measurement is propagated through the calculation, then combined with the RSS method. Equation 10 shows the form of sequential perturbation used to determine the uncertainty, U, of a calculated parameter F, a function of measured parameters $a_1 \ldots a_n$ (Figliola and Beasley, 2000).

$$U = \sqrt{\sum_{1}^{n} \left(\frac{|F(a_i + u_i) - F(a_i)| + |F(a_i - u_i) - F(a_i)|}{2} \right)^2} \tag{10}$$

Where:

F: Function $F(a_1, a_2 \ldots a_n)$
U: Overall uncertainty of calculation (function) F
a_i: Measured parameter used in calculation of F
u_i: Related total uncertainty of parameter a_i

3.5.2 Operating Range

Once the condition is stabilized, the point variation is very small. Day-to-day variances serve to shift the measure of the whole range, not the relation of the points within. Across multiple days, conditions may change enough that the noted injection advance limit changes by a degree or two. However, the advance limit of one fuel versus another does not change. The overall numbers may vary, but there is little variation between the limits for different fuels. Condition of the injector can change as a test progresses, affecting the results. As an injector is fouled, the ignition delay becomes longer – achieving the phasing of both the advance and retard limits requires that the injection be advanced further. Between a ‘fresh’ and ‘well used’ injector, this can be several degrees, which would significantly obscure the results.

Achieving meaningful results in this measurement becomes a function of the experimental method and test process. It becomes imperative that the injector be conditioned before the test, and the test procession be carefully controlled so that the injector and combustion chamber are in very similar conditions for the different fuels.

3.5.3 Soot Emissions

Total uncertainty in the smoke measurement is calculated by the RSS combination of instrument uncertainty and measurement variation. Uncertainty due to measurement variation is handled in the manner described earlier. Instrument uncertainty for the smoke measurements is not as straightforward, however. The total instrument uncertainty (1σ) listed in the smokemeter documentation is ± 0.05 percent of full scale range, for paper blackening between 0.5 and 10 FSN within one roll of filter paper (AVL, 415S). While the measurement range this applies to is higher than the measurements taken, the quantity of exhaust gas flowed through the analyzer was increased such that the paper blackening was within the range noted. Further, while multiple rolls of filter paper were used across the duration of this research program, a standard operating condition was always checked for consistency between the rolls. The repeatability noted within these tests implies that there was consistency between rolls. However, even with these issues addressed, the specifications still yield a total uncertainty (95% confidence, 2σ) of ± 0.10 FSN. Unfortunately, this is on the same order as many of the measurements being taken. Additionally, the AVL standard for calibration during service only assigns an uncertainty of ± 0.15 FSN, indicating the uncertainty is even larger than the value quoted in the specifications. Repeatability, however, is quite good and is less of an issue than the measurement uncertainty, but is still factored in to the overall uncertainty calculations.

Due to the equivalence of the range of instrument uncertainty with the measurements being taken, only gross trends and sizeable changes will be discussed. Two different uncertainty ranges will be used in figures showing smoke emissions. For the bulk of the work (which produces low smoke levels), the combination of only resolution and measurement uncertainty will be used (neglecting instrument uncertainty). For the higher smoke data reported in Chapter Seven, the full measurement + resolution + instrument uncertainty will be presented. With each figure presenting smoke data, the uncertainty method used will be denoted in the accompanying caption.

3.5.4 Gaseous Emissions Indices

All of the gaseous emissions are reported on an emissions index basis. As discussed earlier, the emissions index calculations use several exhaust gas emissions in each calculation: CO, CO_2, and HC. The overall uncertainty is therefore a function of all the emissions used in the calculation. The uncertainty for the gaseous emissions is therefore calculated using the sequential perturbation method of combining the uncertainties of each emission measurement used in the overall index calculation.

The uncertainty of the individual gaseous emissions measurements are a combination of the instrument uncertainty and measurement variation. Measurement variation is calculated in the manner noted previously. Instrument uncertainty is the combination of uncertainties for a given analyzer: resolution (display uncertainty), sensitivity (calibration uncertainty), repeatability (variation in measurement accuracy over one day/test), and drift (day-to-day change in measurement accuracy). These component uncertainties are combined using the RSS method to determine an overall instrument uncertainty. For each of the gaseous emissions, and related analyzers, the component and total instrument uncertainty is listed in Table 3.

Measurement	Resolution	Sensitivity	Repeatability	Drift	F.S. Range	Overall
CO	0.1 %FS	0.5 %FS	0.5 %FS	<1 %FS	1 %	0.013 %
CO2	0.1 %FS	0.5 %FS	0.5 %FS	<1 %FS	15 %	0.20 %
EGR CO2	0.1 %FS	1.0 %FS	1.0 %FS	<1 %FS	10 %	0.18 %
NO_x	0.1 %FS	0.5 %FS	1.0 %FS	<1 %FS	100 ppm	1.5 ppm
O2	0.1 %FS	1.0 %FS	1.0 %FS	<1 %FS	25 %	0.44 %
HC	0.1 %FS	0.5 %FS	1.0 %FS	<1 %FS	1000 ppm	15 ppm

%FS means percent full scale of the instruments full scale range (F.S. Range)

Table 3: Instrument uncertainties of the gaseous emissions analyzers

3.5.5 Other Emissions-based Calculated Parameters

Since equivalence ratio, intake oxygen concentration, and combustion efficiency are calculated parameters, their respective uncertainties are calculated with sequential perturbation. Given that both parameters are principally a function of exhaust gas emissions concentrations, their uncertainty is calculated in the same manner as the gaseous emissions indices as noted above in Section 3.5.4. The equivalence ratio calculation uses the stoichiometric air:fuel (AF) ratio computed from the fuel carbon-hydrogen ratio. The uncertainty for the calculated stoichiometric AF ratios comes from the uncertainties listed in the SAE International Standard covering determination of fuel C:H ratio and stoichiometric ratio (SAE, J1829). The magnitude of the uncertainty arising from the stoichiometric AF ratio calculations is insignificant compared to the uncertainty brought by the emissions measurements.

3.5.6 Ignition Delay

Since there are different ways to specify the ignition delay measurement, the uncertainty of each component of the measurements will be discussed separately. As before, the total uncertainty results from RSS combination of the appropriate measurement component.

The start of injection was measured by monitoring the transition in injector signal current using a current probe. The instrument uncertainty for the current sensor in this application is negligible, as it can reproduce transitions greater than 20 ns, corresponding to 0.0002 crank angle degrees. The repeatability of this instrument is also exceptional. There might be bias errors in the measurement, but they are universally applied. Thus the only significant uncertainty for this measurement is the test variation. Start of injection never varied by more than ± 0.1 degrees, so this is used as the uncertainty for the start of injection measurement.

Establishing the uncertainty for the start of cool-flame combustion, RoHR=0, was a tedious examination of individual rate of heat release curves. Individual rate of heat release curves were calculated for each of the 200 cycles in a representative case, and the variation across the each cycle was compiled. Due to the labor intensive nature of this process, a single typical operating case was examined, and the results are taken to be representative. The variation across engine cycles is also judged to be large enough to dwarf any instrument uncertainty for this particular measurement. The uncertainty used for all case of the RoHR=0 point is ± 0.5 degrees.

Uncertainty for the location of 10% MFB is two standard deviations of the 200-cycle values calculated within the heat release program.

3.5.7 Combustion Phasing

Uncertainty for the location of 50% MFB, used as the metric for combustion phasing, is calculated the same as it was for 10% MFB: two standard deviations of the 200-cycle values calculated within the heat release program.

3.5.8 Temperatures

Temperature measurements are taken exclusively with K-type thermocouples from Omega. The uncertainty for the thermocouples used is ± 2.4 °C or 0.75% of measurement value, whichever is larger. This quoted uncertainty is used for the instrument uncertainty, and combined with the measurement variation using the RSS method.

CHAPTER 4

FUEL CETANE NUMBER EFFECT

4.1 Introduction

Cetane number is an obvious property to vary in a diesel fuels study, as it is one of the foremost methods of quantifying diesel fuel. It is a qualitative measurement of basic ignition behavior and ignition quality which effectively lumps all fuel properties into one main parameter. Given the potential importance of ignition behavior to novel diesel combustion modes, examination of cetane number behavior is critical. The wide variation in fuel properties seen in the field is well represented by the significant variation in cetane number.

The fuel cetane number is varied across a relatively small range which covers what fuels are available in the field. Initial focus is the effect of cetane number on combustion phenomena and behavior. Implications for combustion and emissions of varying cetane number are then detailed within the context of combustion phasing. Additionally, other engine parameter effects are examined relative to the fuel behavioral results. The range of injection timing and combustion phasing which yield acceptable operation is also reviewed. Finally, combustion and emissions behavior is framed through a more commonly referenced context, injection timing, to elucidate perceived trends.

4.2 Test Methodology

4.2.1 Test Fuels

A set of four test fuels is used for this portion of the study: three US ultra-low sulfur diesel (ULSD) certification fuels of varying cetane number, and one light distillation Swedish Environmental Class 1 (MK1) diesel fuel. The three US certification fuels were blended by the supplier to possess cetane numbers across an approximate range of 40-50, while matching in other fuel properties. The Swedish MK1 fuel is a lighter distillation, higher cetane, arctic fuel. It is included in the fuel matrix to have a higher cetane number fuel which is only composed of petroleum without any additives or alternative compositions. Further, Swedish MK1 fuel was the test fuel used in related previous premixed diesel combustion development work at the University of Michigan conducted by Lechner (2003) and Jacobs (2005), along with related studies by Knafl (2007), Han (2007), and Busch (2007). The test fuels are abbreviated in figures as follows: low cetane ULSD (LCN), mid-cetane ULSD (MCN), high cetane ULSD (HCN), and Swedish MK1 (MK1). All three US certification fuels are classified as 2-D diesel fuels based on their distillation 90% recovery points (T90) falling between 288 °C and 338 °C, while the Swedish MK1 is classified as a 1-D diesel fuel since its T90 point is less that 288 °C (ASTM, D975). All test fuels were supplied by the Haltermann Products division of Dow Chemical Company. Specifications of the test fuels are given in Table 4, with the first subtable giving bulk fuel properties and the second subtable indicating the breakdown of the hydrocarbon types present in each fuel on a volume basis. Distillation curves for the test fuels are shown in Figure 7.

	Low CN	Mid CN	High CN	Swedish MK1
Cetane Number	42	47	50	53
Cetane Index	42	45	48	52
Sulfur (ppm)	8	11	10	12
Density (g/ml)	0.85	0.84	0.85	0.81
LHV (MJ/kg)	42.5	42.8	42.4	43.5
H:C Ratio (-)	1.81	1.86	1.86	1.97
T50 (°C)	257	262	281	224
T90 (°C)	307	308	311	268

	Low CN	Mid CN	High CN	Swedish MK1
Alkanes (%)	72	80	76	95
Olefins (%)	2	1	3	1
Aromatics (%)	26	19	21	3

Table 4: Properties of the four cetane number test fuels, including bulk fuel properties and volume percent of hydrocarbon types.

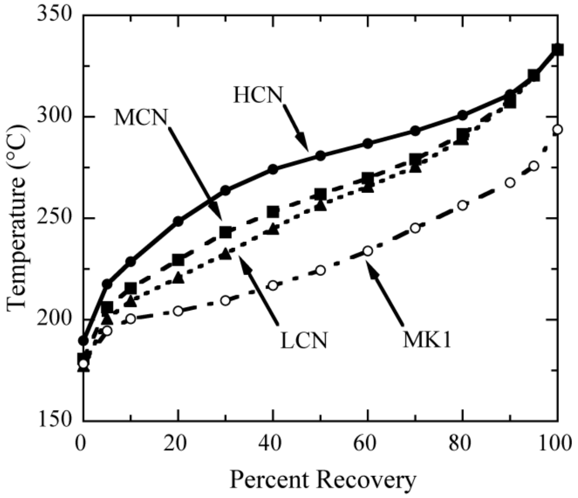


Figure 7: Distillation curves for the four cetane number test fuels. Error bars are withheld for figure clarity. Uncertainty levels are set by the ASTM D86 standard (ASTM, D86), with uncertainty range as follows: ± 3-6 °C (repeatability), and ± 8-16 °C (reproducibility).

4.2.2 Operating Conditions

The testing conditions used for this portion of the work center around the base condition: 1500 rpm with a 5 bar IMEP, as described in detail within Chapter 3. At this condition, several parameters were varied to examine the engine behavior, including EGR fraction, injection timing, and injection pressure. EGR was tested at three different mass fractions: 40, 43, and 45%, with the bulk of the reported results at 40%. Tests with EGR at 43% are often not displayed, as the behavior at 43% falls neatly between that of 40% and 45% EGR. At each EGR level, the injection timing was swept from the timing advance limit (90 dB noise), or two degrees advanced from it for some fuels, to the basic operability retard limit (onset of loss of recoverable power) in increments of 1-2 degrees. For the bulk of the tests, injection pressure was maintained at 1000 bar. It was isolated as a variable and swept from 800 to 1400 bar in 200 bar increments during selected tests.

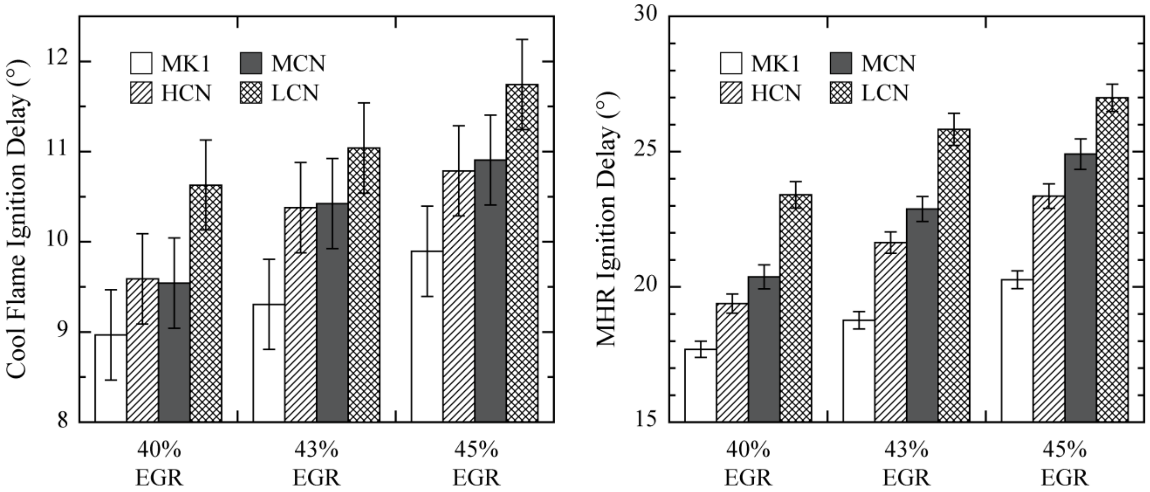
Though the conditions were specified in terms of a set EGR mass fraction at a fixed intake manifold pressure, there are other metrics commonly used to identify operating conditions, including air-fuel ratio and inlet oxygen concentration. For the two EGR levels with results presented here, the average equivalence ratio and intake oxygen concentration across all injection timings and fuels tested was calculated and is reported here for reference. At the 40% EGR level, the mean equivalence ratio is 0.78 ± 0.05 and the mean intake oxygen concentration is 15.2 ± 0.5%. For the 45% EGR level, the mean equivalence ratio is 0.85 ± 0.05 and the mean intake oxygen concentration is 14.2 ± 0.5%. Minor increases in fueling as injection timing is retarded increase the equivalence ratio throughout the range noted, resulting in a corresponding decrease in intake oxygen content due to the reduced oxygen content of the recirculated exhaust gas.

4.3 Results and Discussion

4.3.1 Effect on Combustion Behavior

Ignition Delay

The behavior of the two ignition delays (cool-flame, ID_{CF}, and main combustion, ID_{MHR}) is similar with respect to fuels and other operating parameters: both fuel cetane number and EGR have a notable impact on the low and high temperature ignition delays. Increasing EGR steadily increases the ignition delays as expected. The effect of injection timing is at most secondary with the main heat release ignition delay (slightly increasing with retard on injection timing but within uncertainty), and not significant with cool-flame ignition delay. Reflecting this, the mean ignition delay across varied injection timings is calculated for a given fuel and EGR level and shown in Figure 8.



a. b.

Figure 8: Mean ignition delays for each fuel at varying EGR mass fractions. (a) Cool-flame ignition delay. (b) Main combustion ignition delay. Ignition delays averaged across timing sweep at given EGR level.

Decreases in fuel cetane number increase both the cool-flame and main combustion ignition delays. There is, however, relative parity between the cool-flame ignition delays for the high and mid cetane fuels. The cetane numbers of these two fuels are close and the uncertainty in the cool-flame ignition delay measurement is substantial due to high cycle-to-cycle variation in the start of combustion location. The effect of cetane number on the MHR ignition delay is more clear, with distinct differences between each fuel of different cetane number. The difference in MHR ignition delay between fuels is relatively proportional to their separation in cetane number. The high temperature ignition process, being controlled primarily by the fuel ignition chemistry, is notably very dependent on the cetane number. This is expected, since cetane number is inherently tied to a measurement of ignition delay (ASTM, D613).

Cool-Flame Behavior

One of the defining characteristics of premixed diesel combustion, and of most diesel-fueled low temperature combustion strategies, is the presence of a distinctly identifiable cool-flame heat release. Also known as Low Temperature Heat Release, LTHR, the cool-flame is a small combustion heat release occurring prior to the main, high temperature, heat release. Cool-flames are present with most diesel fuels, and some diesel-like gasoline. Since gasoline and diesel are both petroleum blends, extremes of each can act similarly – very low octane gasoline is very similar to high cetane diesel fuel. Prior researchers note the cool-flame heat release for HCCI type operation with gasoline-like petroleum fuels exhibiting an octane number lower than 83 (Christensen et al., 1999), and for diesel-like petroleum fuels with a cetane number higher than 34 (Bunting et al., 2007). The amount of cool-flame heat release in each case increases with decreasing octane number and increasing cetane number, respectively.

It should be noted that prior research shows cool-flame reactions occur during diesel combustion of appropriate fuels, not just during HCCI type operation (Garner et al., 1956). However, under conventional conditions, the high temperature heat release starts at nearly the same time as the low temperature heat release and overshadows it. In premixed diesel combustion, and other similar combustion modes, the main high temperature heat release is delayed enough that the low temperature heat release is separately visible.

The cool-flame reactions are reported to primarily consist of hydrogen abstractions involving the normal paraffin and, to a lesser extent, the branched paraffin content of the diesel fuel (Curran et al. 1998). However, the simplest paraffin, methane, does not have the two stage ignition process that yields a cool-flame (Downs et al., 1953). The cool-flame reactions are exothermic, releasing the energy shown in the apparent heat release traces. As the temperature increases, the reaction rate constants of the cool-flame chemistry become less favorable (negative with increasing temperature). The reactions slow to a stop once they reach this condition, referred to as the negative temperature coefficient, NTC, region. Frequently with premixed diesel combustion, the high temperature heat release is delayed such that the cool-flame reactions are allowed to progress well into the NTC region (completion) prior to the onset of the main combustion event.

All tested fuels, regardless of cetane number, release the same quantity of energy during cool-flame combustion: 30 ± 5 Joules or approximately 6% of the total heat release (485 ± 25 J). The cool-flame combustion duration varies with the cetane number, with higher cetane number fuels displaying a shorter cool-flame region, as demonstrated in Figure 9. The intensity of the cool-flame heat release, however, scales correspondingly to yield the constant energy release.

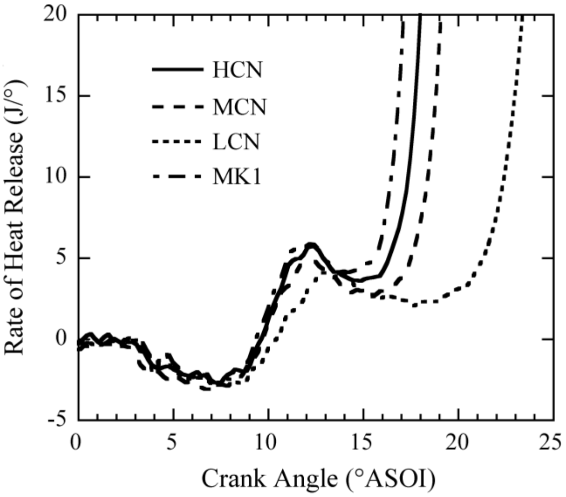


Figure 9: Rate of heat release traces showing behavior in cool-flame region. Cool flame is the heat release following the endotherm caused by fuel evaporation and heating but prior to the main heat release. Condition is 40% EGR, 1000 bar injection pressure, 15 °BTDC injection timing. Plotted against crankangle degrees after start of injection (ASOI).

The high EGR levels used in these tests allow the cool-flame to proceed to the NTC region prior to the onset of main combustion. Since cool-flame reactions are thought to be a function of the normal and branched alkane portion of a fuel (Bunting et al., 2007) and proceed to relative completion prior to main combustion, the apparent cool-flame heat release for the tested fuels (with comparable alkane contents) are equivalent.

Given the relative differences in fuel properties, specifically the different distillation characteristics noted in Figure 7, there is concern that actual cool-flame heat release behavior is masked in the apparent heat release curves plotted. A fuel's higher cool-flame heat release may be obscured by increased heat losses from fuel evaporation and heating. Considering the size of the measured endotherm preceding the cool-flame combustion, magnitude of the expected heat losses due to fuel heating and vaporization, quantity of fuel injected, and difference in specific heat and specific heat of vaporization between fuels, the magnitude of this effect is judged to be insignificant and easily covered by the uncertainty quoted.

Combustion Phasing

At a fixed injection timing and EGR level, higher cetane number fuels cause combustion with an advanced combustion phasing, as quantified by the location of 50% MFB, denoted as CA50. Accordingly, matching combustion phasing between fuels requires different injection timings for different cetane number fuels, with lower CN fuels needing earlier injection timings, as demonstrated in Figure 10.

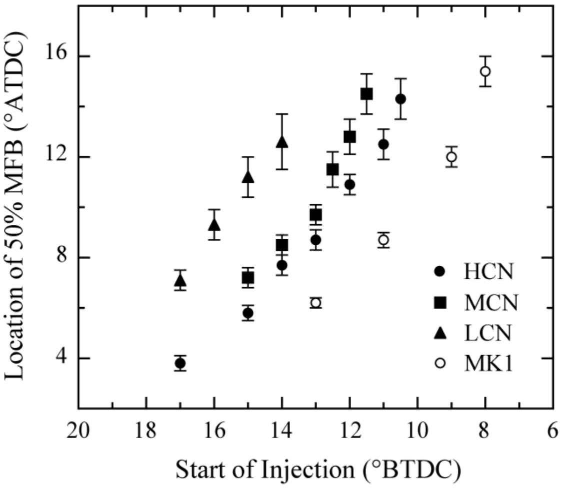


Figure 10: Location of 50% MFB versus injection timing. Injection timing sweeps at 40% EGR, 1000 bar injection pressure, varied fuels.

Many engine parameters besides fuel cetane number affect the combustion phasing. Changes to any one of the main test parameters used within this testing, including EGR fraction, injection pressure, and injection timing, shift combustion phasing. Increasing the EGR fraction retards the combustion phasing due to the increase in ignition delay noted earlier. Increasing injection pressure advances the combustion phasing due to improved spray breakup and shorter physical mixing time, yielding a shorter ignition delay and more rapid combustion (Plee and Ahmad, 1983). Retarding the injection timing produces slightly more than 1:1 retarding shift in combustion phasing. Other engine parameters have an effect as well. Parameters held constant within this set of tests could, if varied, shift the combustion phasing as well. Some parameters classically understood to shift the combustion phasing include intake oxygen concentration, compression ratio, intake pressure, and intake temperature. These parameters have a strong effect on the ignition delay, with increases in any of them leading to a shorter ignition delay and earlier combustion phasing. These are merely several well-known and primary engine testing parameters, and this is not meant to be viewed as an all-inclusive list. Other parameters usually held constant within engine testing do have an effect as well. Within this work, two non-control parameters, injector condition and coolant temperature, were found to shift combustion phasing during secondary tests. The condition of the injector makes a large difference in the ignition delay and progressively the combustion phasing. As testing hours increase, deposits on the injector (fouling) lead to progressively longer ignition delays and retarded combustion phasing. Changing the coolant temperature also has an effect: reducing coolant temperature by 25 °C increases the ignition delay and retards the combustion phasing by three degrees across the range of conditions. Given the sensitivity to these parameters, it is likely that variations in many other engine parameters held constant in these tests have an effect as well.

4.3.2 Emissions as a Function of Combustion Phasing

With the PCI combustion strategy and fuel used, gaseous emissions, in particular NO_x ($NO + NO_2$), are principally a function of the EGR fraction and combustion phasing. Fuel cetane number does not have a direct effect on gaseous emissions: it is only one of many parameters that shift combustion phasing. These resulting shifts in combustion phasing drive the change in emissions. Changes in EGR fraction affect the gaseous emissions in the manner predicted by previous literature: increasing the fraction of cooled EGR decreases NO_x emissions while increasing emissions of carbon monoxide (CO), and hydrocarbons (HC) (Ladommatos et al., 1996-1, 1996-2, 1997-1, 1997-2).

NO_x emissions, in particular, are highly dependent on combustion phasing and independent of cetane number. The NO_x generated by each fuel follows the same trend, with NO_x levels decreasing with a retard in combustion phasing within the range of injection timing values tested. There are no significant differences between the NO_x emissions from the different cetane number test fuels at a particular EGR level and combustion phasing, as demonstrated in Figure 11.

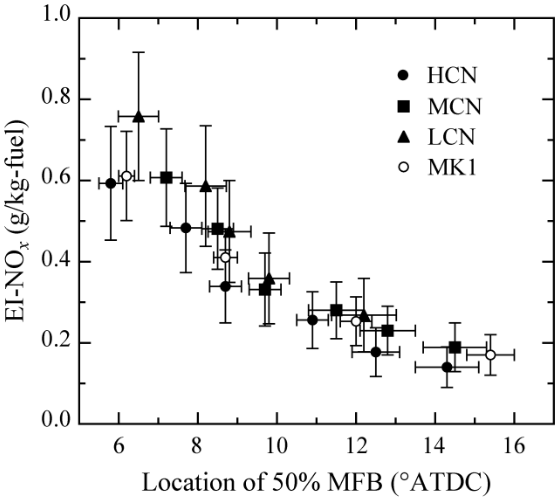


Figure 11: NO$_x$ emissions versus combustion phasing at 40% EGR. Injection timing sweeps at 1000 bar injection pressure, varied fuels.

The cylinder pressure and rate of heat release traces for a given condition follow the same path independent of fuel. Indicative of this is peak cylinder pressure, shown in Figure 12, which displays a linear relationship with combustion phasing, independent of fuel cetane number.

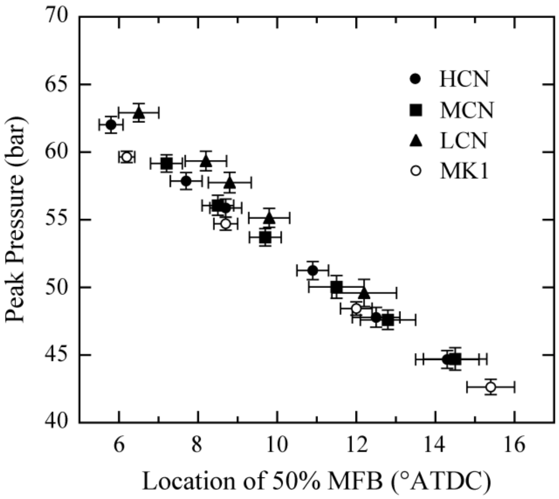


Figure 12: Peak pressure versus combustion phasing. Injection timing sweeps at 40% EGR, 1000 bar injection pressure, varied fuels.

When the combustion processes follow similar overall progressions, NO$_x$ emissions are similarly independent of fuel. Thermal NO$_x$ production is a function of the cylinder conditions, not explicitly the fuel properties. Of the principal NO$_x$ formation mechanism, thermal NO$_x$ is widely understood to be the most significant contributor. Prompt NO$_x$

formation, taking place in the early stages of combustion, contributes to the overall NO_x emissions but not at levels as significant as the thermal NO_x mechanism. Thus, the NO_x formation is primarily dictated by the thermal mechanism, which is controlled by cylinder conditions, primarily local temperature and equivalence ratio (Kamimoto, 1988). If overall cylinder conditions, especially temperature, are similar between combustion resulting from the different fuels, the overall NO_x emissions will be similar as well. Bulk equivalence ratio and cylinder gas temperature vary with EGR fraction and combustion phasing, but are comparable across the fuel set when these parameters are constant.

Equivalence ratio is indicative of the amount of oxygen available to participate in the NO_x formation reactions. Thermal NO_x formation takes place in the post-flame combustion gases – higher local equivalence ratios indicate less oxygen available in the post-flame gas for NO_x production. At a given EGR fraction in this testing, the global equivalence ratio for all tested fuels remains approximately constant (as noted with test values given in Section 2.2), but increasing slightly as injection timing (and therefore combustion phasing as well) retards, due to the increase in fueling rates required to hold engine load constant. Since equivalence ratio increases slightly with combustion phasing, this may contribute to the decreased NO_x formation. However, since NO_x formation is more strongly dependent on the local equivalence ratio than the global equivalence ratio, this may be insignificant. While the equivalence ratios can be calculated for the overall (global) mixture, the local equivalence ratios (the critical parameter) cannot be determined with the current experimental setup. Thus, their values become a matter of speculation. However, since the overall combustion process, including equivalence ratio, displays consistent behavior between fuels, it is reasonable to presume that local equivalence ratio behavior is also consistent between combustion of the different test fuels.

The strong connection between thermal NO_x formation and cylinder gas temperature is well reported – thermal NO_x formation increases with increasing gas temperature, especially in lean mixtures above 2000 K (Kamimoto, 1988). As noted before with equivalence ratio, the dynamic and inhomogeneous nature of the combustion process means there will be significant spatial variations in NO_x formation within the chamber. Accordingly, local temperatures are the critical factor rather than global temperatures.

The current test setup does not yield details of local gas temperatures throughout the chamber and cycle. The methods for calculating the bulk (global) cylinder gas temperature over a cycle from the cylinder pressure measurements induce significant uncertainty into the results, which is especially problematic given the magnitude of the combustion changes and resulting emissions. The uncertainty in the calculated cylinder temperature dwarfs any useful trends, making calculated bulk gas temperature results of little utility for analysis. However, it is understood, based off classical thermodynamic and combustion knowledge, that the later combustion phasing results in lower peak cylinder gas temperatures, which in turn yields decreased NO_x formation. By phasing combustion later into the expansion stroke, peak cylinder pressures are lower (as indicated in Figure 12 noted prior) and cylinder temperatures are expected to be likewise. This decrease in combustion temperature decreases thermal NO_x formation, resulting in lower NO_x emissions, the trend noted within these results. Since there do not appear to be significant bulk differences in the combustion behavior (especially between peak cylinder pressure) of the four different fuels at matched combustion phasing (for the tested operating mode at a given EGR fraction), the cylinder temperature behavior is expected to be comparable. Accordingly, if combustion temperature behavior matches between different test fuels at a common operating condition, NO_x emissions will be equal as well, which is the trend noted in the presented data.

Further, the later combustion phasing itself reduces NO_x formation. The later combustion phasing restricts the available time between the point when the bulk of NO_x formation starts (after the peak rate of heat release point) and when the NO_x reaction chemistry is 'frozen' by the cylinder expansion (Szybist and Bunting, 2005). The thermal NO_x formation process is a slow developing process with a long time constant – decreasing the available time for the formation process to occur reduces NO_x produced by this mechanism. Combustion phased later retards the start of NO_x formation, decreasing the available time for NO_x formation and resulting in decreased NO_x production.

As the EGR fraction increases, the magnitude of the NO_x emissions decrease, condensing the data while continuing to demonstrate the relationship between NO_x emissions and combustion phasing. The decrease in magnitude with increasing EGR, demonstrated in Figure 13, follows the predicted trend (Ladommatos et al., 1996-1, 1996-2, 1997-1, 1997-2). Increased EGR fraction lowers the intake oxygen concentration by diluting the intake charge (replacing oxygen with EGR species), thus increasing the cylinder equivalence ratio, leading to decreased NO_x emissions (Ladommatos et al., 1996-1). Further, the water and CO_2 components of the EGR mixture serve as thermal sinks, absorbing energy and decreasing cylinder temperatures (Ladommatos et al., 1996-2, 1997-1, 1997-2). Finally, the increased EGR fraction lowers the ratio of the specific heat of the cylinder charge, resulting in lower compression temperatures which subsequently decreased peak combustion temperatures (Jacobs, 2005). Again, no significant fuel differences are noted.

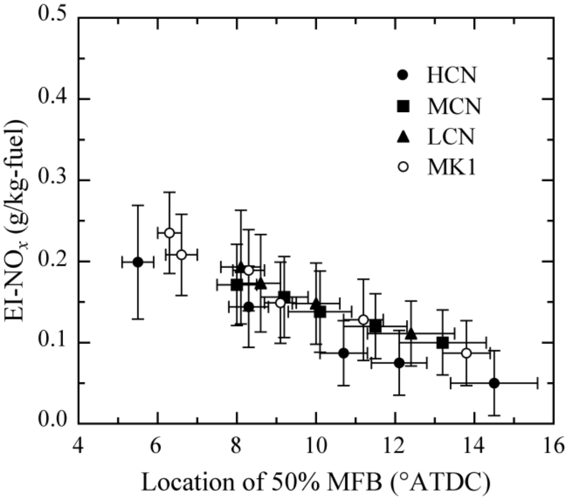
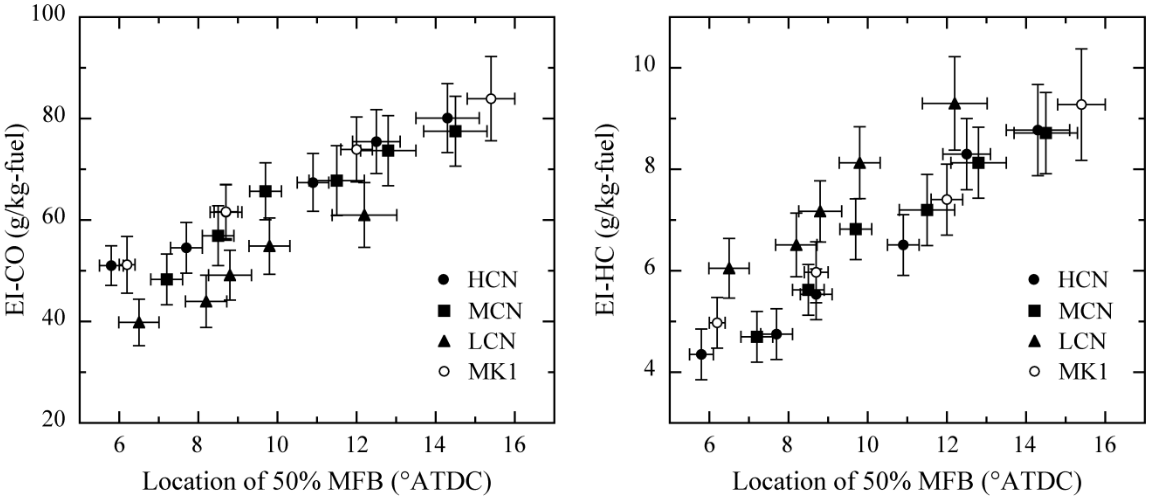


Figure 13: NO_x emissions versus combustion phasing with 45% EGR. Injection timing sweeps at 1000 bar injection pressure, varied fuels.

The other principal emission of concern for compression ignition engines, particulates, is very insensitive to any of the tested parameters, with all smoke measurements in the range of 0.10-0.15 FSN. The low combustion temperatures and fairly well mixed conditions minimize the soot emissions – some soot is still formed within localized regions, however, where the local temperature and equivalence ratio are more favorable to soot formation (higher local temperature, richer mixture conditions). The low measured smoke levels fall within the instrument uncertainty of the smokemeter used for the measurements, making it impossible to ascertain any significant differences between the test fuels at the given operating condition. This issue has been reported before in previous studies (Risberg et al., 2005). However, smoke measurements only account for the carbon soot emissions, and do not include any measure of the soluble organic fraction (SOF) of the particulate emissions. The SOF may be a substantial element of PM emissions, and one which does vary with fuel changes. Equipment capable of measuring the SOF of the particulates was not available for the present tests, so no conclusion can be drawn about their behavior.

Emissions of carbon monoxide and hydrocarbons also show similar strong relations to combustion phasing, with both CO and HC increasing with a retard in combustion phasing, as shown in Figure 14.



a. b.

Figure 14: CO (a) and HC (b) emissions versus combustion phasing at 40% EGR. Injection timing sweeps at 1000 bar injection pressure, varied fuels.

However, there are secondary fuel effects to CO and HC emissions: the low cetane fuel made preferentially lower CO emissions and higher HC emissions. This is not the result of degraded combustion quality, which would have led to simultaneous increases in CO and HC, rather than inverse changes seen here. It is attributed to three possible sources: differences in exact fuel hydrocarbon composition, disparities in the cool-flame behavior, and possible overleaning during the longer ignition delay. A combination of one or more of these was responsible for the phenomena noted.

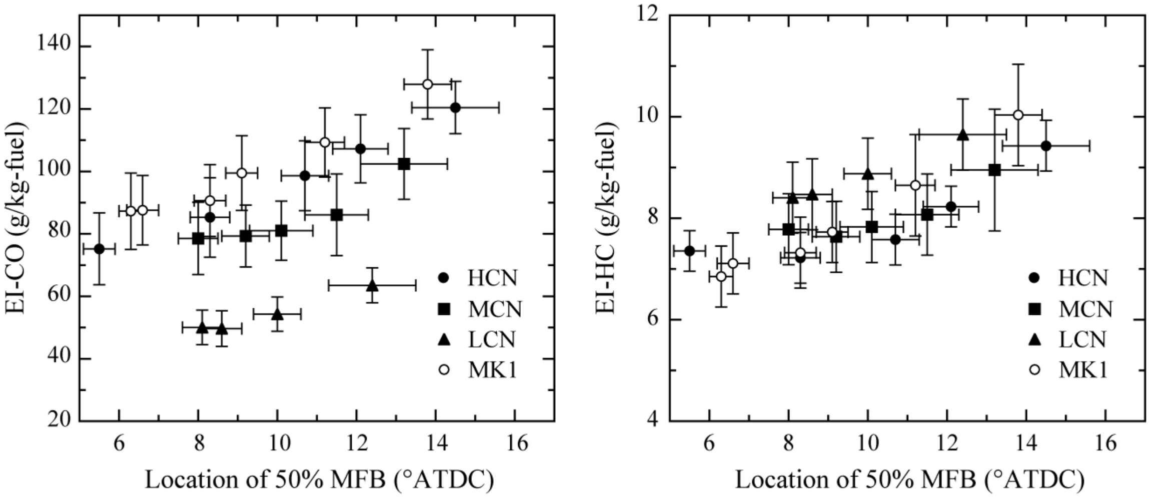
The different behavior of the low cetane fuel is partially attributed to differences in the exact hydrocarbon composition of this particular fuel. It is postulated that the specific fuel composition of the low cetane test fuel is such that, during combustion, certain hydrocarbon species preferentially remain as unburned hydrocarbons rather than partially oxidize to CO. Specifically, heavier and less reactive aromatic hydrocarbons could be responsible. All the fuels contain aromatic hydrocarbons, but the low cetane fuel has the highest level of these hydrocarbon species and the lowest cetane number. Reflecting this, the low cetane fuel is believed to have a higher quantity of unreactive hydrocarbons. Total aromatic content of the low cetane fuel is 26%, higher than the other three fuels (HCN: 19%, MCN: 21%, MK1: 3%).

The spread in emissions behavior may also be related to differences in the cool-flame portion of combustion. Similar CO and HC emissions behavior is noted by others (Szybist and Bunting, 2005), albeit with a larger spread of CO-HC fractions due to a significantly larger spread of tested cetane number. Their principle explanation focuses on the distinct differences in cool-flame combustion (including the lack of an observable cool-flame for their tested low cetane fuels). Heat release analysis in the present work indicates similar cool-flame heat release levels between the fuels, but the low cetane fuel has a longer duration, less intense cool-flame. The level of CO produced during the cool-flame with the low cetane fuel may prompt the same effect noted by Szybist and Bunting, to a lesser magnitude.

Further, the increase in HC emissions with the low cetane fuel could be related to overleaning due to the longer ignition delay. As the ignition delay increases, there is increasing risk that the fuel will mix to the point where it is too lean for combustion to occur. Overleaning has been shown to increase hydrocarbon emissions (Greeves et al., 1977).

One additional possibility is that the differences in HC emissions behavior could be a measurement artifact. Flame ionization detectors (FIDs) used for hydrocarbon measurements do not have equal measurement responses to all hydrocarbon species. Hydrocarbon species with a lower (C_1, C_2) carbon number than the calibration gas (C_3H_8) show an increased measurement response with the FID relative to their true value (Horiba, 090934). Likewise, hydrocarbon species with higher carbon numbers (C_{4+}) show a decreased response (Horiba, 090934). Accordingly, if the composition of hydrocarbon species varies significantly between fuels, the hydrocarbon emissions results could be artificially skewed. Further examination, in the form of hydrocarbon speciation with a gas chromatograph, of the hydrocarbon composition resulting from combustion of the different fuels could illuminate whether this effect impacts the results in a significant fashion.

As EGR fraction was increased beyond the 40% level shown, the disparity between the low cetane fuel and the other fuels with respect to CO and HC emissions increased, further highlighting this effect, as shown in Figure 15. The overall CO and HC emissions behavior remains consistent at higher EGR fractions as well, displaying the same trends as noted at 40%. However, as the EGR fraction increases, the magnitude of CO emissions increases, but HC levels remain relatively constant.



a. b.

Figure 15: CO (a) and HC (b) emissions versus combustion phasing at 45% EGR. Injection timing sweeps at 1000 bar injection pressure, varied fuels.

4.3.3 Emissions as a Function of Ignition Timing

Differences in the test fuels, which represent a spread of cetane numbers, primarily reflect as changes in ignition behavior, not combustion behavior. The high temperature combustion process, once initiated, is very similar between all of the fuels, regardless of cetane number. The time from high temperature ignition to 50% MFB, the overall rate of heat release, and the cylinder pressure behavior are very similar between the test fuels. This is demonstrated by the linear relationship between the location of 10% MFB (start of main combustion criteria) and 50% MFB (combustion phasing), as shown in Figure 16.

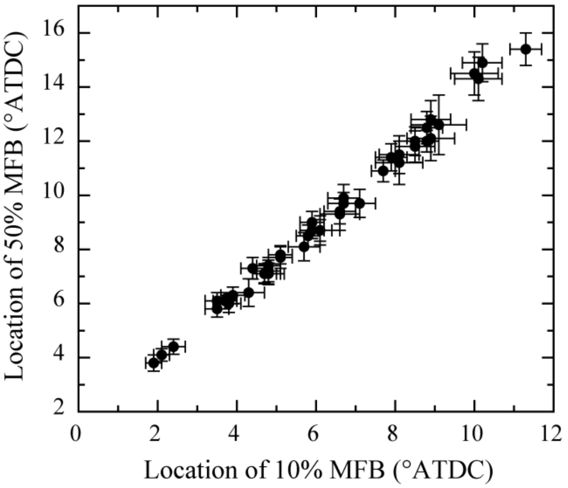


Figure 16: Combustion phasing versus start of combustion. Injection timing sweeps at 40% EGR, 1000 bar injection pressure, varied fuels.

The bulk of high temperature combustion is the same for all the fuels. Thus, the relation between emissions, primarily NO_x, and combustion phasing (CA50) is preserved between emissions and start of high temperature combustion, as demonstrated in Figure 17.

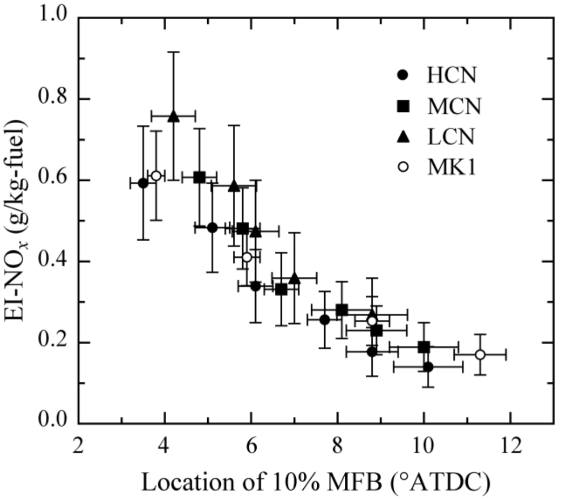


Figure 17: NO_x emissions versus start of combustion. Injection timing sweeps at 40% EGR, 1000 bar injection pressure, varied fuels.

Once ignition occurs, combustion proceeds at similar rates for each fuel. As noted earlier, the same amount of energy is released during the cool-flame portion of combustion for each fuel. At the start of high temperature combustion, all four fuels start at approximately the same cylinder conditions: same pressure, temperature, EGR fraction, and all are well mixed given the long ignition delay. With matched starting conditions, the combustion proceeds in similar fashion for each of the test fuels, resulting in similar combustion characteristics and gaseous exhaust emissions. The results of a prior paper, which fixed the start of combustion in their examination of cetane number and EGR effects on combustion, demonstrate parity between the NO_x values of the different fuels (Li et al., 2006). This reflects a similar effect to the ones noted here: by aligning combustion, the overall combustion was similar and NO_x emissions equivalent.

4.3.4 Maximum Rate of Pressure Rise and Combustion Noise

Other important engine parameters besides emissions also demonstrate strong dependence on combustion phasing. Factors relating to the overall sound level of the combustion process are important for satisfying both hardware durability and vehicle customer requirements. The maximum rate of pressure rise is characteristic of the combustion process and noise level produced. Within the range of injection timings tested, the maximum rate of pressure rise decreases with a retard in combustion phasing, as demonstrated in Figure 18 below.

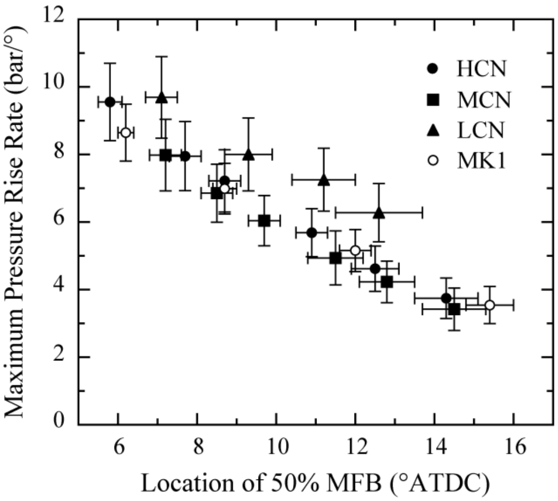


Figure 18: Maximum pressure rise rate versus combustion phasing. Injection timing sweeps at 40% EGR, 1000 bar injection pressure, varied fuels.

It is notable that all four fuels exhibit complementary behavior – no significant fuel dependent differences are present in the results. Phasing the combustion later within the cycle (retarding the combustion phasing) results in decreased maximum pressure rise rates. When combustion is phased later (for combustion occurring after TDC), combustion occurs as the cylinder volume is expanding, with the cylinder expansion partially offsetting the combustion pressure rise. This opposing expansion mutes the sharp pressure rise from combustion, decreasing the peak cylinder pressure rise rates as displayed in Figure 19. This is expected behavior, but the complementary behavior of the test fuels (and lack of fuel dependent effects) demonstrates that this parameter is principally related to bulk cylinder conditions rather than combustion fuel effects, and dictated primarily by combustion phasing.

Combustion noise level reflects the dependency of maximum pressure rise rate on combustion phasing. Combustion noise, as measured with an AVL Combustion Noisemeter, shows a similar strong dependence on combustion phasing with little dependence on fuel type. Combustion noise is highest at the earliest combustion phasing and decreases with a retard in combustion phasing for the range of tested injection timings. All four test fuels exhibit similar noise behavior within the tested range of injection timings, as shown in Figure 19.

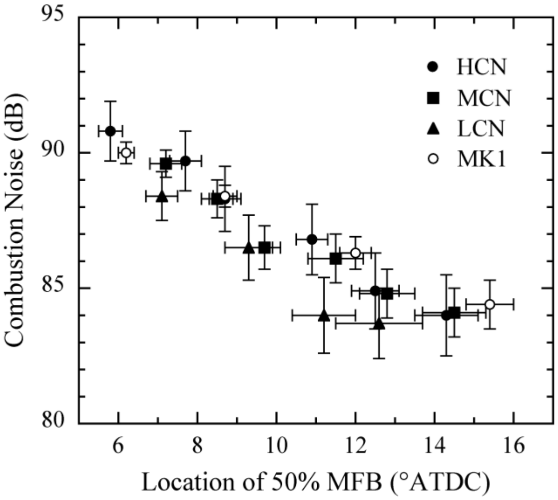


Figure 19: Combustion noise versus combustion phasing. Injection timing sweeps at 40% EGR, 1000 bar injection pressure, varied fuels.

The combustion noise measurement (described in greater detail in the Experimental Methods chapter) filters the signal from the cylinder pressure sensor to simulate the sound dampening of a representative engine block and the aural response of a human ear, measuring the resulting pressure level in decibels. Accordingly, the signal is a function of the cylinder pressure and, therefore, will be closely related to the maximum rate of cylinder pressure rise. Thus both parameters demonstrate matching behavior sharing a common explanation.

4.3.5 Combustion Efficiency

The efficiency of the combustion process is also a distinct function of combustion phasing and an important parameter to consider during analysis of an operating condition. Emissions and efficiency are frequently at odds – decreased NO_x and PM emissions often come at the expense of fuel economy, especially with the premixed diesel combustion modes (Jacobs, 2005). Understanding the combustion efficiency as a function of combustion phasing is therefore important.

Standard metrics used to evaluate efficiency, including quantity of fuel injected per cycle and specific fuel consumption, require accurate fuel flow measurements. Unfortunately, the fuel flow measurements on the test engine used in this study are woefully inadequate to yield accurate and precise results. Due to its large flow capability, the fuel flowmeter used has a listed instrument uncertainty of ± 0.1 g/s. The fuel flow at the light load operating condition tested is around 11 mg/cycle, or 0.14 g/s. Thus the instrument uncertainty is around 75% of the measured value. The measurement uncertainty will easily cover any trends within fuel flow measurements. There is significant fluctuation in the measured data resulting from the oversized fuel flowmeter which obscures all trends associated with fueling rate.

Since direct measurement of fuel consumption does not yield usable data, examination of other parameters linked to engine efficiency are required for comparison. Using exhaust emissions data, it is possible to calculate combustion efficiency, the percentage of the injected fuel which is completely combusted to CO_2 and water. This can then be used, along with other parameters, to assess efficiency and fuel consumption behavior. The formula used to calculated combustion efficiency from exhaust species concentrations is given in Equation 7 (Chapter 3, Section 3.6). Combustion efficiency decreases with retarding combustion phasing within the range tested for all four test fuels as shown in Figure 20. All four fuels demonstrate similar behavior.

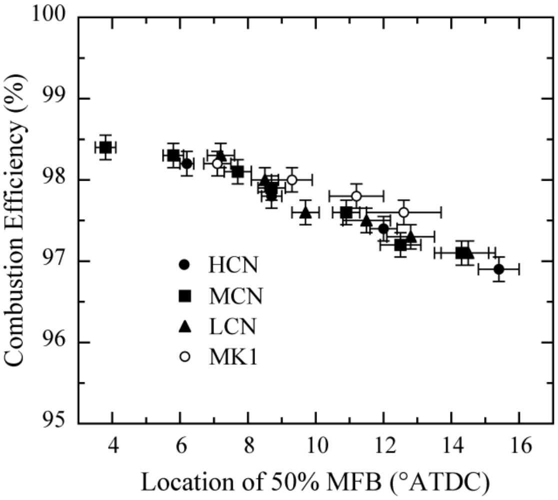


Figure 20: Combustion efficiency versus combustion phasing. Injection timing sweeps at 40% EGR, 1000 bar injection pressure, varied fuels.

As shown, similar levels of combustion phasing occur for all four test fuels, and all are decreasing over the range of combustion phasing tested. This trend is complemented by the CO and HC emissions trends, both of which increase with a retard in combustion phasing. Both CO and HC are products of incomplete combustion: increases in them imply fuel is not being fully combusted. If combustion efficiency is decreasing with a retard in combustion phasing, it is likely that overall efficiency could be following a similar trend. Further support comes from an examination of the fuel injection duration. As combustion phasing is retarded for a given fuel in these tests, the fueling rate increases to maintain the fixed IMEP load condition. If fueling was not adjusted, the most retarded injection timing conditions would have a 2% (0.1 bar) lower IMEP than the most advanced timings.

To further illustrate this, fuel injection durations are normalized as a function of each fuel's injection duration at the combustion phasing yielding 90 dB combustion noise. The combustion phasing yielding 90 dB combustion noise is a standard condition used in these tests and is the most advanced combustion phasing common between fuels. Each fuel is normalized against its own injection duration at the 90 dB point to account for the differences in fuel energy content and density that exist between test fuels. Figure 21 demonstrates the change in relative injection timing as a function of combustion phasing. Y-axis error bars are not displayed as the injection durations plotted are commanded (absolute, discrete) values, and the overall trend is more important than the exact value.

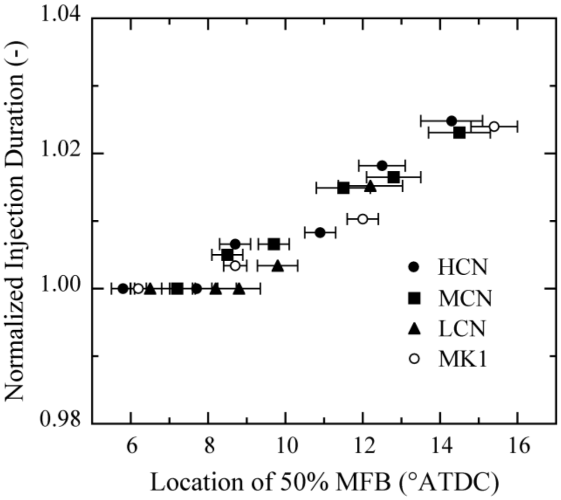


Figure 21: Normalized injection duration versus combustion phasing. Injection timing sweeps at 40% EGR, 1000 bar injection pressure, varied fuels. Commanded injection durations are normalized against the injection duration which yields 90 dB combustion noise for a specific fuel.

From this figure, it is apparent that maintaining a constant engine load while retarding combustion phasing requires increasing the fuel injection duration. Thus, fueling is increased as injection timing is retarded for a constant load, implying an increase in fuel consumption. This matches the trend partially inferred from the emissions and largely suspected. As combustion is phased later in the expansion stroke (all combustion occurring in these tests was phased after TDC), the combustion chamber expansion rate increases, leading to lower combustion pressures and resulting work output. Retarding combustion phasing over the range tested here decreases the thermodynamic efficiency of the engine, which when coupled with decreased combustion efficiency, decreases the overall thermal efficiency and increases fuel consumption.

4.3.6 Effect of Injection Pressure on Emissions

Injection pressure effects are studied to identify potential cetane number variations and add context to the previous results. For one test fuel, the US high cetane fuel, injection timing was held constant at the value yielding 90 dB noise at 1000 bar, and then the injection pressure varied from 800 to 1400 bar in 200 bar increments. Principally, varying injection pressure changes the combustion phasing. The subsequent combustion and gaseous emissions behavior is dictated by the combustion phasing, not specific injection pressure effect. As shown in Figure 22, increasing the injection pressure advances the combustion phasing by around one degree in combustion phasing per 200 bar increase in injection pressure.

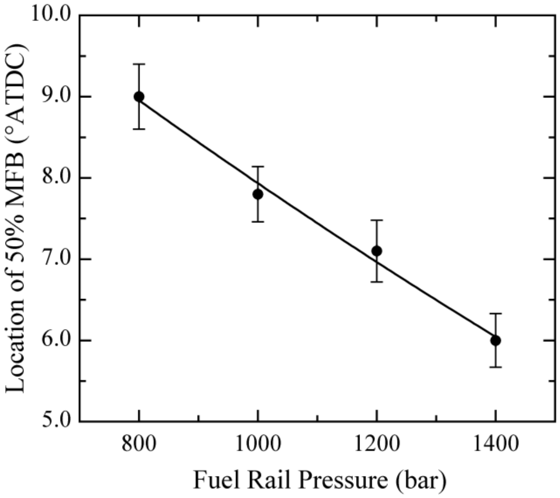
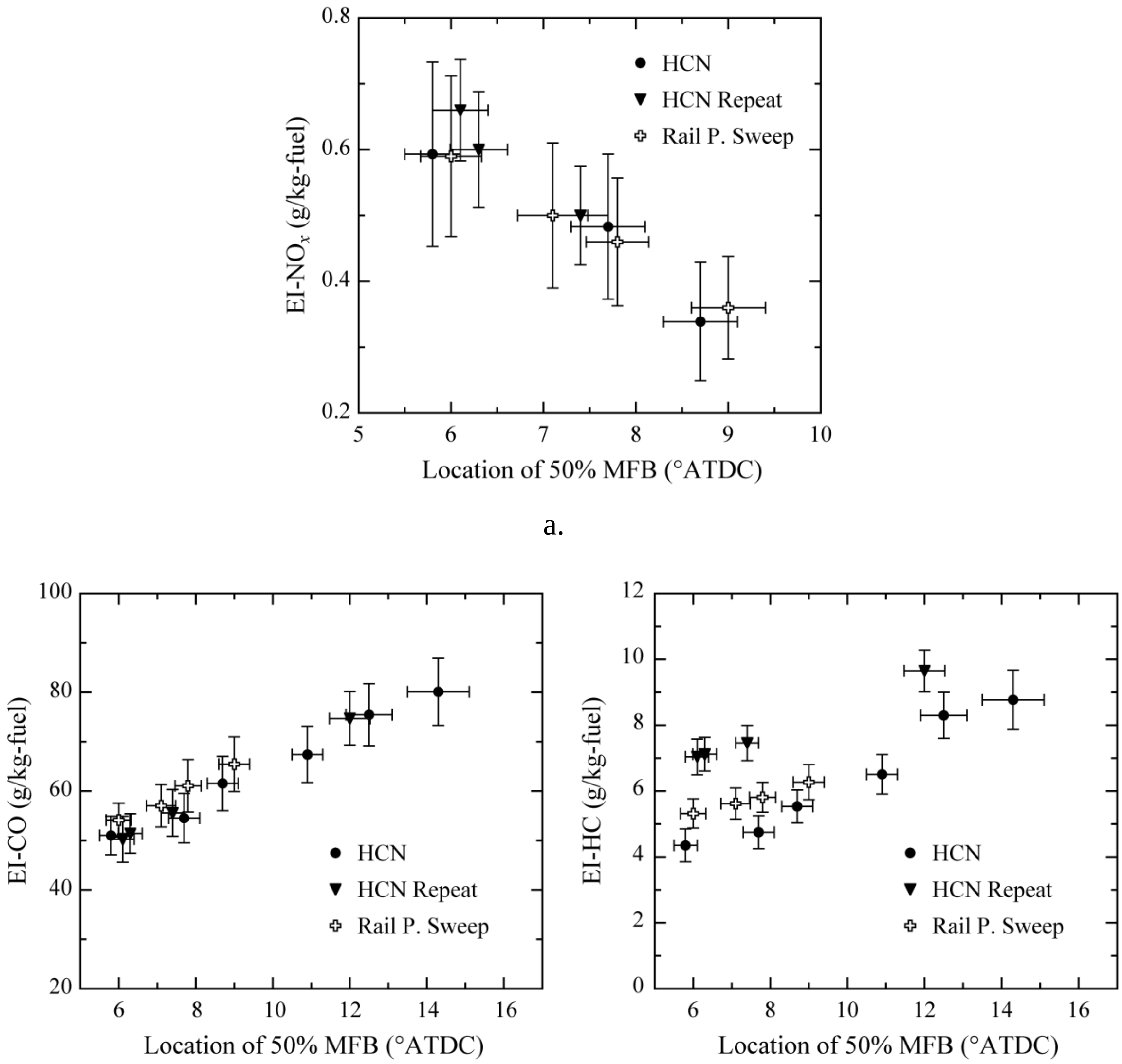


Figure 22: Combustion phasing versus injection pressure. US high cetane fuel, 40% EGR, 15° BTDC injection timing.

This shift in combustion phasing precipitates a change in gaseous emissions within the range of values predicted by combustion phasing. This is demonstrated in Figure 23, showing the injection pressure effect within two sets (principal plus repeated test) of data taken by varying the fuel injection timing. EGR fraction is constant between all tests shown. The gaseous emissions are still principally a function of EGR and combustion phasing. Injection pressure is simply another parameter which shifts combustion phasing.



a.

b.

c.

Figure 23: Injection pressure effect on gaseous emissions referenced to combustion phasing sweep. (a) NO$_x$, (b) CO, (c) HC. US high cetane test fuel, 40% EGR. Injection pressure sweep conducted at 14 °BTDC injection timing. ‘HCN’ and ‘HCN Retest’ were identical timing sweeps conducted a week apart.

Smoke emissions, however, demonstrate a dependency on injection pressure, though the relation is step-wise rather than continuous. As demonstrated in Figure 24, there is little difference in the smoke emissions produced with injection pressures between 1000 and 1400 bar, but a significant increase at 800 bar. This indicates there is a minimum injection pressure required to yield proper spray breakup resulting in low smoke combustion. This minimum pressure is around 1000 bar – any increase in injection pressure above this value does not significantly change the smoke emissions. However, there is a significant increase in soot emissions when the injection pressure is lower than this minimum value.

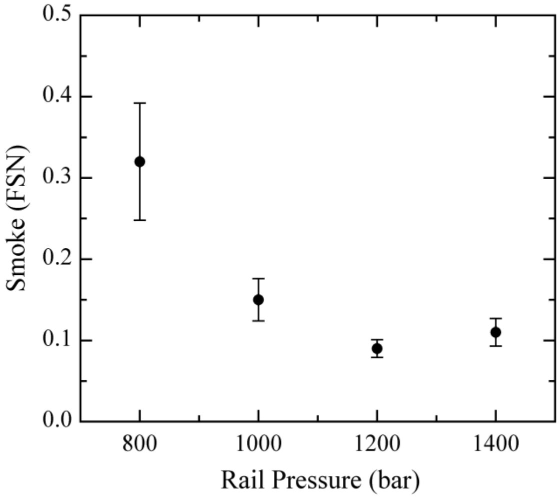


Figure 24: Smoke emissions versus injection pressure. US high cetane fuel, 40% EGR, 15 °BTDC injection timing.

This effect is related to injection spray breakup and fuel-air mixing. Once injection pressure is high enough to yield sufficient spray breakup and mixing to prevent locally rich regions, which would produce significant soot during combustion, increasing injection pressure further does not help. If all fuel-rich regions are eliminated by having sufficient spray breakup and mixing, then further improving the mixture formation by using a higher injection pressure cannot further reduce these fuel rich zones. However, decreasing the injection pressure below what is necessary to provide proper spray breakup and mixing, will result in increased fuel-rich regions and subsequent soot formation.

4.3.7 Acceptable Injection Timing Range

As noted before, ignition delay is strongly a function of cetane number. Thus, as cetane number varies so does the time between injection and the combustion process. This initiates a concern regarding fuel compatibility of premixed diesel combustion strategies. Most current conventional diesel engine control systems set a fixed injection timing based on the commanded load (pedal position). If injection timing is fixed, combustion phasing will shift with variations in cetane number, and the magnitude of these shifts may push combustion into suboptimal operating regimes. Combustion phased earlier than desired leads to excessive and unacceptable combustion noise and NO_x emissions. Combustion phased too late in the cycle results in excessive CO and HC emissions or, if late enough, instability and misfire. To address these concerns, this portion of the work examines the range of injection timing which yields acceptable combustion, as determined by a series of criteria reflecting operability concerns, an expansive and highly inclusive set of operating limits. Injection timings falling within these limits will achieve stable combustion with acceptable combustion noise levels.

Requiring combustion noise levels to not exceed limits, set to insure acceptable NVH conditions in a vehicle, limits the injection timing advance. A common rule is to maintain combustion noise less than 90 dB. If held at these levels, vehicle noiseproofing adequately mitigates engine sound so it is unobtrusive in the vehicle cabin. Reflecting this production implementation guideline, the advance limit is set by requiring combustion noise, as measured with an AVL 450S Combustion Noisemeter, remain less than 90 dB.

The retard limit is defined to reflect misfire and basic operability limits. This defines the retard limit as the point where a further retard in injection timing results in a non-recoverable loss in power. As injection timing is retarded, there is a point where it is no longer possible to maintain the specified load condition of 5 bar IMEP. Increasing fueling at this point does not recover load but rather creates higher exhaust CO and HC emissions. Injection timing limit is one degree advanced from the condition where this occurs. Retarding the timing one degree further (two degrees retarded from the listed limit) results in additional power loss and frequent misfires. Another degree further retarded (three degrees retarded from the stated limit) results in complete misfire – no combustion in any cycles.

The operating window existing between the advance and retard limits discussed above is shown in Figure 25 for each of the test fuels at 40%, 43%, and 45% EGR mass fractions and 1000 bar injection pressure.

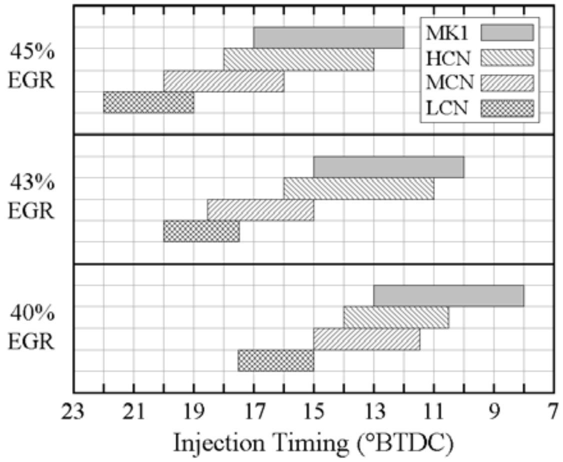


Figure 25: Acceptable injection timing window for the test fuels at different EGR levels and 1000 bar injection pressure. Injection advance limit: combustion noise less than 90 dB. Injection retard limit: loss of recoverable power.

At a given EGR fraction, there are no common injection timings where combustion falls within the constraints for all four fuels. It should be noted that the advance limit is a ‘soft’ constraint – the engine will operate at this condition, just not meet the established noise limit. However, the retard limit is a ‘hard’ limit since the engine cannot be made to achieve the operating condition at injection timings further retarded from the limit. Relaxing the noise constraint allows fuel compliant operation at a fixed injection timing. However, combustion noise resulting from the higher cetane fuels would exceed presently desired levels.

The injection timing ranges shown above were run at one injection pressure – 1000 bar. Testing conducted in a preceding (preliminary) experiment indicated that varying fuel injection pressure did not produce more favorable and overlapping operating windows, as the injection pressure changes simply shifted the operating window without resizing it. Increased injection pressure shifted the retard limit, allowing use of more retarded injection timings, but the effect was counteracted by a subsequent and comparable shift in the advance limit. Increasing the injection pressure decreased the main ignition delay and resulted in a sharper, and therefore noisier, heat release event. Reflecting this initial insight, only one injection pressure was used for the current examination.

Further complicating the use of a fixed injection timing control strategy with variable fuels is that engine load varies with combustion phasing for a fixed injection quantity. As noted before in Section 3.5, when injection timing (and therefore phasing) is retarded for a given fuel in these tests, the fueling rate must be increased to maintain the fixed IMEP load condition. The increase is relative to combustion phasing, and the relative position within the operating window. Hence, to maintain load at a given injection timing, the low cetane fuel requires a longer injection duration than high cetane fuel because the resulting combustion is phased later in the operating window. When fueling is not adjusted, the most retarded injection timing conditions have a 2% (0.1 bar) lower IMEP than the most advance timings. This further exacerbates the difficulty of finding a fuel compliant injection condition. The injection timing range which allows fueling to remain constant while maintaining load is very narrow (at most three crankangle degrees, but usually less and often nonexistent), and not close to overlapping between different cetane number fuels.

Remapping the operating window in terms of combustion phasing (location of 50% mass burned fraction, CA50), rather than injection timing, results in identical operating windows for all four test fuels. At all EGR fractions, and with all injection pressures, the advance limit (90 dB) occurs at a CA50 of 7 ± 1 °ATDC, while the retard limit (loss of recoverable power) is at 15 ± 1 °ATDC, independent of fuel cetane number. Cumulative data illustrating these limits is shown in Figure 26. The 90 dB noise limit is marked, and the misfire/operability limit is denoted by the lack of data with a CA50 later than 15 °ATDC.

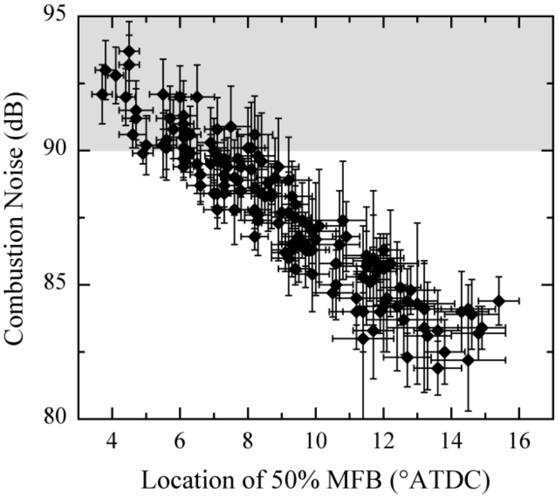


Figure 26: Combustion noise versus combustion phasing. All tested data plotted, including variations in fuel cetane number, injection timing, injection pressure, and EGR flow rate. Gray band covers data points in excess of the 90 dB noise limit.

4.3.8 Perceived Emissions Trends with Fixed Injection Timing

The central conclusion presented in Section 3.2, and one of the main results of this study, is that gaseous emissions from this combustion mode trend with combustion phasing. In more simplistic studies, results are frequently presented in relation to injection timing, a common control variable. In relation to current or future studies which examine fuel cetane number effects on premixed diesel combustion using fixed injection timing, this section seeks to demonstrate the perceived trends associated with varying the fuel cetane number.

It is important to note that, within this section, only results stemming from the US certification fuels will be discussed at the sole matching injection timing: 15 °BTDC. The Swedish MK1 fuel was not tested at an injection timing that matches the US fuels, due to combustion operation limits which were part of the original testing criteria (note related discussion in Section 3.7). In cases where clear trends are present, data for the Swedish fuel tests may be extrapolated and presented for further illustration and support.

As shown before in Figure 10, combustion phasing varies as a function of injection timing and cetane number. For a matched injection timing, combustion phasing advances as cetane number increases, as demonstrated by the cylinder pressure and heat release traces shown in Figure 21. This relation can be further confirmed by combining the relations for main ignition delay versus cetane number (Figure 8) and 50% versus 10% mass fraction burned (Figure 16).

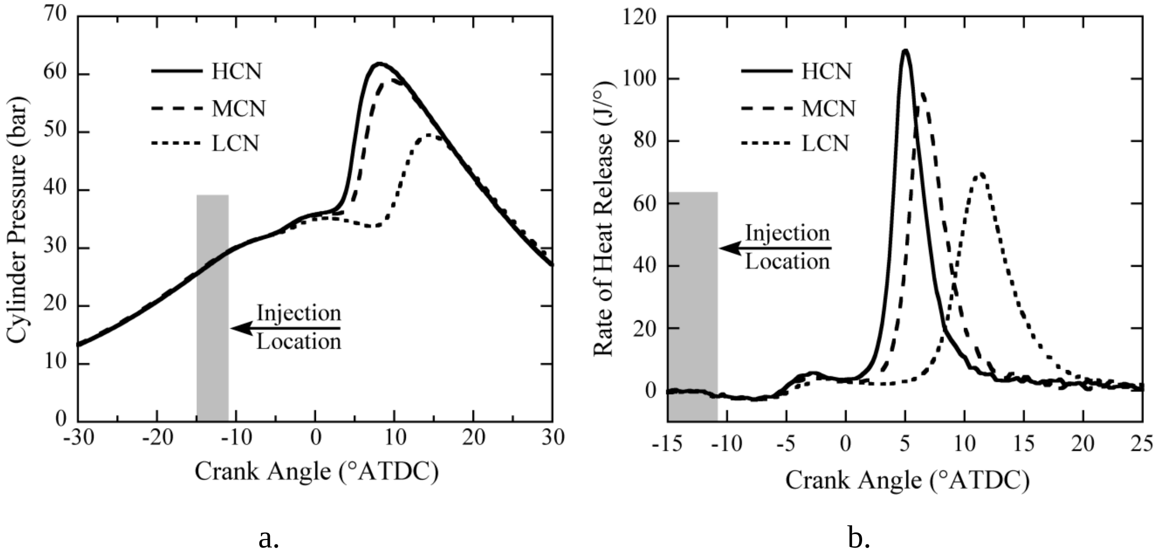
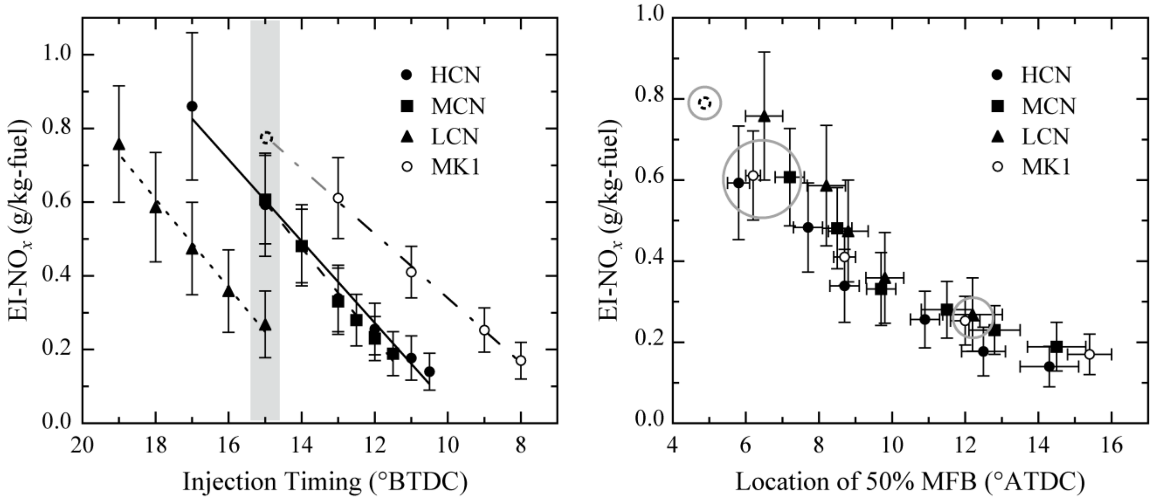


Figure 27: Cylinder pressure and rate of heat release traces at fixed injection timing. (a) Cylinder pressure, (b) Rate of heat release. US certification fuels, 40% EGR, 15 °BTDC injection timing.

Combustion phasing differences, and the related differences in combustion conditions shown in the above figure, manifest themselves in the emissions data. The main critical emissions, NO_x, was shown earlier (Figure 11) to strongly be a function of combustion phasing. With the difference in combustion phasing between fuels for fixed injection timing, NO_x emissions appear to be a function of fuel cetane number. This is shown in Figure 28 (a) below, where NO_x values for the higher cetane fuels are higher than the lower cetane fuels. There is little difference between the mid and high cetane fuels, as their combustion phasing at the matched point is not drastically different, and there is uncertainty/variation in the NO_x measurements. Given the strong linear trends between NO_x and injection timing demonstrated, a NO_x value for Swedish fuel at the matched condition has been extrapolated to further illustrate the apparent trend.

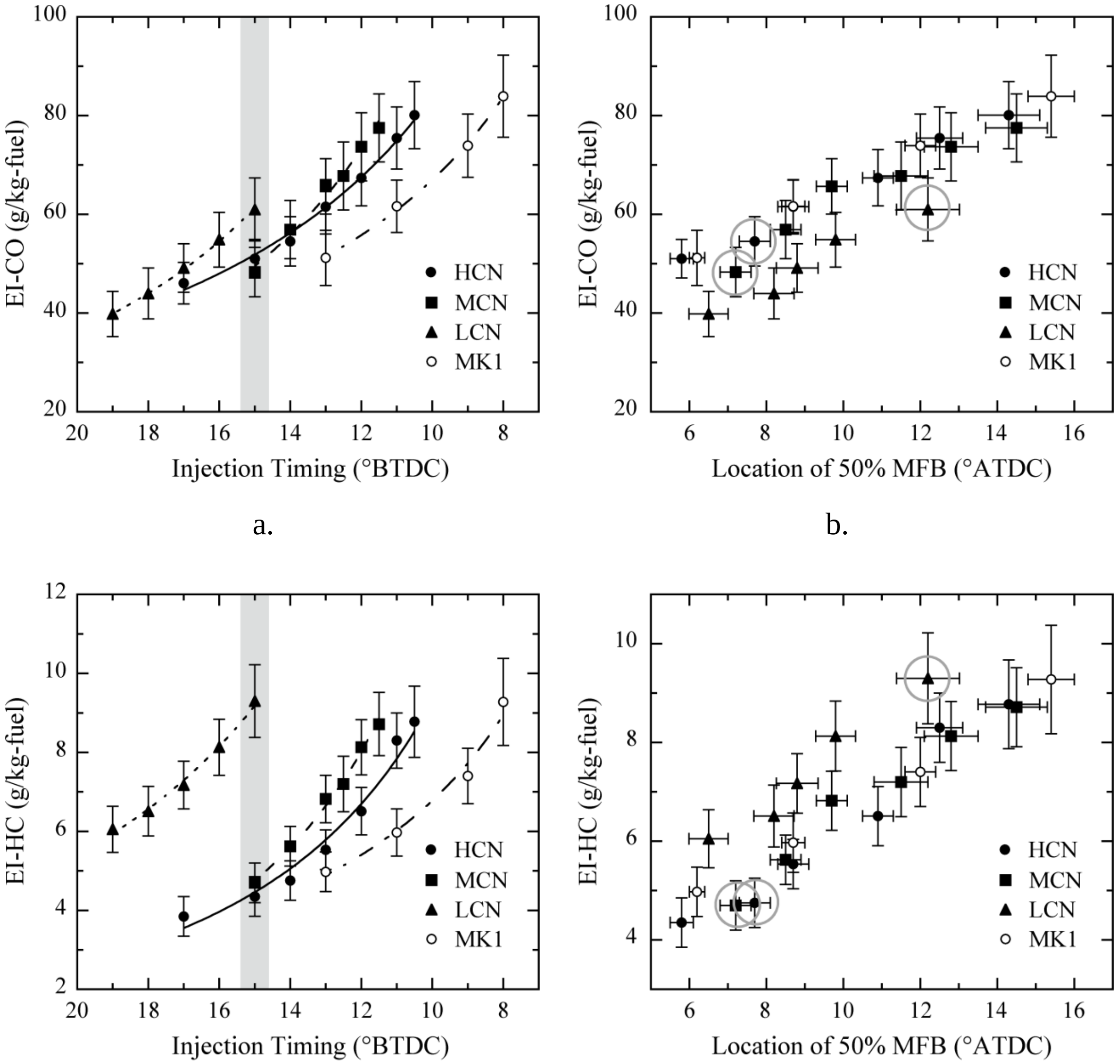
However, the related combustion phasing trend in Figure 28 (b) makes it apparent that what appears as a difference in the fixed injection timing plot is simply the result of combustion phasing differences.



a. b.

Figure 28: Perceived cetane number effect on NO$_x$ emissions with fixed injection timing. (a) Apparent NO$_x$ effect, (b) NO$_x$ effect within context of combustion phasing. Injection timing sweeps with US certification fuels. Apparent effect noted at only overlapping injection timing: 15 °BTDC. Swedish fuel extrapolated to matching timing – actual data not measured.

The same effect manifests in the CO and HC emissions as well, as demonstrated in Figure 29. There is not a substantive difference in the CO values, as the low-cetane fuel produces preferentially lower CO emissions. However, because the low cetane fuel produces notably higher HC emissions for a given phasing, and is phased later (which also increases HC emissions), the HC emissions are dramatically higher for a fixed injection timing condition. Again, the perceived trends with cetane number at fixed injection timing are explained the differences in combustion phasing.



a. b.

c. d.

Figure 29: Perceived cetane number effect on CO/HC emissions with fixed injection timing. (a) Apparent CO effect, (b) CO effect within context of combustion phasing, (c) Apparent HC effect, (d) HC effect within context of combustion phasing. 40% EGR. Injection timing sweeps with US certification fuels. Apparent effect noted at only overlapping injection timing: 15 °BTDC.

4.4 Summary and Conclusions

Fuel cetane number strongly affects the ignition delay and combustion phasing of this single-injection premixed diesel combustion mode. Increasing cetane number results in a shorter ignition delay, which for a given injection timing results in earlier combustion phasing.

Gaseous emissions, particularly NO_x, resulting from this premixed diesel combustion strategy are principally a function of the cooled EGR fraction and the combustion phasing. Fuel cetane number does not directly impact these emissions. Rather, changes in cetane number shift the combustion phasing – the corresponding shift in bulk combustion behavior alters the gaseous emissions. When combustion phasing and EGR fraction are matched, fuel cetane number has no effect. Fuel hydrocarbon composition has, in certain cases, a secondary effect on CO and HC emissions, but the bulk effect remains EGR and combustion phasing.

Additionally, the most important fuel property is cetane number. Though not sequentially varied, fuel distillation does not appear to have an impact on the combustion process or emissions. Both the Swedish MK1 and high cetane US fuel possess distillation curves differing from the other two fuels (which are, themselves, closely matched). However, their combustion and emissions behavior is comparable, indicating that fuel distillation is relatively unimportant.

Basic operability and production environment constraints restrict the operating window and demonstrate the impact of varying cetane number on the combustion mode. Fuel compliant behavior at fixed injection timing is not delivered for the fuels tested here. Across a ten-point range of cetane number, no injection timings yield combustion meeting noise and operability constraints at the tested operating conditions. When characterized in terms of combustion phasing, the operating window becomes very consistent. All fuels show the same operating window independent of fuel cetane number: the noise based advance limit is reached at a CA50 of 7 ± 1 °ATDC, and the loss of power based retard limit at 15 ± 1 °ATDC.

CHAPTER 5

EFFECT OF 2-ETHYLHEXYL NITRATE CETANE IMPROVER

5.1 Introduction

5.1.1 Overview

A common cetane improving additive, 2-ethylhexyl nitrate (2-EHN, EHN, also known as iso-octyl nitrate, ION) is used to improve diesel fuel ignitability in small concentrations. It is commonly produced by several different manufacturers; the exact product used in these tests was manufactured by the Ethyl Corporation and marketed under the name HiTec 4103. The more formal chemical formula is $C_8H_{17}NO_3$, with the basic structure an ethyl hexane molecule with one of the hydrogen atoms replaced with an NO_3 nitrate radical. The chemical structure of the molecule is shown in Figure 30.

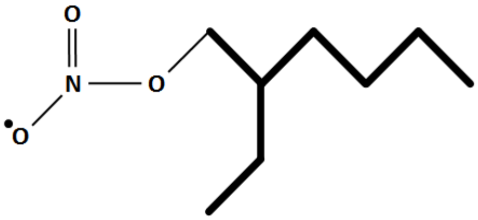


Figure 30: Chemical structure of 2-ethylhexyl nitrate molecule.

As mentioned initially, 2-ethylhexyl nitrate has also been referred to as iso-octyl nitrate. Technically, this is not entirely correct, as iso-octyl nitrate has a slightly different chemical structure even though the chemical formula is the same. The difference is the base compound of iso-octyl nitrate is iso-octane rather than ethyl hexane, which involves slightly different configuration of the carbon branches. The same nitrate radical is present in both compounds and, consequently, both react in a similar fashion with a similar chemical mechanism. Ostensibly, they are equivalent compounds, and the terms are used interchangeably.

EHN, though a nitrate compound, is rather stable at room temperature conditions. The kinetics of its decomposition reaction give very slow reaction rates at temperatures below 100 °C (Bornemann et al., 2001). Additionally, of interest for its use in diesel engines, the decomposition reaction rates are even slower when EHN is in a fuel solution at high pressure (Bornemann et al., 2001). This is very important because it infers that the EHN will remain stable within the fuel injection system, only decomposing within the cylinder after injection.

Generally, the additive doping concentration remains relatively low to achieve a specified increase in cetane number. The increase in cetane number responds in a non-linear fashion with additive concentration, and is dependent upon the base fuel, with higher cetane number base fuels seeing a larger increase in cetane number for given additive concentration. For basic quantification, adding 1500 ppm by volume of 2-EHN to low sulfur diesel fuel with a cetane number of 36-52 yields a 5-6 point increase in cetane number (Ethyl, 2004).

5.1.2 Ignition Improvement Behavior

The addition of EHN to diesel fuel increases the ignitability, and therefore the cetane number, of the fuel. The addition of EHN improves ignition (makes fuel more ignition prone) because it causes the creation of radicals participating in the ignition process (Li and Simmons, 1998). Adding to the stock of these ignition precursors promotes ignition. However, once ignition occurs the effect of the EHN is mute and the combustion process is dictated by the properties of the bulk fuel (Higgins et al., 1998). Further, the primary effect of EHN is on the low-temperature (cool-flame reactions) portion of the diesel combustion process. If the pre-ignition conditions feature higher temperatures, the cool-flame portion is quickly overtaken by the high temperature portion faster, and EHN has less of an effect on the combustion process (Higgins et al., 1998).

The reaction process is identified from the works of Zaslonko et al. (1988), Pritchard (1989), Clothier et al. (1990, 1993), and Stein et al. (1999). The process described is simplified to show the overall process: the details of formation/decomposition processes of intermediate species (or those not intimately involved in the ignition improving effect) are not discussed, as they exceed the scope of necessary detail. With temperatures in the range of 450-550 K (175-275 °C), EHN decomposes into formaldehyde (CH_2O), nitroheptane (C_7NO_2), nitrogen monoxide and dioxide (NO or NO_2), and assorted radicals. As temperature exceeds 650 K (375 °C) the nitroheptane decomposes, further increasing the concentration levels of formaldehyde and nitrogen dioxide (NO_2). The NO_2 reacts through two separate sets of reactions listed below, one with the formaldehyde formed from EHN decomposition and the other with unburned diesel fuel, to form hydrogen nitrite, HNO_2.

$$NO_2 + H_xC_y \xrightarrow{yields} HNO_2 + H_{x-1}C_y$$

(Nitrogen dioxide reaction with diesel fuel)

$$NO_2 + CH_2O \xrightarrow{yields} HNO_2 + CHO$$

$$NO_2 + CHO \xrightarrow{yields} HNO_2 + CO$$

(Nitrogen dioxide reactions with formaldehyde)

The HNO_2 dissociates into NO and the hydroxyl radical (OH). The hydroxyl radical plays a role in the chemical reaction initiating combustion. Increasing the concentration of OH radicals improves the likelihood of ignition, thereby improving the ignition quality and perceived ignitability of the fuel. It should also be noted that this overall reaction is self sustaining (cyclic) to a degree. Thermal decomposition of EHN results in the formation of NO_2 and formaldehyde, which then react to form the HNO_2. This subsequently decomposes leaving NO which, if oxidized to NO_2, can continue to react with formaldehyde or petroleum molecules to form additional HNO_2.

5.1.3 NO_x Formation Mechanism

Examination of the EHN decomposition process described previously illuminates that NO and NO_2 are formed by the initial decomposition, and the final reaction products include NO. This implies that introducing EHN into the combustion process results in an additional NO_x formation mechanism that would otherwise not be present. In contrast to the prompt and thermal NO_x mechanisms, which emanate from the nitrogen in the cylinder air charge either reacting with the hydrocarbon fuel to form NO (prompt NO_x

formation) or being directly oxidized (thermal NO_x formation), the EHN NO_x mechanism results from nitrogen contained within the fuel.

5.1.4 Testing Motivation

The addition of a new NO_x formation mechanism would suggest that fuels laden with EHN would be likely to have higher NO_x emissions. The results of some initial engine tests suggested that this could be correct. Accordingly, a series of more structured in-depth tests were conducted to quantify the effect of fuels doped with 2-EHN on premixed diesel combustion and emissions, specifically NO_x emissions.

5.2 Testing Methodology

5.2.1 Test Fuels

Two sets of fuels were prepared to examine the impact of EHN on premixed diesel combustion. Both fuels sets were designed so that cetane number was matched between a fuel doped with EHN and one that consisted solely of petroleum components. Using the basic test fuels, two sets of fuels were prepared at differing cetane levels. The pairings are as follows:

Set A:
  Swedish MK1
  US ULSD High Cetane, doped with 15% (volume) n-cetane
  US ULSD High Cetane, doped with 1150 ppm (volume) 2-ethylhexyl nitrate
Set B:
  US ULSD Mid Cetane
  US ULSD Low Cetane, doped with 900 ppm (volume) 2-ethylhexyl nitrate

The first set of fuels (Set A), are three different fuels with equivalent cetane numbers of approximately 53. Swedish MK1 is a light distillation fuel, with a natural cetane number in the desired range. The US ultra low sulfur diesel (ULSD) fuel used as a base fuel had a natural cetane number of around 48. In two cases, addition of a doping compound was used to increase the cetane number to match the Swedish MK1. In one case, normal cetane (n-cetane), possessing a cetane number of 100, was added at a concentration of 15% by volume to achieve the desired cetane number increase while maintaining the fuel as only composed of petroleum. The other case featured the addition of 2-ethylhexyl nitrate at a concentration of 1150 ppm by volume.

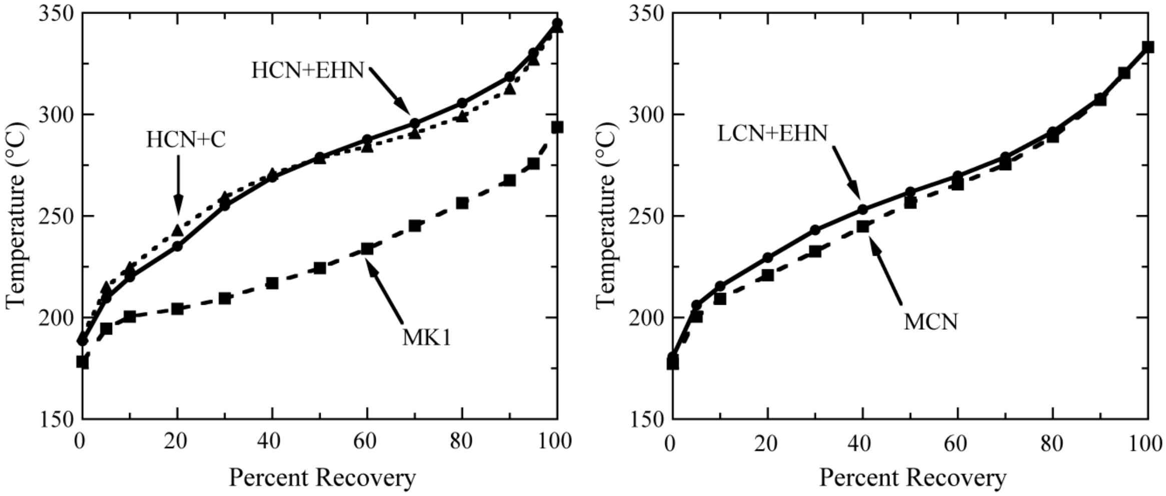
The second set of fuels (Set B), consist of two US ULSD fuels with final matching cetane numbers of approximately 47. The ULSD mid-cetane fuel achieved this 47 cetane number without the use of additives, and served as the undoped petroleum-only fuel. Addition of 900 ppm by volume of 2-ethylhexyl nitrate to the ULSD low-cetane fuel, which had a cetane number of 42 prior to doping, yielded an equivalent cetane number, and the matching EHN doped fuel in the pair.

Final fuel specifications are given in Table 5, and their distillation curves shown in Figure 31. Fuels are labeled in the following tables and figures with the abbreviations indicated: Swedish MK1 (MK1), ULSD high-cetane fuel with 1150 ppm 2-EHN (HCN+EHN), ULSD high-cetane fuel with 15% n-cetane (HCN+C), ULSD mid-cetane (MCN), and ULSD low-cetane with 900 ppm 2-EHN (LCN+EHN).

	MK1	HCN+EHN	HCN+C	MCN	LCN+EHN
Cetane Number	53	54	53	47	47
Sulfur (ppm)	12	16	14	8	8
Density (g/ml)	0.81	0.85	0.84	0.85	0.85
LHV (MJ/kg)	43.5	42.4	43.0	42.8	42.5
H:C Ratio (-)	1.97	1.86	1.91	1.86	1.81
T50 (°C)	224	279	279	262	257
T90 (°C)	268	319	313	308	307

	MK1	HCN+EHN	HCN+C	MCN	LCN+EHN
Alkanes (%)	95	72	75	80	72
Olefins (%)	1	5	4	1	2
Aromatics (%)	3	23	21	19	26

Table 5: Properties of the EHN test fuel sets.



a. b.

Figure 31: Distillation curves for different test fuels. (a) Matched set of 53 CN fuels. (b) Matched set of 47 CN fuels. Error bars are withheld for figure clarity. Uncertainty levels are set by the ASTM D86 standard (ASTM, D86), with uncertainty range as follows: ± 3-6 °C (repeatability), and ± 8-16 °C (reproducibility).

Fuel doping was achieved by dispensing approximately 25 gallons of the respective fuel into a 55 gallon metal storage drum. The amount of additive or doping hydrocarbon required to achieve the desired cetane number was then added. The fuels were mixed using a pneumatic, drum-mounted, immersion mixer spinning at 2000 rpm for 20 minutes. Given the supplier specification for this mixer of a 50 gallon per minute flowrate through the mixing propeller, the twenty minute mixing time would result in the entire contents of the drum being cycled though the mixing blades 40 times, enough to insure thorough mixing.

5.2.2 Experimental Conditions

The testing conditions for this set of tests are a restricted subset of the ones used previously, consisting of injection timing sweeps at 40 and 45% EGR, with injection pressure fixed at 1000 bar. Prior testing indicates that injection pressure is not a particularly influential variable, so it is eliminated to shorten the testing schedule. Additionally, the 43% EGR case is also dropped, as prior testing indicates combustion behavior at 43% tends to fall exactly between the behavior at 40% and 45% EGR. Removing the 43% case shortens the testing process, which is important because of concerns stemming from initial tests that EHN doped fuels cause excessive combustion chamber fouling, which can negatively impact the test results. Minimizing the testing time is a strategic move to help negate this impact.

Thus the two primary tested EGR levels are 40% and 45%. Much of the testing for other parts of the work covered in the dissertation was conducted at 40% EGR, so it remains a natural choice for inclusion. The 45% EGR case is selected because very low levels of NO_x are produced during it. Additionally, the fact that varying the injection timing or combustion phasing does not notably affect the NO_x emissions indicates that thermal NO_x formation is essentially eliminated with this high level of EGR. If thermal NO_x was forming, NO_x emissions should correlate with cylinder pressures/temperatures, which are affected by combustion phasing. Results show that they do not, indicating minimal thermal NO_x formation. Minimizing the NO_x formation levels should make the EHN effect more clearly visible.

5.3 Results and Discussion

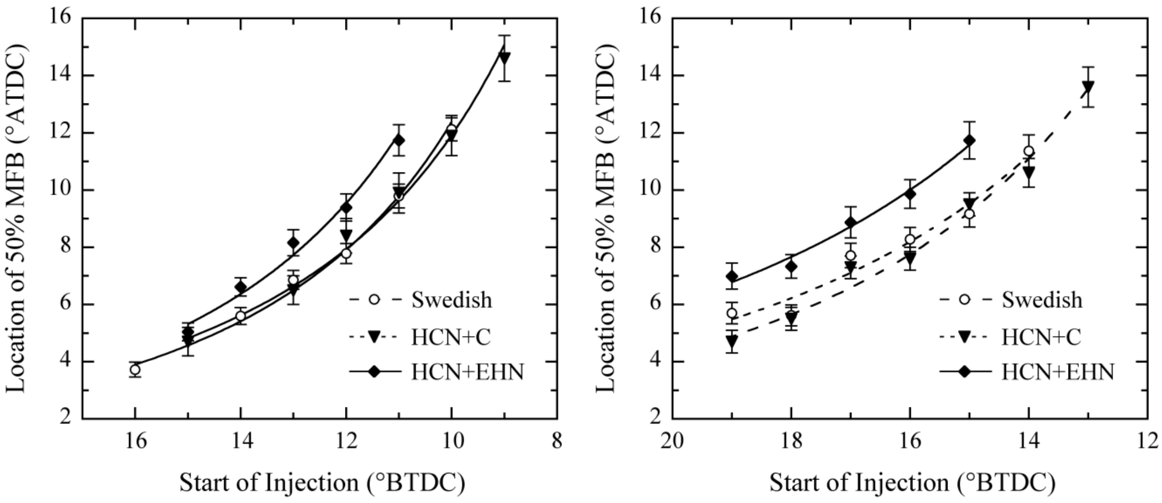
5.3.1 Injector Fouling

In all tests conducted as part of this study (the tests yielding the results presented here, along with initial exploratory tests), the EHN laden fuels demonstrated behavior consistent with injector fouling of a substantially more accelerated and severe nature than the other test fuels. The exact nature of this effect is hard to quantify, but the end results are apparent. Inspections of the injector after tests with the EHN-doped fuel revealed visual indication of substantial injector fouling. The injector deposits were more substantial than what resulted from using the other fuels which lacked EHN. Unfortunately, photographic documentation was not taken to visually demonstrate the effect. Thus, the fouling is not demonstrated *a priori*, but rather through observed combustion and emissions behavior. Combustion degrades over time as injector deposits (fouling) affect the fuel spray coming from the injector nozzle. This effects changes in the combustion behavior and engine emissions for the EHN doped fuels in contrast to the petroleum only fuels. The effects on individual results (combustion and emissions) are noted in their respective section.

It is important to note that increased engine fouling from EHN use is not generally noted within the literature. No studies of EHN treated fuels report fouling issues, though this is not a direct indication that no fouling problems existed. Only one study formally examined engine durability issues with EHN laden fuels, and it was conducted by Ethyl, one of the common producers of EHN and the maker of the EHN product used in these tests (Kulinowski et al., 1998). Their testing consisted of 1000 hour engine durability studies on a pair of Detroit Diesel Series 60 heavy duty truck engines, with one engine fueled with untreated diesel fuel and the other with the same fuel treated with a very high concentration (7500 ppm) of EHN. Measurement of combustion surface deposits and injector flowrates indicated that EHN did not have a negative effect – and actually may have lead to decreased deposits and fouling. However, there are several important caveats: this testing was conducted on a 1993 series heavy-duty engine without EGR over a durability testing cycle with fuels of vastly different cetane number. Issues of fouling are more pronounced when operating in premixed diesel combustion modes with high EGR rates – the lack of EGR in the Kulinowski et al. compared to the current study's high rate may yield diverging trends. Further, the operating modes of the durability test, though not explicitly described, are likely vastly different from the operating modes in the current work, leading to different deposit formation issues. Finally, the two fuels tested in the durability study had vastly different cetane numbers: there was a nine point difference in cetane number between the untreated (42.5) and treated (51.5) fuel. In an engine of the vintage used in the durability study, this cetane number difference gives vastly different combustion characteristics between the two fuels. The possible improvement in durability criteria may result more from the notably higher cetane number than anything directly related to the additive.

5.3.2 General Combustion Behavior

The EHN doped fuels initially act in a very similar manner to the petroleum-only fuels of equivalent cetane number. The ignition delay and the time from start of injection to location of 50% MFB is constant between the fuels at the beginning of testing. However, after the onset of what is understood to be injector fouling, the EHN-doped fuels behavior diverges from that of the petroleum only fuels.



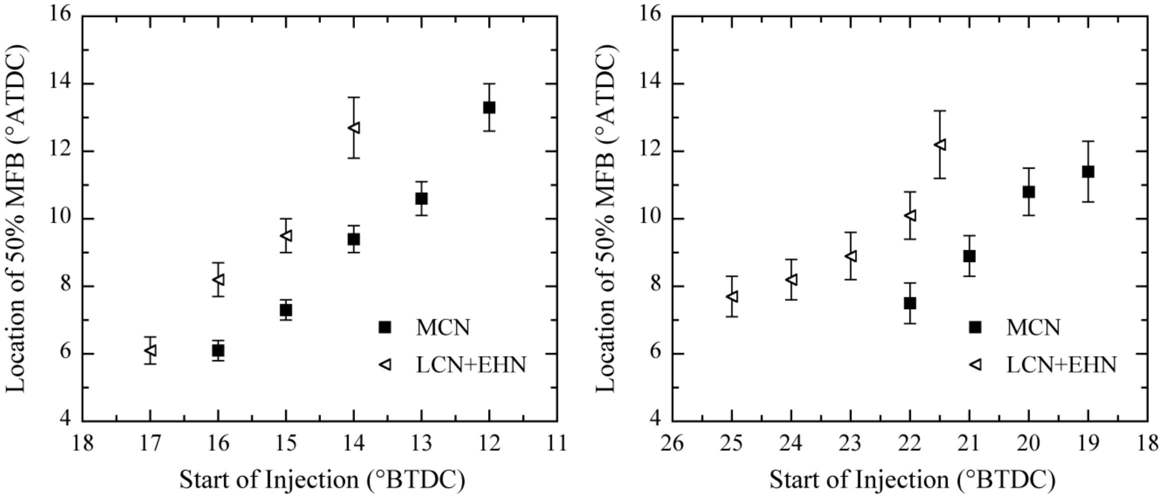
a.

b.

Figure 32: Location of 50% MFB (CA50) versus start of injection for fuels with matching cetane number of 53. (a) 40% EGR condition. (b) 45% EGR condition. There is a time-dependent injector fouling effect on the HCN+EHN fuel data set, resulting in the increasingly delayed 50% MFB location. Timing sweeps were run in retarding direction, with the 40% EGR dataset run before the 45% EGR case. Injection timing sweeps at 1000 bar injection pressure. Fitlines solely for illustrative purposes – no specific relation implied.

In Figure 32 (a), both petroleum fuels follow very similar trends, while the HCN+EHN fuel is similar at the advanced conditions but diverges as timing is retarded. However, this is not an effect of timing, but of test time. In all testing, injection timing sweeps occur in the retarding direction – starting at an advanced timing and retarding back – for reasons of hydrocarbons emissions measurement hysteresis. Thus, inherently, there is a time aspect to the sweep as well. As test time with the EHN-doped fuel increases, the injector becomes increasingly fouled: excessive deposits form at the tip, increasing the ignition delay. The effect noted in Figure 32 (a) is this fouling occurring real time during the test: as the injector progressively fouls, the ignition delay increases, as does the time from the start of injection to the location of 50% MFB. By the end of timing sweep, the injector has essentially reached a fully fouled equilibrium condition, and the offset between the curves remains constant. Advancing the timing back to the advanced condition yields a different ignition delay and time from injection to CA50 than at the test start. This fully-fouled condition is confirmed by later testing at 45% EGR, shown in Figure 32 (b), where the offset between the EHN-doped fuel and the petroleum-only fuels remain relatively constant.

The same phenomenon is present with the matching set of lower cetane fuels, though the offset is larger, as shown in Figure 33. It is believed that bulk fuel differences between the low cetane fuel and the mid cetane fuel are larger than the differences noted between the higher cetane fuels. This exacerbates the magnitude of these shifts.



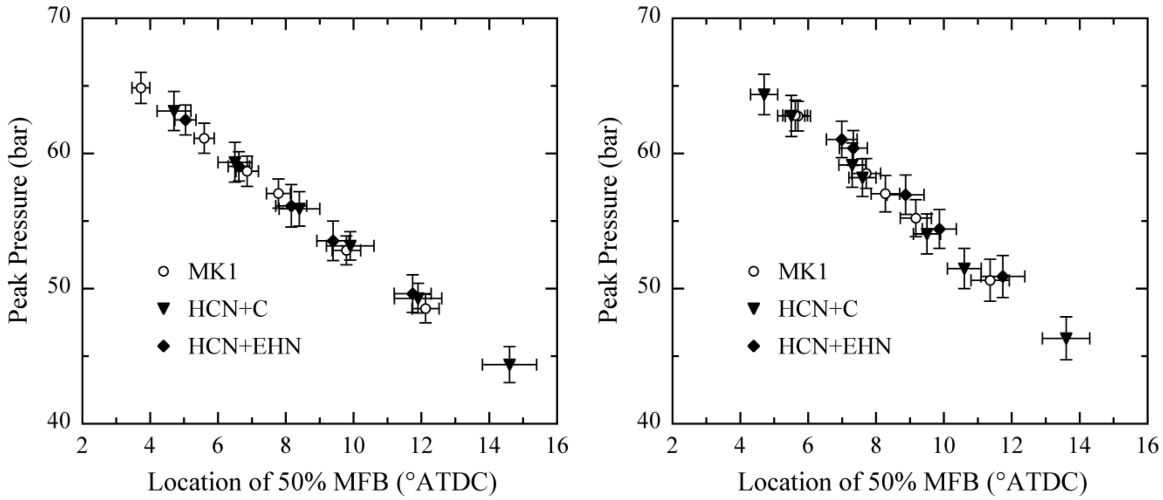
a.

b.

Figure 33: Location of 50% MFB (CA50) versus start of injection for fuels with matching cetane number of 47. (a) 40% EGR condition. (b) 45% EGR condition. Injection timing sweeps at 1000 bar injection pressure.

5.3.3 Cylinder Pressure – Cylinder Conditions

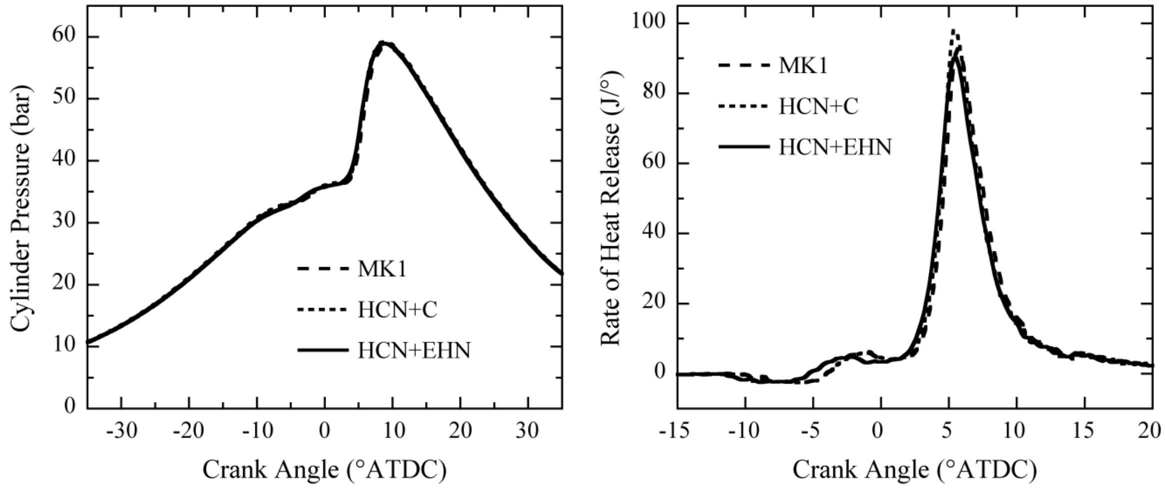
Results of previous fuel tests indicate that at a given operating condition with matching EGR rate, cylinder conditions are identical when combustion phasing is matched. The current set of test fuels also exhibit this behavior. Figure 34 demonstrates that peak cylinder pressure correlates very well with the combustion phasing, the location of 50% MFB. This indicates that cylinder conditions will be very similar for a given combustion phasing independent of the fuel type used.



a. b.

Figure 34: Peak cylinder pressure versus location of 50% MFB (CA50) for fuels with matching cetane number of 53. (a) 40% EGR condition. (b) 45% EGR condition. Injection timing sweeps at 1000 bar injection pressure.

Furthermore, cylinder pressure and heat release traces for the different test fuels overlap when the combustion phasing is matched, further indicating that cylinder conditions are similar/same independent of the fuel type. A representative example set is shown in Figure 35. Data from the matched set of fuels with lower cetane number showed identical behavior.



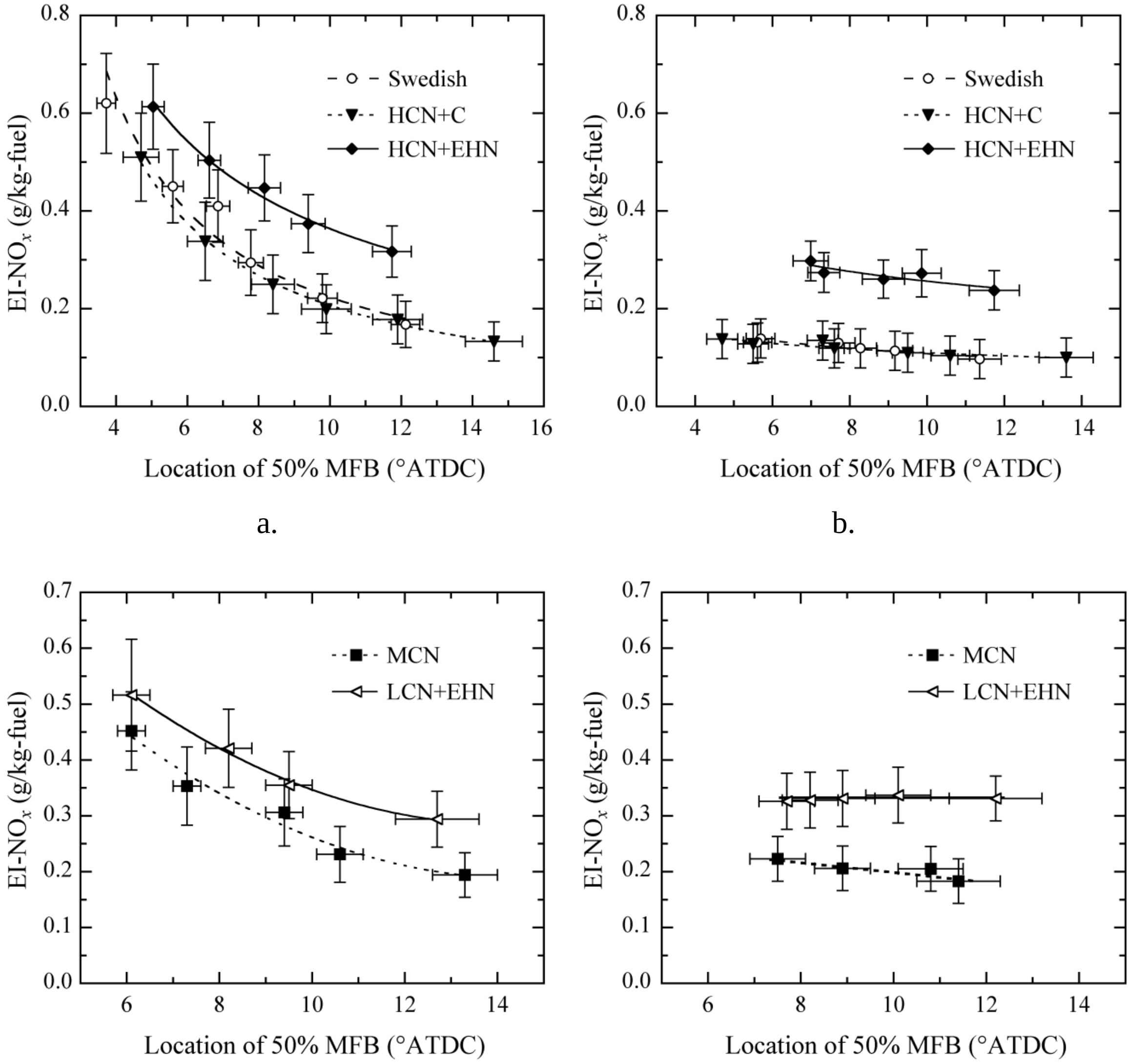
a. b.

Figure 35: Representative matching cylinder pressure (a) and rate of heat release (b) traces for the 53 CN set of test fuels. Injection timing as follows: Swedish fuel and HCN+C (HCN doped with 15% n-cetane) at 13 °BTDC, and HCN+EHN (HCN doped with 1150 ppm 2-EHN) at 14 °BTDC.

These sets of fuels follow the same basic behavioral pattern identified in the study of cetane number effects: the combustion follows a virtually identical heat release and cylinder pressure process when combustion phasing is aligned, independent of fuel. There are slight differences in the cool-flame region because the start of injection is advanced with the EHN fuel to compensate for the fouled injector, but the bulk portion of the combustion is similar. The cool-flame heat release energy remains equal (28 ± 6 Joules, 6% of total mass fraction burned), so main combustion is unaffected.

5.3.4 NO_x Emissions

The fuels doped with 2-ethylhexyl nitrate produce significantly higher levels of NO_x emissions than the petroleum-only fuels. The increase in NO_x emissions is present in the results of both sets of fuels, and at both tested EGR levels, as shown in Figure 36.



a.

b.

c.

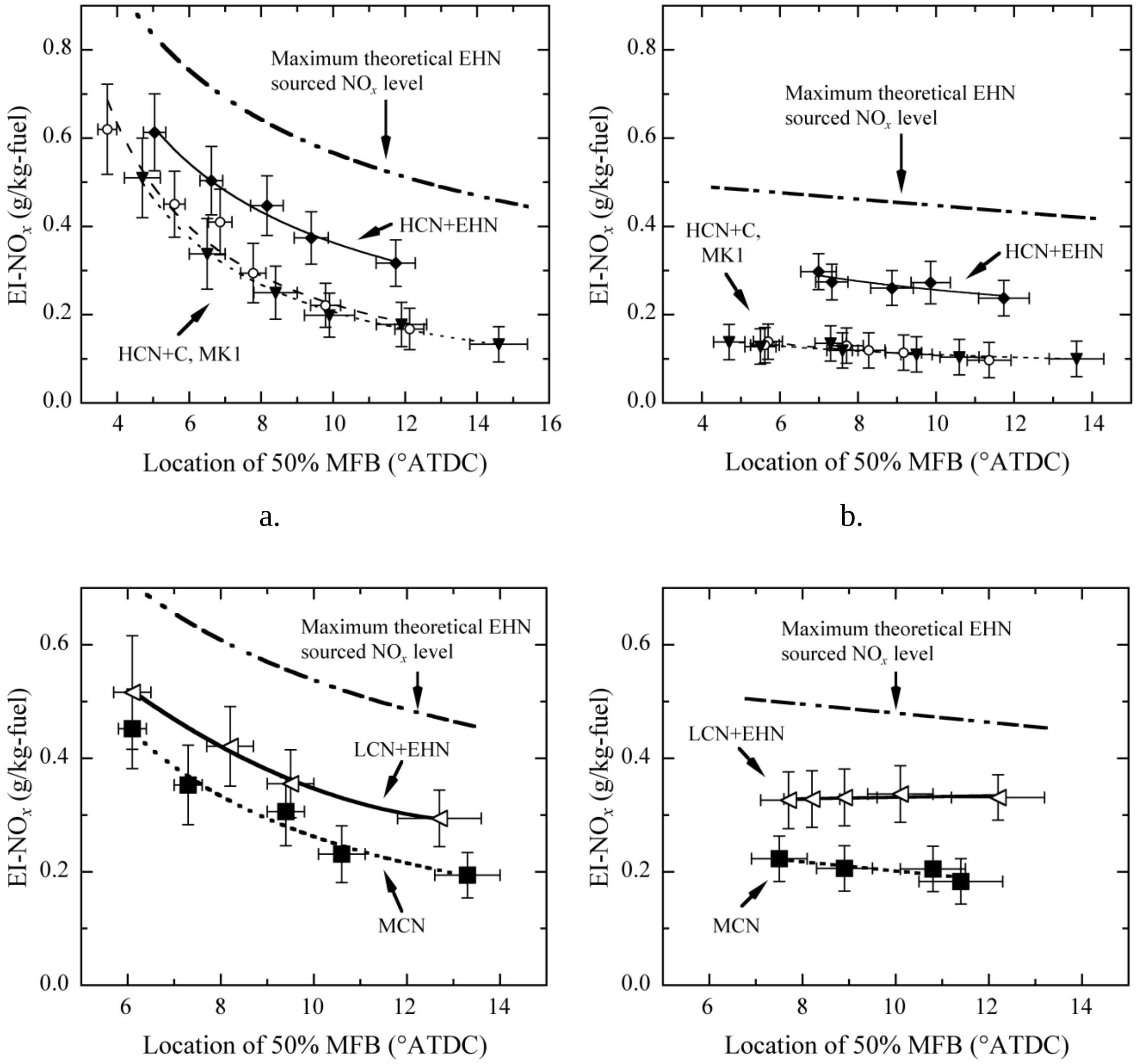
d.

Figure 36: NO$_x$ emissions as a function of combustion phasing for matching cetane test fuels. Higher cetane (53 CN) fuels at (a) 40% EGR, (b) 45% EGR, and lower cetane (47 CN) fuels at (c) 40% EGR, (d) 45% EGR. Injection timing sweeps at 1000 bar injection pressure. Fitlines solely for illustrative purposes – no specific relation implied.

In all cases, NO$_x$ emissions from the EHN doped fuel are higher than those from the petroleum-only fuels. The 0.10-0.15 g/kg-fuel difference in NO$_x$ emissions corresponds to approximately a 6 ppm increase in exhaust NO$_x$ concentration, over a 5-15 ppm base level. The NO$_x$ increase is especially notable at the 45% EGR condition, where NO$_x$ emissions are minimal and independent of combustion phasing. The NO$_x$ concentrations at this EGR level are nearly double those from the petroleum-only fuels.

The NO_x emissions should be similar since the combustion phasing is matched according to the behavioral trend presented in Chapter 4. Thermal NO_x formation should be identical since the pressure traces match. At 45% EGR, the combustion phasing independent NO_x levels indicate there is minimal thermal NO_x formation. Given the similar behavior between the EHN-doped and petroleum-only fuels, it would be expected that the prompt NO_x formation would be similar, as well. If prompt NO_x formation is equivalent, and thermal NO_x formation equivalent (or nonexistent), the difference in NO_x emissions must result from a different mechanism than normally present. Both thermal and prompt NO_x formation mechanisms involve the nitrogen found in the combustion air. The believed source of the increased NO_x emissions with the doped fuels is from the nitrogen found in the EHN cetane improver: a new fuel-borne NO_x formation mechanism. Revisiting the decomposition reactions that lead to the ignition improving characteristic of EHN, the final reaction products are the OH radical (the part which causes improves ignition quality) and NO. Thus, inherent to the action of the EHN improver is a NO_x formation mechanism.

The overall maximum level (*i.e.* worst case) of NO_x production from EHN additive can be calculated from the decomposition reactions: every molecule of EHN contains one nitrogen atom, so each mol of EHN yields at most 1 mol of NO. Using the EHN concentration of each fuel (1150 ppm by volume for the high cetane fuels, 900 ppm by volume for the mid cetane fuels), the maximum possible mass of NO which can be created from the EHN is 0.34 g/kg-fuel and 0.27 g/kg-fuel, respectively. The increase noted in NO_x emissions (0.10-0.15 g/kg-fuel) is covered by both these formation levels, indicating the NO_x from EHN decomposition can account for the full difference in NO_x emissions. This relation is illustrated in Figure 37, which shows the NO_x emissions along with curves representing the maximum level of NO_x which could result from the EHN. These curves for the 53 CN fuels result from adding the maximum possible NO_x increase (0.34 g/kg-fuel) to the average NO_x value at a given phasing from the two petroleum-only fuels (MK1 and HCN+C). For the 47 CN fuels, these curves result from adding the maximum possible NO_x increase (0.27 g/kg-fuel) to the NO_x values from the MCN fuel.



a. b.

c. d.

Figure 37: NO$_x$ emissions with bounds of theoretical maximum NO$_x$ produced from EHN decomposition. High cetane (53 CN) fuels at (a) 40% EGR, (b) 45% EGR, and lower cetane (47 CN) fuels at (c) 40% EGR, (d) 45% EGR. Bounds calculated assuming all nitrogen from EHN in fuel exits as NO$_x$. Fitlines for illustrative purposes – no specific relation implied.

The difference between the maximum possible formation and measured NO$_x$ emissions is accounted for by partial completion of the decomposition reactions and shifts in NO$_x$ equilibrium reactions. All of the classical NO$_x$ formation mechanisms present in combustion are equilibrium reactions: the sudden influx of NO from the fuel increases the NO concentration, shifting the reaction equilibrium. Thus, NO$_x$ which would have been formed due to the normal mechanism does not form, leading the lower than expected NO_x levels. Also, the analyzer used to measure NO_x emissions only measures the concentrations of NO and NO_2. The nitrogen from the fuel which does not show up in the exhaust as NO_x is simply leaving in the form of other nitrogen compounds which are not measured by the NO_x analyzer.

Trying to identify the relative fraction of these two effects is fraught with peril. Two primary factors make further subdivision of the effects difficult: (1) the magnitude of the difference in NO_x level between maximum and viewed results, and (2) the highly dynamic and inhomogeneous nature of the diesel combustion process. The magnitude of the difference between measured and calculated maximum possible NO_x level is on the order of 6-8 ppm. Accurately subdividing this into subcategories of effects (partial decomposition reactions vs. NO_x equilibrium shift) will be difficult simply because the magnitude examined is small, especially relative to the uncertainty of the measurements. Second, the in-cylinder dynamics of the diesel combustion process are extremely complex, with large variations in temperature, fluid motion, particle interaction, and composition, which are all factors that exert strong influence on the chemical reactions and NO_x formation behavior. Fully accounting for these effects is required to reasonably subdivide the small difference in NO_x levels, and yet doing so is highly impractical. Potentially, fully characterizing all nitrogen containing species in the exhaust of the engine when operated on fuels with and without EHN additive may offer some inference as to the relative percentage of the two effects. The relative complexity of the experiment should be weighed against to the likelihood of generating useful results before undertaking, however.

These results indicating that EHN leads to higher NO_x emissions contrast the findings of previous research with EHN, which conclude that EHN addition does not increase NO_x emissions, and in many cases results in a slight decrease (Ullman et al., 1995; Spreen et al., 1995; Gairing et al., 1995; Li et al., 1997; Starr, 1997; Higgins et al., 1998; Higgins and Siebers, 2001; McCormick et al., 2002; Szybist et al., 2005; McCormick et al., 2005). The principal differences between these published cases and the current research work is the magnitude of the engine-out NO_x emissions, and the type of diesel combustion employed.

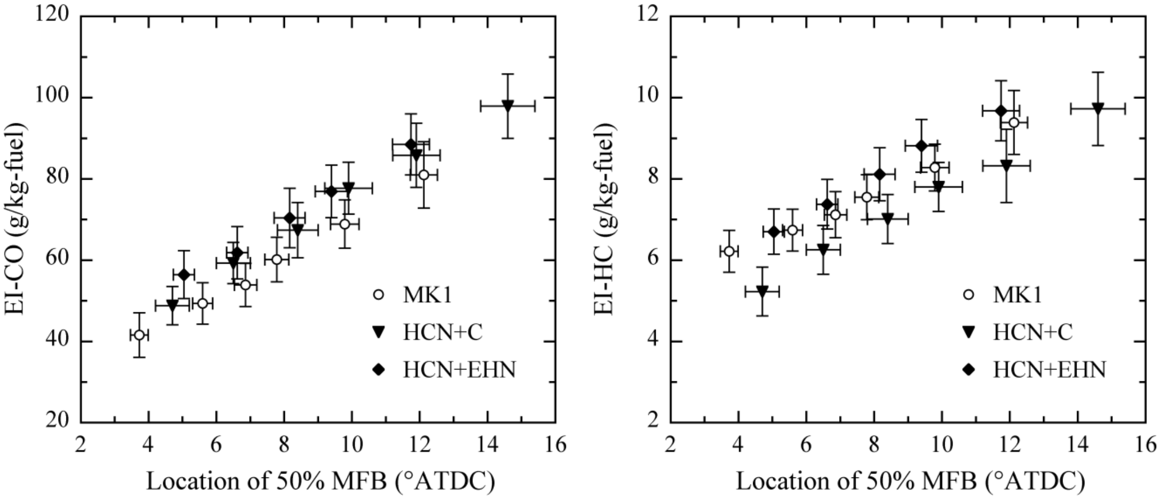
The magnitude of NO_x emissions in published studies is substantially higher than the range produced here. Normalizing the literature results into g/kg-fuel emissions indices demonstrates how much higher the NO_x levels in those tests were. For the first nine references, comprised of tests on older heavy duty and industrial diesel engines, the NO_x emissions are in the range of 25-45 g/kg-fuel, two orders of magnitude higher than the test results of this work. The final reference (McCormick et al., 2005), used a more recent heavy duty diesel engine in a multi-mode test, producing NO_x emissions of approximately 10 g/kg-fuel, still substantially more than the levels of NO_x found in this test. The amount of NO_x formed by the EHN decomposition is insignificant compared to the overall emission level in the prior tests, and would be usurped by the experimental uncertainty and condition variation. However, in the current case, where high rates of EGR are used to minimize the thermal NO_x formation, the amount of NO_x formed by EHN decomposition becomes increasingly significant.

With the exception of the most recent reference (McCormick et al., 2005) the combustion mode used in all these earlier studies is classified as conventional diesel combustion. Given the dates of publication and test engines used, it is unlikely any of these engines use significant quantities of EGR for NO_x reduction. With conventional diesel combustion, featuring both a premixed and diffusion portion of combustion, increasing fuel cetane number decreases mixing time and, as a result, the premixed portion of combustion. By decreasing the amount of premixed combustion, overall peak pressures and temperatures decrease, causing decreased thermal NO_x formation. As such, the decrease in thermal NO_x formation, due to the higher cetane number causing a reduction in premixed fraction, likely overshadows any NO_x production from EHN decomposition. The more recent (2004 calibration) heavy duty diesel engines used in the last reference (McCormick et al., 2005), which were likely using some levels of EGR and multiple fuel injections, the EHN did not alter NO_x emissions. This is expected since cetane number has been shown to have little effect on the combustion of engines using multiple injections (Massa et al., 2007). The cetane improving quality of EHN therefore did not affect the combustion in a manner which would change the thermal NO_x formation.

However, one source in the literature indicates partial support for EHN doping leading to increased NO_x emissions. A principal components analysis study conducted on a diesel HCCI engine reports that, for all other parameters being held equal, increasing the concentration of EHN added to the fuel increases NO_x emissions (Bunting et al., 2007). Their study tested a series of fuels with varied properties, then analyzed the results to correlate between different individual parameters. Accordingly, the authors of this prior study give only modest confidence in the reported correlation between EHN concentration and NO_x emissions. The relation published in their study suggests that the concentration of EHN found in the test fuels of the current study should yield approximately a 0.05 g/kg-fuel increase in NO_x emissions, less than the measured increase of 0.10-0.15 g/kg-fuel. However, the relation in the Bunting et al. paper was determined using only three different EHN concentrations: 200, 3200, and 5000 ppm. There is a sizeable gap between the two bracketing concentrations (200, 3200) to those tested here (900, 1150). Due to the sensitivity of the equilibrium NO_x equilibrium reactions, which are affected by the increased NO_x production, it is possible that the higher concentrations of EHN improver yield similar levels of NO_x emissions as the lower ones tested here. Remember, the NO_x emissions measured are less than the theoretical maximum amount which would be generated if there was complete conversion and no destruction of all the EHN to NO_x. Increased NO_x destruction is likely with the higher EHN concentrations, muting the level of NO_x emissions with the higher EHN concentration. At an EHN concentration of 200 ppm, it will be very difficult to measure any significant level of NO_x increase. Consequently, the reported correlation for NO_x emissions may not be accurate in the range between 200 and 3200 ppm. The shape of the correlation presented is likely not representative within this range.

5.3.5 Carbon Monoxide and Hydrocarbon Emissions

The EHN additive does not have a direct impact on the carbon monoxide (CO) and hydrocarbon (HC) emissions levels. Results initially follow the expected trend, with both CO and HC emissions increasing with a retard in combustion phasing. However, due to combustion fouling, there are EGR specific differences. At 40% EGR, the CO and HC emissions were equal between the EHN treated and petroleum only fuels. This behavior was noted for both the matching high and low cetane sets of fuels. Carbon monoxide and hydrocarbon emissions are shown for the 40% EGR case with the three matching high cetane fuels in Figure 38.

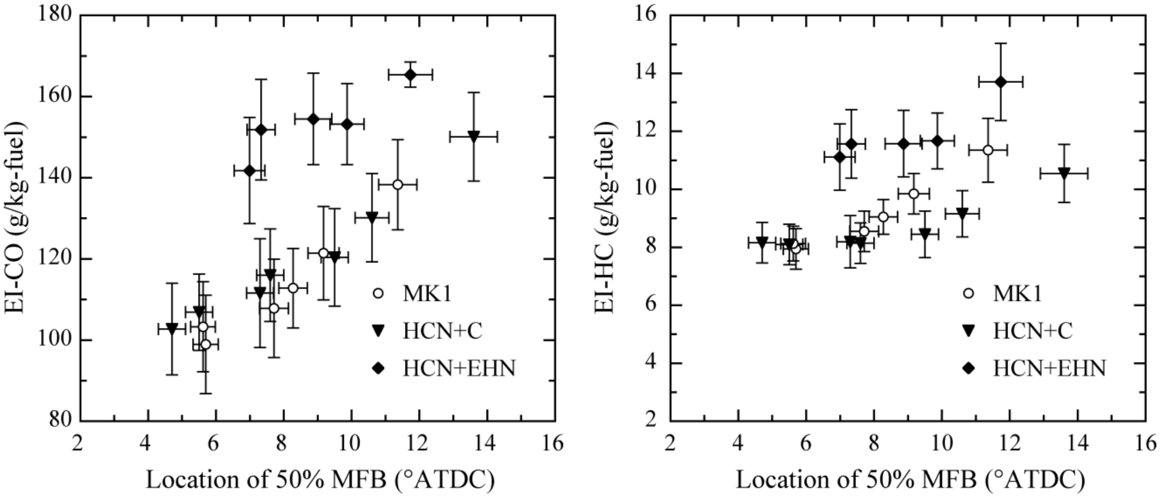


a. b.

Figure 38: Carbon monoxide (a) and hydrocarbon (b) emissions for matched high cetane (53 CN) fuels at 40% EGR. Injection timing sweeps at 1000 bar injection pressure.

There is minimal difference in the trends between fuels of matching cetane number, and the EHN doped fuel does not show any unique behavior at this condition. This indicates that the EHN additive does not chemically alter combustion in a manner which directly affects the CO and HC emissions like it does with NO_x. The emissions trends are consistent with expectations based on previous tests of varying cetane number fuels. At this EGR condition, shifts in phasing due to combustion fouling (as noted earlier) merely alter combustion phasing, with resultant emissions varying accordingly. Emissions of all fuels overlap within uncertainty.

However, this does not hold true at the higher EGR level, due to increased injector fouling and intolerance of the combustion at 45% EGR to poor mixture formation. As deposits build on the injector, there is reduced penetration and breakup of the fuel spray, similar to a reduction in injection pressure. At the higher EGR rate, there is insufficient oxygen distribution and bulk gas temperature to maintain acceptable combustion. Accordingly, both CO and HC emissions increase significantly, as demonstrated in Figure 39.



a. b.

Figure 39: Carbon monoxide (a) and hydrocarbon (b) emissions for matched high cetane (53 CN) fuels at 45% EGR. Injection timing sweeps at 1000 bar injection pressure.

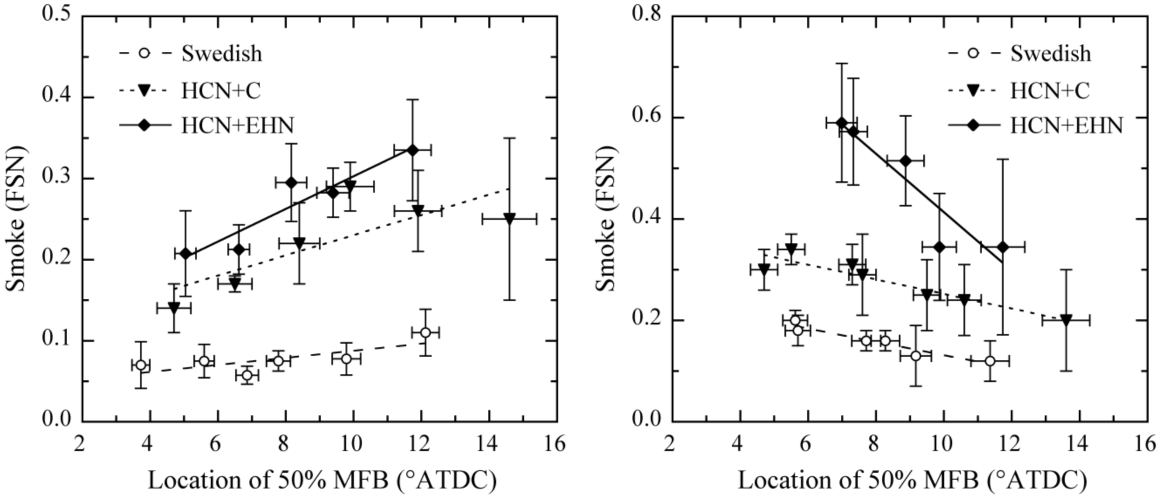
The high (45%) EGR case is significantly less tolerant to suboptimal mixture preparation resulting from the fouled injector. Both CO and HC emissions are simultaneously higher, which is an indication that combustion performance has been compromised. Symptomatic of this, there is also an increase in the number of 'partial burns' for the EHN doped fuel as well. A 'partial burn' is defined as a cycle where the final mass burned fraction is less than 90% of the expected heat release. The Swedish and HCN+C fuels average less than one partial burn per 200 measured cycles, while the HCN+EHN average around three partial burns per 200 measured cycles, with a maximum of nine at the most retarded case. This is a clear indication of poor combustion quality, reflected by the increased HC and CO emissions.

5.3.6 Particulate Emissions

Discussion of particulate emissions must begin with reinforcing the measurement uncertainty caveat: the measurement uncertainty of the smokemeter used for PM measurement is subtantial. As discussed in more detail in the Chapter 3, the instrument uncertainty alone is in excess of ± 0.15, which is significant compared to the magnitude of the measurements. Error bars only include the resolution and measurement uncertainties for clarity (ignoring instrument uncertainty), but differences of less than

0.15 FSN are not judged to be very significant. Thus, the smoke results are more useful in terms of trends, not specific values.

The smoke emissions for the high cetane set of fuels at the two EGR levels are shown in Figure 40. The EHN doped fuels generate higher smoke emissions at both EGR levels than the two petroleum-only fuels. The same behavior was present in the results of the lower cetane pair of test fuels as well. Two main factors explain the observed differences in smoke emissions: variations in the fuel aromatic concentration and injector fouling.



a. b.

Figure 40: Smoke emissions for matched high cetane (53 CN) fuels. (a) 40% EGR, (b) 45% EGR. Injection timing sweeps at 1000 bar injection pressure. Fitlines solely for illustrative purposes – no specific relation implied.

Initial observation suggests that smoke emissions increase with increasing fuel aromatic content – the aromatic content of the three test fuels shown were 4% (Swedish), 21% (HCN+C), and 23% (HCN+EHN). However, substantial literature sources indicate that changes in fuel aromatic content do not affect soot emissions when the fuel cetane number is constant (Lee et al, 1998; Ladommatos et al., 1997; Kidoguchi, 2000). Additionally, the differential in fuel aromatic content does not scale with the observed differences in smoke emissions at the 45% EGR condition. The difference in aromatic concentration between the HCN+EHN and HCN+C fuels is only due to the doping component (15% n-cetane, a saturated paraffin, dilutes the aromatics of the HCN+C fuel). The exact aromatic compounds present in these two fuels are the same since they share a common base fuel. A two percent difference in concentration of the same set of aromatics does not explain the difference in smoke emissions noted at 45% EGR.

The most substantial increase in smoke emissions is at 45% EGR condition. This is also where the largest increases in CO and HC emissions occur, which are tied to a decline in combustion quality due to injector fouling. As deposits on the injector increase, fuel sprays achieve less penetration, breakup, and mixing. This is the same result a decrease in injection pressure causes (for relevant discussion, see injection pressure effects discussion in Chapter 4, Section 3.6). The effect may be identical, with deposits acting to throttle the fuel injection. Accordingly, the behavior is similar to a decrease in injection pressure: increasing smoke emissions. However, there are two concerns with this theory. First, the smoke number decreases with combustion phasing from significantly higher than the other fuels at advanced phasings to approximately the same level at retarded phasing locations. Second, symptoms indicate the injector fouling occurred during the 40% EGR tests, which do not display the same level of increased smoke emissions. For this to be an issue of injector fouling, there is clearly also a secondary EGR effect present.

The phasing dependency of smoke emissions is common at high EGR levels. The smoke emissions for all the fuels decrease as combustion phasing is retarded. This behavior, smoke emissions decreasing with phasing at 45% EGR, shows in the results of the lower cetane matched pair of fuels, along with the varied cetane number petroleum fuels from earlier in this work, and in prior research by Jacobs et al. (2005). At 45% EGR, the cylinder temperatures drops below the soot formation threshold as combustion phasing is retarded. Thus, even when injector fouling should cause notably higher smoke emissions (as evidenced by the high smoke numbers at advanced phasings), the magnitude is limited by combustion conditions not promoting soot formation. Additionally, the smoke measurements only indicate carbon soot emissions – examining particulate matter as a whole (including the soluble organic fraction, SOF) may have yielded a more consistent increase in PM emissions with the EHN.

The second concern, that injector fouling occurs during the 40% EGR conditions but is not reflected in the smoke measurements, can be reasonably explained. The smoke emissions for the EHN treated fuel trend higher than the petroleum-only fuels at 40%

EGR. The offset is not as significant as at higher EGR levels, and is nearly covered by measurement uncertainty, but it is still present. Furthermore, there is an observed and documented effect of EGR affecting the behavior of smoke measurements, and the observed trend falls within this phenomenon. It is expected that the effect would be amplified at the higher EGR condition.

5.4 Summary and Conclusions

The presence of 2-EHN within the fuel introduces a new fuel-borne NO_x formation mechanism into the combustion process, which significantly increases NO_x emissions in a premixed diesel combustion mode. The increase in emissions is not reported by prior researchers due to their use of a conventional combustion mode and large magnitude of the NO_x emissions in their tests, both of which lead to other effects overshadowing the NO_x formed by the EHN decomposition. The NO_x emissions levels resulting from premixed diesel combustion are low enough to reveal a consistent increase in NO_x emissions that is directly tied to the addition of 2-EHN to the test fuel.

The use of 2-ethylhexyl nitrate causes significantly worse injector fouling under the specified test conditions than petroleum-only (undoped) fuels. Observed changes in combustion and emissions behavior lead to this assertion. Test results indicate that 2-ethylhexyl nitrate is not *directly* responsible for changes in carbon monoxide, hydrocarbon, or smoke emissions. However, especially at high EGR rates (45% in this case), injector fouling caused by the 2-EHN in the test fuel leads to distinct increases in all three emissions compared to fuels without the additive.

CHAPTER 6

PREMIXED DIESEL COMBUSTION LOAD LIMITS AND FUEL EFFECTS

6.1 Introduction

Though desired, it is understood that premixed diesel combustion will not be used throughout the full operating range of future diesel engines. The intent is for it to supplant conventional combustion in the light to mid load range. Even within this range, different premixed diesel combustion strategies will be used based on their characteristics, advantages, and deficiencies. Thus, premixed operating modes will always be limited to a range of engine speeds and loads. Combustion modes, like the one used within this dissertation’s study, often classified as a ‘late’ injection premixed diesel combustion (PCI) strategy, are envisioned to be used for the upper portion of the load range covered by premixed combustion modes, with ‘early’ injection strategies covering the lower range. Early injection strategies are very similar in nature to the strategy used here, differing primarily in that they utilize significantly earlier injection timings and increased EGR levels. The resulting combustion is phased closer to TDC for reduced CO, HC, and PM emissions and improved efficiency over comparable conventional or late injection premixed strategies, but uses higher EGR levels to maintain low NO_x emissions. However, noise constraints limit their use to lower engine loads. As load increases beyond the limits of the early injection premixed strategies, late injection PCI becomes more advantageous. Eventually, emissions from premixed combustion modes become excessive and require transition to more conventional diesel strategies for high load operation.

After studying the fuel effects on the emissions of a premixed diesel combustion mode at a fixed engine load (5 bar IMEP), the effect on the operable load range is examined to both further determine the effects of fuel type and bring global perspective and overall context to the project.

6.2 Test Methodology

6.2.1 Test Fuels

The main four fuel test matrix was used for this portion of the work: three US ULSD certification fuels of varying cetane number (low – 42 CN, medium – 47 CN, high – 50 CN) plus Swedish MK1 (53 CN) diesel fuel. These are abbreviated in figures as LCN, MCN, HCN, and MK1, respectively. Further discussion, relevant fuel properties, and distillation curves for the test fuels can be found in Chapter 4, Section 2.1, specifically Table 4 and Figure 7.

6.2.2 Operating Conditions and Test Procedures

Load testing was conducted starting with the main operating condition used in the bulk of the work: 1500 rpm with 5 bar IMEP. Engine speed was held constant at 1500 rpm throughout the load sweep. Intake and exhaust manifold absolute pressures were maintained at 100 kPa and 110 kPa, respectively. The turbocharger on a multi-cylinder version of this engine would likely be affected by a sweep in load – higher loads yield higher exhaust energy which could translate to higher boost levels (depending on the turbocharger boost map and variable geometry turbine control maps). However, attempting to include this effect dramatically increases the complexity of the study while further complicating the results. Accordingly, the intake manifold pressures were held constant for simplicity and to isolate the load trends. Injection pressure was held constant at 1000 bar through the bulk of the load sweep. However, it was increased as part of a parametric study of the high load operating condition, the details of which are discussed later in this section.

EGR mass fraction was maintained at 40% throughout the load sweeps. This does not, however, indicate that equivalence ratio and intake oxygen concentration were held constant throughout the tests. In fact, both these parameters vary across load. Since EGR mass fraction, intake boost level, and engine speed were all held constant while the fueling was altered, the equivalence ratio varies with fueling (and therefore, engine load). As a consequence of the changing equivalence ratio, the oxygen concentration within the exhaust gas (and accordingly the EGR flow) varies with load. Given the substantial flow of EGR, changing the oxygen concentration in the EGR flow alters the intake oxygen concentration as well, so it too varies with load. Of course, there is some interrelation between equivalence ratio and intake oxygen concentration. These last two parameters, equivalence ratio and intake oxygen concentration, are discussed in further detail (including figures detailing their variation with engine load) within the result discussion in Section 3.1.

The load sweeps began with the engine operating at the baseline operating load used in previous portions of this work: 5 bar IMEP. The load was initially decreased from the 5 bar IMEP condition by reducing the injection duration in increments of 20-30 μs. Load was decreased until a limit was reached – typically combustion stability. Combustion was viewed as unstable when the COV of IMEP exceeded 4% or the engine began misfiring. While operating at the 5 bar IMEP condition, injection timing was adjusted so that combustion noise was at the 90 dB limit (approximate location of CA50: 7 ± 1 °ATDC). This injection timing was maintained throughout the load decrease.

After reaching the minimum load level, fueling was increased to yield 5 bar IMEP, and the condition allowed to stabilize for a period of time, with data taken to insure combustion behavior returned to match the starting conditions. When combustion and related emissions returned to initial levels, load was increased by extending the duration of the injection pulsewidth in 20-30 μs increments. However, increasing the injection duration often leads to increased combustion noise, which was counteracted by retarding the injection timing to bring the combustion noise back under the 90 dB limit. Load was increased until one (or more) of the four (very generous) operating limits were reached: (1) smoke measurements exceeded 2.0 FSN (visible smoke limit), (2) IMEP reached a maximum level (increasing fueling no longer brought about an increase in load), (3) hydrocarbon measurements exceeded 1000 ppm-C_3, (4) engine began misfiring. The test was suspended when the engine achieved one or more of these limits (most fuels reached limits 1-3 simultaneously at a particular load). It is important to note that these are very generous limits – it was felt that emissions based restrictions would be the load limiting factor, but that these limits could be applied during data postprocessing following the conclusion of testing. The justification behind the second and fourth operating limits (peak load, misfire) should be self explanatory. The smoke and hydrocarbon emissions criteria bear explanation. The smoke limit of 2.0 FSN is a general industry guideline from historical tests – it is the point where smoke emissions become visible (which was to be avoided). The use of a particulate filter (DPF) will likely be required to meet the stringent PM emissions regulations which are part of new regulations. By maintaining smoke emissions less than 2.0 FSN, particulates are within a range which can be effectively treated by the DPF. The 1000 ppm-C_3 hydrocarbon limit is an arbitrary limit, but HC emissions of this level are excessive, and will be difficult to convert in a DOC to meet the regulated standards. It is felt that operating modes producing HC emissions higher than this are of little utility.

Once a high load limit was achieved, injection timing and injection pressure adjustments were made to evaluate whether the peak load could be increased or emissions reduced. Injection timing was retarded by two degrees (advancing the timing would cause combustion noise to exceed 90 dB), while maintaining other engine parameters (including injection duration). If the engine was no longer exceeding any of the set limits, fueling was subsequently increased until a limit was again reached, establishing a new load limit. A similar procedure was used when injection pressure was increased to 1200 and 1400 bar. However, with higher injection pressure, the injection duration was reduced to give initially comparable fueling rates. Further, the injection timing was retarded, when necessary, to maintain the combustion noise less than 90 dB.

Coupling the data taken from these tests with inferred DOC behavior allows for an examination of the load range of the utilized combustion mode, analysis of fuel cetane number effect on this load range, and understanding the critical limits of the combustion mode.

6.3 Results and Discussion

Examination of emissions behavior is central to this analysis, since engine load limits are defined primarily by emissions criteria. The primary limiting emissions species are smoke, HC, and CO. NO_x emissions are less relevant to this study as (1) they remain less than the specified emissions standards throughout the tests, and (2) NO_x emissions are a strong function of combustion phasing, which was not explicitly constant in these load sweeps. With combustion phasing not constant, NO_x emissions are a function of a secondary variable.

6.3.1 Smoke Emissions

Particulates, reported as a filter smoke number, are a strong function of engine load as shown in Figure 41. At conditions with an IMEP lower than approximately 450 kPa, the smoke emissions are essentially zero (FSN < 0.05, within the values found when measuring background levels). Smoke rises steadily until 550 kPa IMEP, at which point the smoke emissions hook sharply up to the FSN = 2 limit within a 20-30 kPa IMEP span. This is similar behavior to what is noted by Knafl (2007), who evaluated load limits using similar combustion strategies with different engine conditions. The results from his tests show similar trending behavior: negligible smoke emissions in the low load level with strongly increasing smoke emissions at the higher load levels.

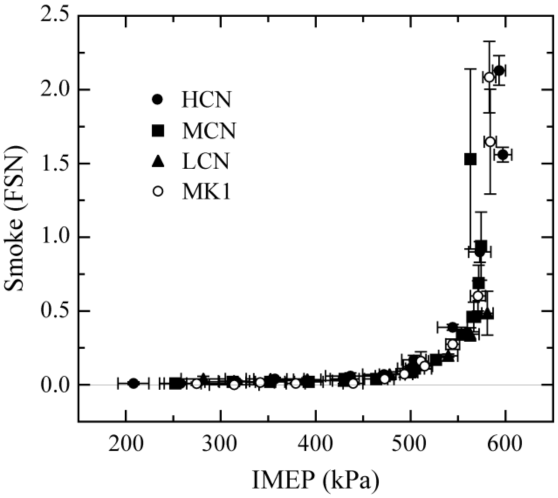


Figure 41: Smoke emissions versus engine load for four primary test fuels.

At light load operating conditions, locations of rich conditions are minimized due to the low volume of fuel delivered with adequate injection pressure for spray breakup and a long enough ignition delay to provide optimized mixing. As fueling increases, there are more regions with unfavorable (fuel rich) fuel:air ratios, which produce soot (Khan et al., 1973; Dec, 1997). At the upper operating limit, increases in fueling yield a sharp increase in soot emissions without any increase in engine load, since the overall cylinder equivalence ratio approaches unity (stoichiometric conditions) as shown in Figure 42.

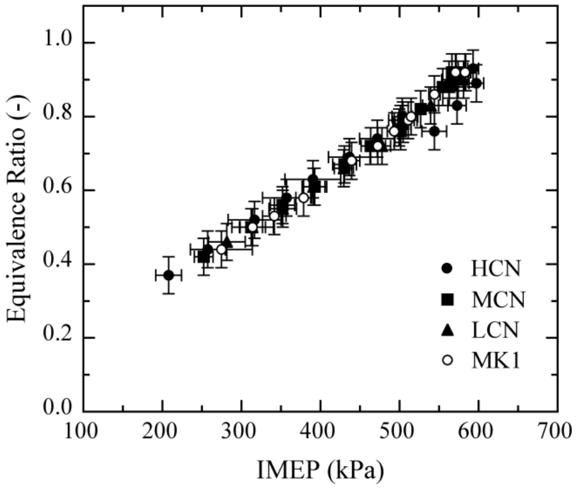


Figure 42: Equivalence ratio (ϕ) versus engine load for the four primary test fuels.

At the peak load conditions the overall cylinder equivalence ratio is very near stoichiometric (0.9). With the overall mixture near stoichiometric, it is virtually certain that there are fuel rich regions within the cylinder. As equivalence ratio approaches unity, the size and number of these regions increases, yielding higher soot formation and engine-out smoke emissions. Equivalence ratio is a function of engine load (fueling), but independent of fuel properties.

All four test fuels yield very similar soot emissions trends. The only deviation occurs as load reaches the upper operating limit. The low cetane test fuel never produces the strong spike in soot emissions as it reaches the upper operating limit – its soot emissions, while increasing with load in this range, peak around a smoke number of 0.5, rather than 2.0 as produced by the other fuels. However, given the steepness of the other curves (increase in smoke number per increase in IMEP), it is possible a small increase in fueling (if it were possible) would increase the soot emissions in a complementary fashion, yielding a similar ending trend as with the other fuels. However, further increases in fuel lead to increased combustion instability, preventing substantiation of this theory. It is also possible that the lack of high soot emissions results from the longer ignition delay apparent with this fuel. Increased ignition delay should allow for improved fuel mixing, resulting in a decrease in soot emissions due to fewer rich regions. However, given that overall equivalence ratio is near stoichiometric, the mixture must be virtually homogeneous to eliminate rich regions, and this seems unlikely.

A further extension of the change in equivalence ratio involves examination of the intake oxygen concentration as a function of load. Since boost levels, engine speed, and EGR fraction are held constant, the intake oxygen concentration will vary alongside equivalence ratio with changes in engine load. This is shown in Figure 43, showing intake oxygen concentration as a function of engine load for the four test fuels.

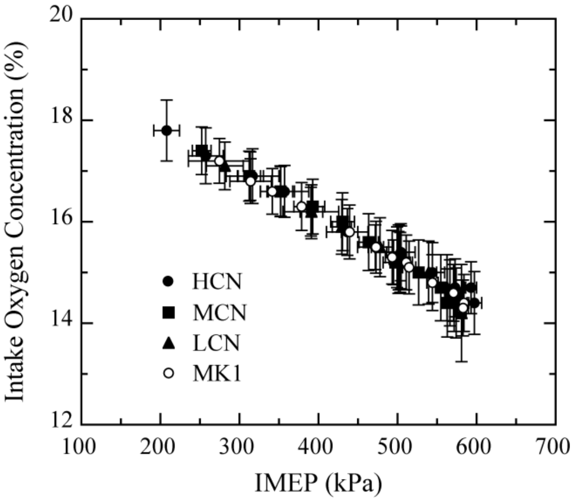
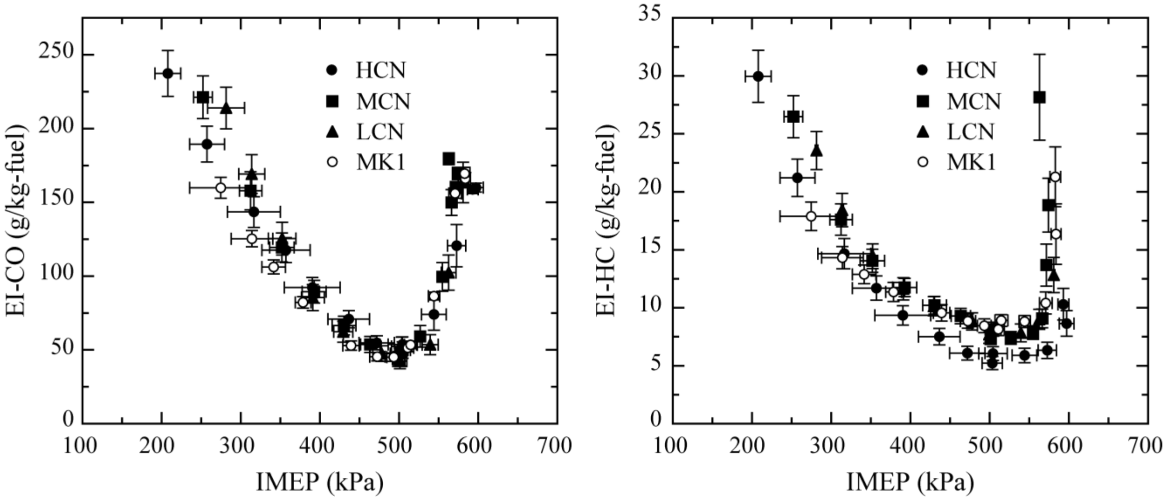


Figure 43: Intake oxygen concentration versus engine load for the four primary test fuels.

The intake oxygen concentration decreases with an increase in load, essentially inverse the equivalence ratio trend. This is understandable because the intake oxygen concentration is a function of equivalence ratio (and vice versa). As equivalence ratio increases towards stoichiometric, the amount of excess oxygen in the combustion process decreases, resulting in a lower concentration of unreacted oxygen in the exhaust gas. Since 40% of the intake charge is recirculated exhaust gas (the balance being fresh air with a constant oxygen concentration), a decrease in exhaust oxygen concentration lowers the intake oxygen concentration. Of course, the parameters are also connected in the opposing manner – as the intake oxygen concentration decreases due to less oxygen in the EGR, the oxygen:fuel ratio decreases, further increasing the equivalence ratio. Equivalence ratio and intake oxygen concentration are linked parameters which behave in the expected manner. There are no resulting differences across test fuels – all fuels show similar behavior.

6.3.2 Carbon Monoxide and Hydrocarbon Emissions

Both CO and HC emissions exhibit similar trends for this combustion mode across a sweep of engine load, as shown in Figure 44. The trends display a minimum around 5 bar IMEP, with a steep increase to higher loads and a more shallow increase as load is decreased. Both emissions trends also sharply increase as the high load limit is reached.



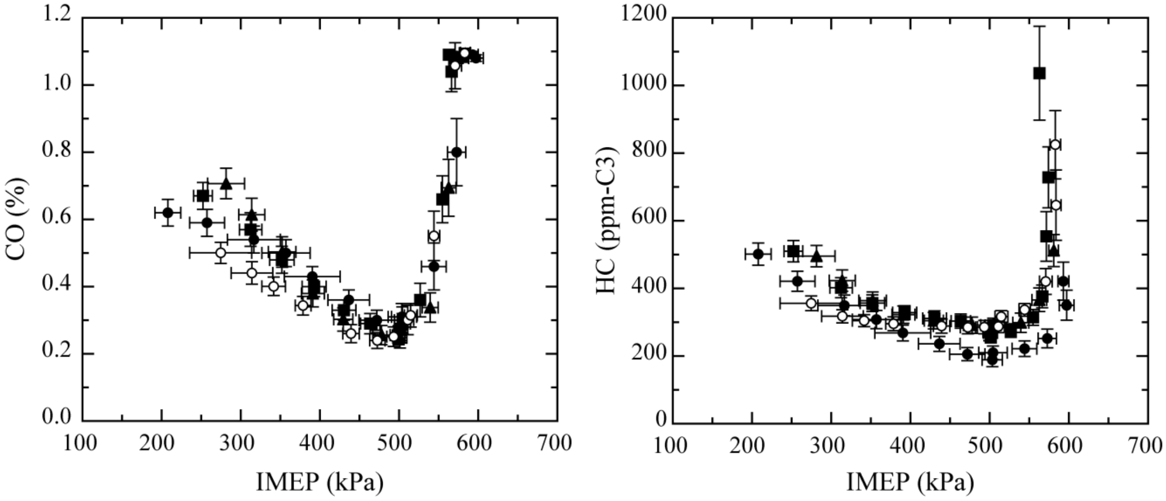
a.

b.

Figure 44: Carbon monoxide (a) and hydrocarbon (b) emissions versus engine load.

At high load conditions, the CO emissions erroneously appear to reach a peak value of around 175 g/kg-fuel. For each fuel, the last several conditions (highest load) yield CO emissions in excess of 1.1%, the saturation concentration for the measurement range of the CO analyzer used. Accordingly, data for all of these high load points indicate a CO concentration of 1.1%, a constant and spurious reading. Given the trend consistency, it is believed that the CO emissions continue to sharply increase with a near vertical slope in the range not accurately measured.

While the measured species concentrations follow a similar trend, the low load effect is strongly magnified by the presentation of results as fuel flow normalized EI emissions indices. The levels of CO and HC slightly trend upward as load is decreased from the 5 bar IMEP condition, but this is amplified by the normalization based off fuel flow rate, which decreases through the same range. The high load range emission trends (sharp increases), being normalized by increasing fueling rates, are actually somewhat muted by the computation of EI emissions indices. Figure 45 shows the raw emissions concentrations as a function of engine load to illustrate this point.



a. b.

Figure 45: Carbon monoxide (a) and hydrocarbon (b) emissions concentrations versus engine load.

The combustion mode appears to be optimized at the 5 bar IMEP condition, which initially incurs pause as to the true value of this study and its observations since 5 bar IMEP was the base condition. However, the end result simply demonstrates the rationale behind comments made in the opening paragraphs of this chapter: there is an optimal load range for implementing the ‘late’ premixed diesel combustion strategy used in this study. Premixed diesel combustion modes are only optimal over a narrow load range. At light loads, where CO and HC emissions increase to high levels, transitioning to an ‘early’ injection strategy should yield more acceptable emissions. However, evaluation of this goes beyond the extents of the current study.

The surge in CO and HC emissions as load increases above 5 bar IMEP is expected, matching the soot emissions trend. As fueling increases towards the limit, the equivalence ratio approaches unity (stoichiometric) as shown in Figure 42. As the overall cylinder conditions approach stoichiometric, less air is available for complete combustion of all the injected fuel. While the overall mixture is always lean, it is not entirely uniform but somewhat stratified. Combustion occurring in locally fuel-rich regions does not have sufficient oxygen for complete combustion, though the overall chamber does. Within these rich regions, the lack of sufficient oxygen for complete combustion results in products of partial combustion: CO, HC, and PM emissions. All three of these emissions can be tied to incomplete fuel oxidation (CO is an incompletely oxidized combustion product, HC is unburned and partially burned fuel, and soot is pyrolyzed fuel).

Moreover, as load increases, combustion phasing is retarded, from both a shift due to the increased quantity of fuel combusted, and injection timing retards used to hold combustion noise under 90 dB. Combustion phasing is shifted due to increased fueling, because the heat release curve follows a similar initial trajectory, only extending higher and longer due to the higher level of heat output from the increased fueling. Accordingly, combustion phasing is retarded as well. Recalling results presented in Chapter 4, both CO and HC emissions increase with a retard in combustion phasing.

As the load decreases below 5 bar IMEP, CO and HC emissions also increase. As engine load decreases from reduced fueling, the combustion temperature decreases as well. As noted within the classic equivalence ratio versus temperature plot (Kook et al., 2005), this moves combustion into a region of increased CO production. As equivalence ratio drops, there is also increased risk of overmixing, creating regions where the fuel-air mixture is too lean for ignition (overleaning). The ensuing lack of combustion results in increased HC emissions. Additionally, the combustion is phased later in the cycle than would be optimum. Recalling results presented in earlier chapters, both CO and HC emissions increase with a retard in combustion phasing. However, the NO_x emissions are close enough to the limits that advancing the combustion phasing forward would result in NO_x emissions exceeding the acceptable limits. To operate effectively with low emissions in this range requires significantly advancing the injection timing – the result of which is ‘early’ premixed diesel combustion. However, to effectively utilize dramatically advanced fuel injections, different levels of EGR are normally used, which substantially change the combustion conditions.

6.3.3 Peak Load Levels

As discussed in the preceding section, all three primary load function emissions (soot, CO, HC) increase sharply at similar load levels. The trends indicate that as fueling is increased beyond this point, higher engine load will not result but emissions will continue to increase. Effectively, the slope of the emissions trend versus engine load becomes vertical. For all four test fuels, this peak load condition was achieved at an IMEP of 570 ± 20 kPa.

6.3.4 Injection Timing Effect on Peak Load

Injection timing effects were examined at the peak load condition by retarding the timing from the 90 dB timing, and redetermining peak load. Injection timing was not advanced, as this would cause combustion to exceed 90 dB. Initially, fueling levels remained constant, but fueling was increased if the load limit criteria were not met or exceeded after the initial timing retard. The effect on soot is displayed in Figure 46.

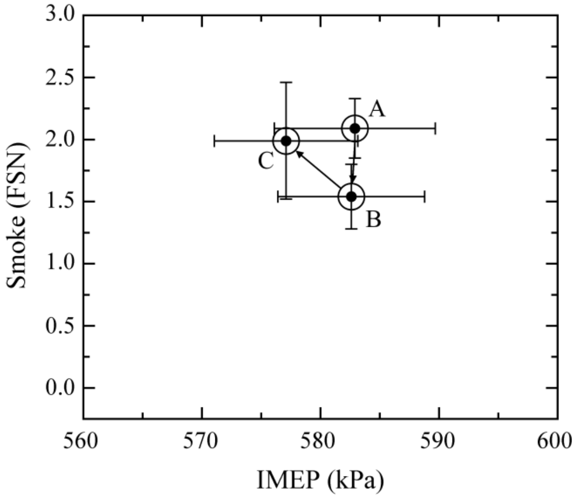


Figure 46: Effect of injection timing on soot emissions and peak load conditions. Swedish fuel showed here – other fuels exhibited complementary behavior. Testing progression as follows: initial baseline point (A), followed by a two degree retard in injection timing (B), followed by increased injection duration (C).

For the two high cetane fuels (ULSD high cetane and Swedish MK1), retarding the injection timing results in lower soot emissions with comparable measured CO and HC emissions at the same engine load. However, when fueling is increased, the result is not increased engine load, but merely increased soot, CO, and HC emissions. At the comparable peak load and soot emissions of 2.0 FSN, the HC emissions are 50% higher than with the earlier injection timing (CO was saturated well before this point and, therefore, indistinguishable). Hence, a shift in the timing of injection (and therefore combustion) makes it possible to operate at the peak load condition with lower soot emissions, but does not allow operation at higher load. It should be noted that soot was exempted from earlier discussion of emissions being solely a function of EGR and combustion phasing. In this case, later combustion phasing results in lower soot emissions. The peak pressure is 500 kPa lower with the retarded combustion (5500 kPa vs. 6000 kPa), indicating cooler combustion which helps to limit soot pyrolysis. Fuel carbon which may have exited as soot under prior conditions, may be partially oxidized to CO and HC with combustion phased later. A slight, though not substantial, uptick in HC emissions is noted (with the CO analyzer saturated, it is not possible to discern changes in CO emissions).

For the low and mid cetane fuel, retarding the injection timing does not yield a notable decrease in soot emissions. The combustion phasing is not substantially changed, nor are the resulting peak pressures. Stability concerns preclude varying the injection timing by two degrees as done with the higher CN fuels. Only a one degree shift can be made with the MCN fuel while maintaining acceptable combustion. For the low-cetane fuel, stability issues prevent retarding injection timing at all - retarding the timing resulted in misfire and extremely unstable combustion. Both these fuels have a significantly increased ignition delay compared to the higher CN fuels (26-29 degrees for LCN and MCN vs. 20-21 degrees for MK1 and HCN), and correspondingly earlier injection timings (21, 17 °BTDC for LCN, MCN vs. 13.5, 14 °BTDC for MK1, HCN). These early injection timings cause the combustion to display similar traits to HCCI, where there is no direct link between the injection timing and the combustion phasing – combustion conditions throughout the delay period have as much an effect on the combustion process as the injection timing. Significant instability (substantial change in combustion and variation of phasing) was notable within the combustion of the low CN fuel at this condition.

6.3.5 Injection Pressure Effect on Peak Load

Increasing injection pressure has a similar effect to retarding injection timing: decreasing the level of smoke emissions but not yielding higher peak load. With higher injection pressure, the smoke levels decrease significantly at a comparable load level. The slight load increase visible for this transition in the accompanying figures is not judged to be overly significant relative to the sizable uncertainty bounds. When fueling is subsequently increased, the result is not an increase in engine load but simply higher soot emissions. This behavior is consistent for all four fuels, for injection pressures of 1200 and 1400 bar. The effect is shown for one fuel, Swedish MK1, in Figure 47.

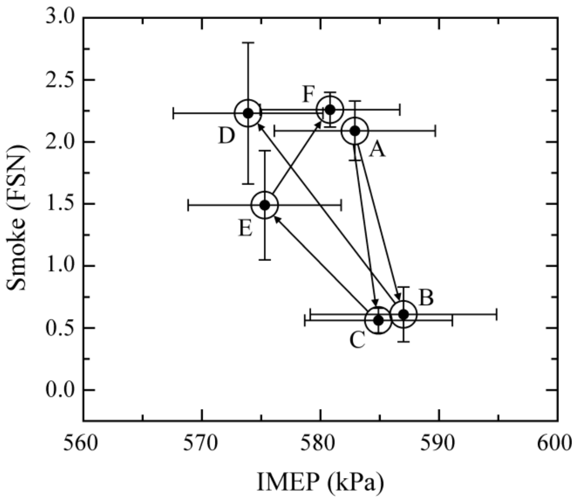


Figure 47: Effect of injection pressure on soot emissions and peak load conditions. Swedish fuel showed here – all other fuels exhibited complementary behavior. Point A is baseline peak load condition taken at 1000 bar injection pressure. Points B-D used 1200 bar injection pressure, while points C-E-F used 1400 bar injection pressure. Testing progression as follows: initial point (A), increases injection pressure (B, C), increased injection duration (D, E-F).

Tests decreasing the injection pressure to less than 1000 bar was not conducted, as prior injection pressure sweeps at 5 bar IMEP show decreasing injection pressure below a certain value (1000 bar in those cases) causes a substantial increase in soot emissions. Since soot levels were already at the limit, making an adjustment previously shown to increase soot emissions was judged to be of little utility.

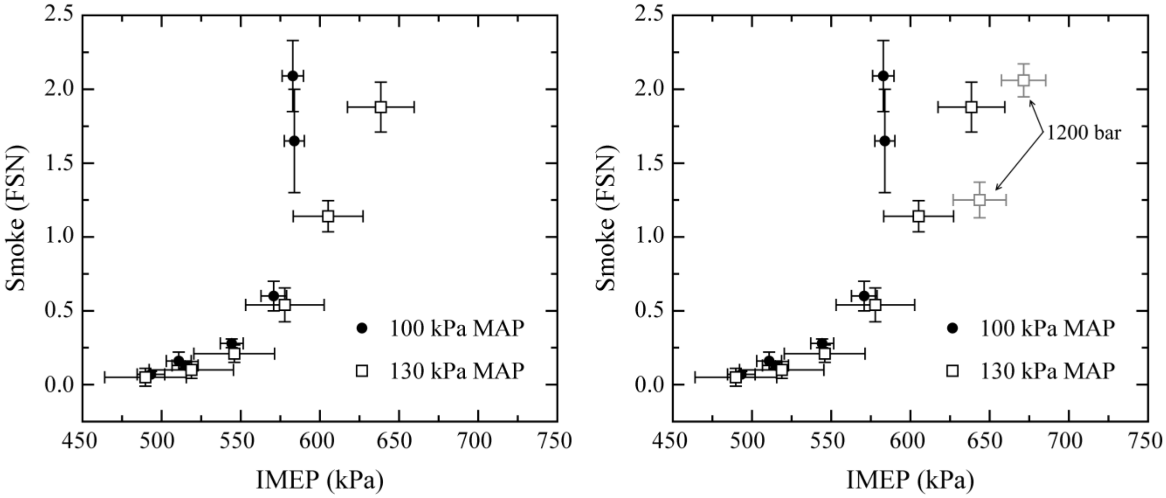
Increasing injection pressure decreases the soot emissions by improving the spray breakup, enhancing the in-cylinder mixing processes and decreasing the quantity of locally rich regions within the cylinder. While global cylinder average temperatures remain reasonably low and the mixture overall is still lean, the in-cylinder mixture is still rather inhomogeneous, and soot forms in the localized rich regions. The low cylinder temperatures prevent substantial post flame soot oxidation, so most soot formed during combustion remains and exits in the exhaust. Enhancing the mixing process by increasing injection pressure reduces these local rich regions and the resulting soot production.

6.3.6 Peak Load Limitations

From the above noted effects, there seem to be two principal factors limiting the operating range: cylinder mixing conditions partially dictating emissions, and overall equivalence ratio dictating peak producible load and partially dictating emissions as well. Increasing peak engine load requires addressing both concerns.

CO, HC, and soot emissions all increase dramatically at higher loads. Various strategies can be used to enhance the mixing process to reduce these emissions. Common strategies include increasing the injection pressure (as demonstrated in this study), increasing the number of holes in the injector nozzle (Alkidas, 1988), increasing cylinder turbulence by increasing chamber swirl/tumble (Khan et al., 1972) or using a turbulence sustaining/enhancing combustion chamber shape (Williams and Tindal, 1980).

Across parameter tests, engine load always peaks at a similar point (in these tests, an IMEP of 570 ± 20 kPa) and is unresponsive to increases in fueling. This suggests a fundamental limitation of the condition, which is not dependent on any of the tested variables. The test variables (fuel CN, injection pressure and timing) are all related to the fuel side of the combustion process. The primary limitation on load results from the air side of the process – fueling is limited by the amount of air within the cylinder and maximum equivalence ratios. Examining the equivalence ratios indicates that combustion is lean overall, but at high loads is moving disconcertingly close to stoichiometric ratios. The closer the overall process is to stoichiometric, the more likely there are to be regions of locally rich equivalence ratios which form CO, HC, and PM. Increasing intake pressure increases the quantity of air within the cylinder, decreasing the overall air:fuel ratio, and improving the volumetric efficiency of the engine. More air mass within the cylinder allows higher fueling levels at the limiting equivalence ratio, resulting in increased energy release, and therefore increased load. A quick test was conducted with lightly boosted intake conditions (130 kPa intake MAP, maintaining a 10 kPa exhaust to intake differential for EGR flow) which confirm that boosting the intake pressure results in higher peak load, as shown in Figure 48 (a). This small increase in intake pressure leads to a 15% increase in load range. At the peak load conditions, the equivalence ratio was 0.85 ± 0.05, essentially the same as the equivalence ratio at the smoke limit for the lower intake pressure condition (0.90 ± 0.05).



a. b.

Figure 48: Smoke versus load conditions for varying intake manifold pressures. (a) Load sweep, (b) Increasing injection pressure at the higher MAP condition.

Figure 48 (b) shows an interesting phenomenon as well: increasing injection pressure (in this case to 1200 bar) yields an increased peak load capacity. Unlike tests at 100 kPa MAP, increasing fueling at the higher injection pressure increases the overall peak load. The increased spray breakup results in improved mixing, and lower smoke emissions. More detailed examination of boosted conditions falls outside the scope of this work, and is left for a more detailed future study.

6.3.7 Emissions-Based Oxidation Catalyst Implications

The CO and HC emissions resulting from the premixed diesel combustion mode investigated within this study are in excess of regulated maximum levels at tailpipe exit for the selected steady state condition. The currently implemented diesel oxidation catalyst (DOC) will be tasked with bringing these emissions down to the legislated levels. The ability of a DOC to reduce high CO and HC emission levels adds a further load range constraint to the limits specified during testing.

An important note regarding the following discussion: error bars are not displayed on figures as uncertainty was not directly computed for each point. It is important to understand that there are substantial assumptions made within the calculations supporting the following discussion. It is acknowledged that the outright accuracy and precision of these calculations may be rather poor. However, the purpose of this discussion is simply to place the combustion results in a more global context, and illustrate the basic requirements and constraints for implementation of the studied combustion strategy.

Furthermore, the following analysis is based on the steady state application of a specific model catalyst referenced in prior research. It is understood and acknowledged that many more issues besides those represented in the following analysis guide DOC development and implementation. Focus areas including startup behavior and transient operation are critical to a full engine and aftertreatment system working together to meet regulated emissions standards. Furthermore, emissions standards measure emissions quantities over a specified test cycle – the steady state approximations used within this analysis are a limited proxy of the full vehicle cycle tests. Accordingly, this analysis will attempt to put the overall emissions levels into context with current and future emissions standards. None of the analysis here conclusively shows that certain emissions regulations can or cannot be met by a full vehicle system – conclusions of this nature are limited to the context of the specific analysis described.

Both US and European emissions laws regulate the emissions of carbon monoxide (CO) and unburned hydrocarbons (HC). Since the advent of recent Euro 4 and Tier 2 emissions regulations, diesel engines have required the use of oxidation catalysts (Diesel Oxidation Catalysts, DOCs) to reduce the engine out emissions of CO and HC to the regulated standards. It is assumed that this will continue to be the case, as the emissions of HC and CO are higher with premixed diesel combustion than with conventional diesel combustion and new emissions regulations further reduce the acceptable output levels of these emissions species. It is therefore imperative that CO and HC produced by the engine not exceed the level which can be reduced by the DOC to the regulated maximums. Understanding the relative magnitude of the emissions within a basic analysis of catalyst performance provides an initial understanding of the concern.

Emissions Limits

Examining the emissions limited operating window involves finding the conversion efficiency required to reduce the measured emissions to levels complying with various regulations. As with NO_x and PM emissions, there are different emissions standards for the United States, California, and Europe. Their respective CO and partially oxidized hydrocarbons regulations are summarized in Table 6. The EPA and CARB standards regulate the level of non-methane organic gases, NMOG, which includes all unburned hydrocarbons with the exception of methane (CFR, 86.1811-04; CCR, 1961). The Euro 5 and 6 standards regulate the sum of unburned hydrocarbons and NO$_x$ emissions (EPC, 715/2007).

Standard	CO		NMOG		HC+NO$_x$	
EPA Tier 2	**3.4**	48	**0.08**	1.0	**-**	-
CARB ULEV	**1.7**	24	**0.04**	0.56	**-**	-
Euro 5	**0.81**	11	**-**	-	**0.37**	5.2
Euro 6	**0.81**	11	**-**	-	**0.27**	3.8
	g/mile	g/kg-fuel	g/mile	g/kg-fuel	g/mile	g/kg-fuel

Table 6: Carbon monoxide and hydrocarbon emission regulations applicable in the United States and Europe. Regulated emissions include carbon monoxide (CO), non-methane organic gases (NMOG), and the sum of NO$_x$ and unburned hydrocarbon emission (HC+NO$_x$). Regulations are defined on a per distance basis: per-mass-fuel basis levels are calculated using Equation 6. Note the US and EU standards are tested on different drive cycles, but end results are comparable.

These emissions standards are set over driving cycles, and therefore specified in terms of emissions per distance (US emissions are in g/mile weighted over the US driving cycles, while the EU standards are g/km on the NEDC driving cycle – while different cycles, they are comparable, as discussed in Chapter 1, Section 2). The regulations are converted to a gram per kilogram fuel basis to match the EI emissions indexes (the method for reporting engine test results) using Equation 11 (Knafl, 2007). An assumed fuel consumption of 45 miles per gallon is used, derived from the stated fuel consumption of an Opel Astra using the parent GM 1.7 Circle-L engine to the one tested here. Fuel density, while varying slightly between the different test fuels used in this study, is assumed to be the average density of the US specification fuels: 0.85 g/cc.

$$EI_{Regulation} = \frac{(EmmReg)(FC)}{\rho_{fuel}} \tag{11}$$

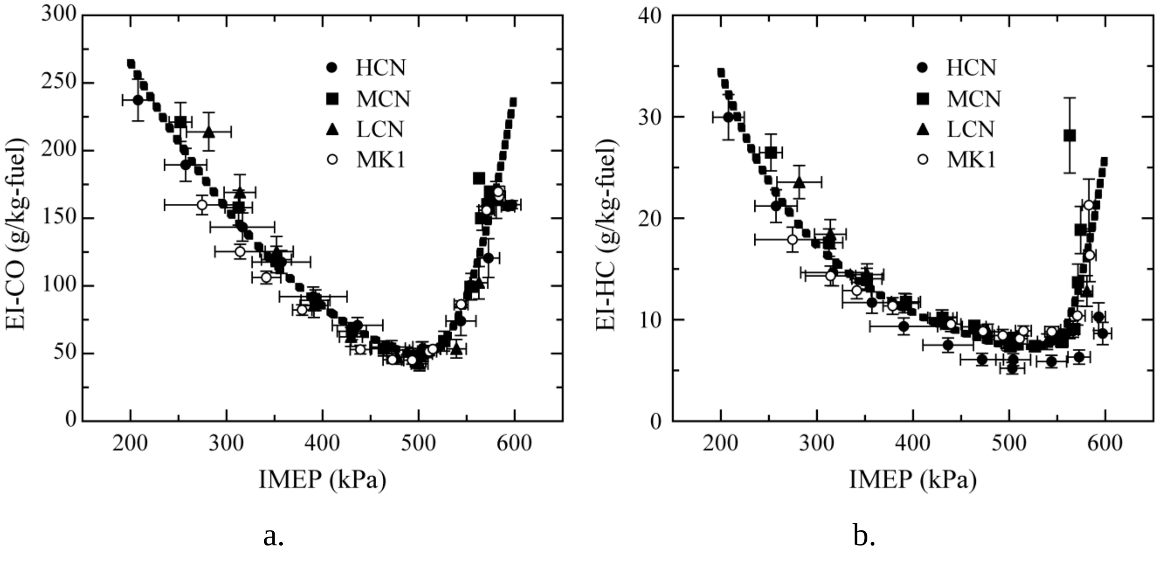
Where:

$EI_{Regulation}$: Emission regulation on per fuel mass basis
EmmReg: Emission regulation on per mile basis
FC: Fuel consumption (assumed 45 mpg)
ρ_{fuel}: Fuel density (assumed 0.85 g/cc)

The experimental hydrocarbon measurements include methane, which is not regulated by the US emissions standards. Previous studies by Jacobs (2005), who used a hydrocarbon analyzer which reported methane concentration, note that around 3% of the hydrocarbon content from a similar combustion mode is methane. Later (unpublished) data taken by Han and by Knafl also show a similar percentage (6 ± 5%) of the hydrocarbons are methane for comparable conditions. The effect on required conversion efficiency is not an overly significant one – approximately 1%. Attempting to elicit further detail becomes increasingly speculative and frivolous since there are enough approximations within the analysis that a 1% change falls within the lumped uncertainty.

DOC Conversion Efficiency

Comparing the measured emissions level as a function of load with the US and European emissions standards, allows the calculation of catalyst conversion efficiencies required to take the engine out emissions down to levels required by a particular emission standards. Given the lack of a strong linear relationship between emissions and engine load and the fuel-to-fuel consistency of the data, a composite average emissions number, representing the average emission at a given load (averaged over the four test fuels), is used. The composite averaged emissions trends are shown in Figure 49, along with the base emissions data.



a. b.

Figure 49: Composite average CO (a) and HC (b) emissions used for calculation of required DOC conversion efficiencies.

To calculate HC conversion efficiencies required to achieve Euro 5/6 standards, a measure of NO_x emissions is necessary as well. As acknowledged earlier, there is spread in the NO$_x$ data for conditions below 5 bar IMEP stemming from the test methodology used, which causes a variation in combustion phasing and therefore NO$_x$ emissions. For loads higher than 5 bar IMEP, the average NO$_x$ value at a given load is used. For IMEP conditions lower than 5 bar IMEP, the NO$_x$ value at 5 bar IMEP of 0.6 g/kg-fuel was used (approximate average, and constant value). Required catalyst conversion efficiencies at varying engine load are calculated from these fuel-average composite emissions for the different regulations, and are shown in Figure 50.

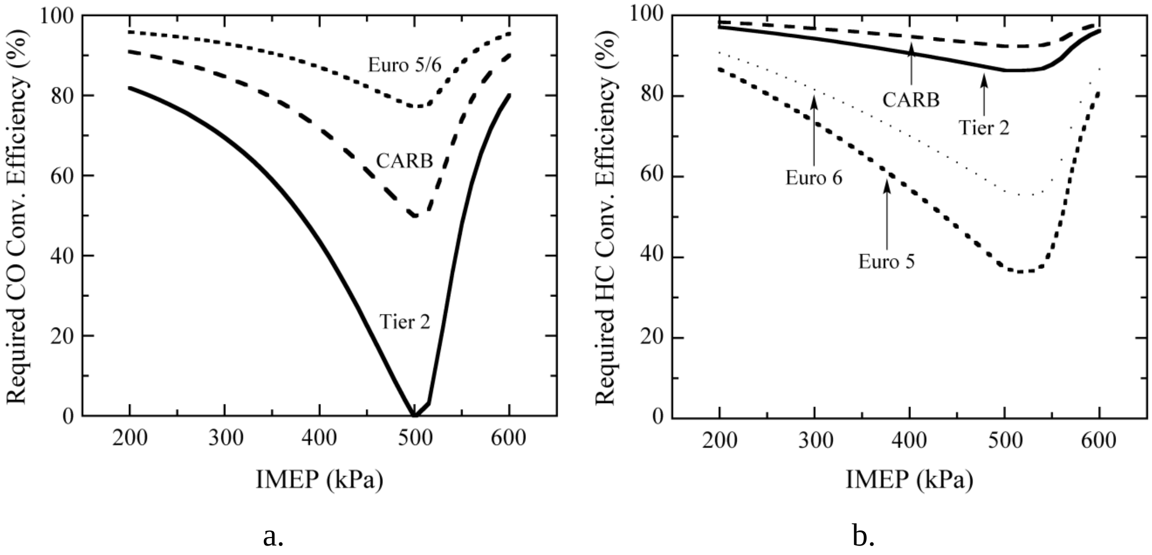


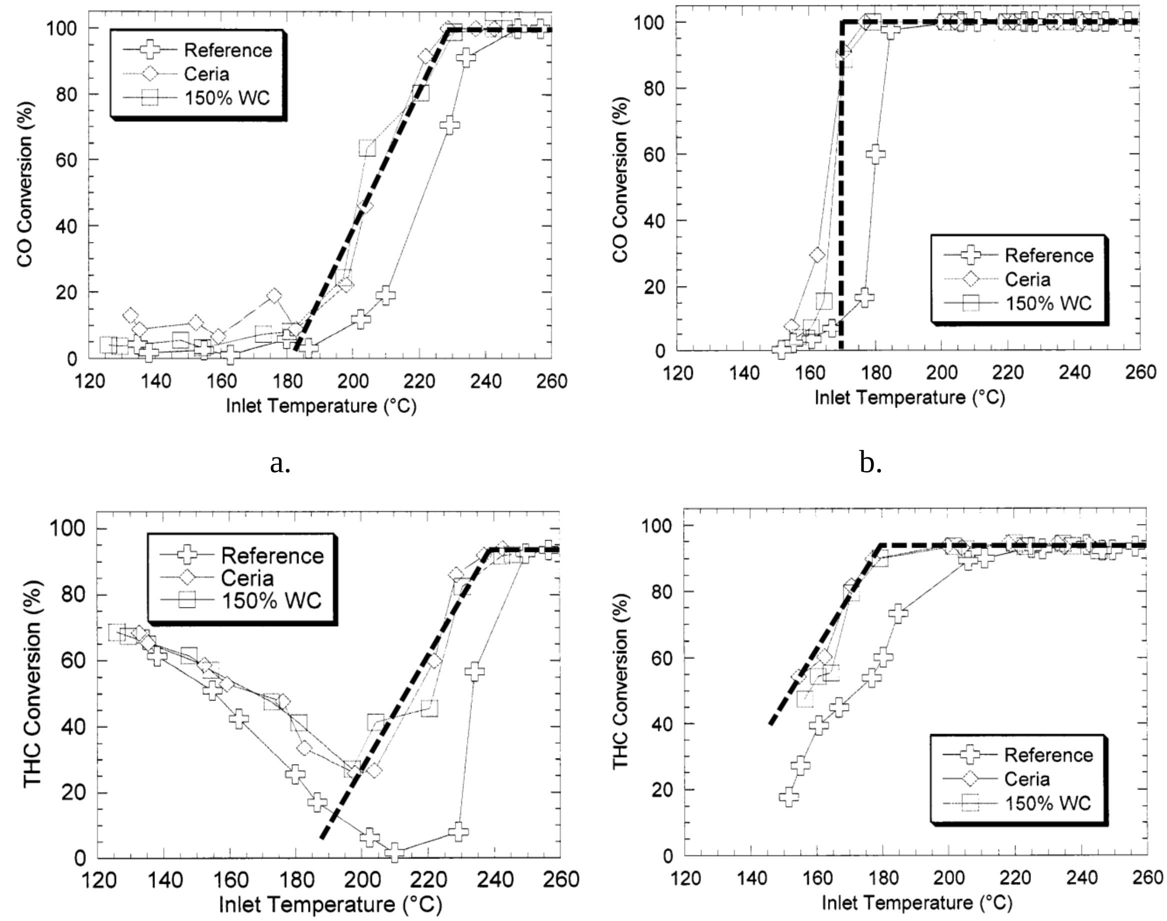
Figure 50: Required DOC conversion efficiency versus engine load for different emissions standards. (a) Required CO conversion efficiency (Euro 5 and Euro 6 specify the same maximum CO levels), (b) Required HC conversion efficiency.

The required conversion efficiencies clearly, and expectedly, reflect the emissions results. There is a substantial increase in required conversion efficiency for loads away from 5 bar IMEP. In the same manner noted in earlier discussion of required DOC behavior, the two US standards (Tier 2, CARB) require very high conversion rates of hydrocarbons: at the loadrange extremes, the DOC is tasked with reducing HC emissions by 98%, a colossal requirement for current DOCs. Prior testing of model DOCs with premixed diesel combustion by Jacobs (2005) and Knafl (2007) show HC conversion efficiencies of 80 and 92% respectively, neither of which would be sufficient based off this analysis. Changes in the catalyst design would be required: different formulations, increased precious metal loadings, and/or larger catalyst volumes.

Operating Range Limitations – Including DOC Temperature Effect

Using results from recent DOC studies which incorporate exhaust temperature effects, it is possible to further examine DOC conversion efficiencies in a more representative way. DOC behavior and conversion efficiencies are well documented to be strongly related to temperature within the light-off/light-down temperature range, which further complicates DOC analysis and predicted requirements. Exhaust temperatures produced by this combustion mode are estimated to fall within the light-off/light-down range based on comparison between single and multi-cylinder engine data. Light-off curves show the conversion efficiencies as the catalyst temperature is increased from a starting point with minimal catalytic activity. Light-down curves show the opposite behavior, starting with a catalyst at full operating temperature and then cooling the catalyst. Examining both curves shows how a catalyst will behave relative to whether it has been warmed to the point of significant catalytic behavior, and vividly demonstrate their temperature sensitive nature.

Light-off and light-down curves as a function of catalyst temperature were generated for several different catalysts subjected to PCI exhaust gas species in a related prior study (Knafl, 2007). Using these results, two-range linear fits are created to approximate the observed behavior of the best catalyst, noted in the figures as ‘Ceria’. This catalyst possesses a washcoat formulation with a 120 g/ft^3 loading of platinum (Pt) and palladium (Pd) at a 3:1 ratio, along with alumina oxide (Al_2O_3), β-zeolite, and cerium oxide (CeO_2) (Knafl, 2007). The light-off and light-down curves for CO and HC, reprinted from Knafl’s dissertation, are shown in Figure 31 with the modeled fits marked.



a.

b.

c.

d.

Figure 51: Light-off and light-down curves for CO and HC when subjected to exhaust gas from a PCI combustion mode. Figures reprinted with permission from Knafl (2007) with two-range fit lines added to represent the catalyst behavior. (a) CO conversion: light-off, (b) CO conversion: light-down, (c) HC conversion: light-off, (d) HC conversion: light-down.

Note that, due to the catalyst formulation containing zeolite, there is a hydrocarbon storage capability in the catalyst as indicated by the perceived catalyst conversion at low temperatures. This is neglected in the present analysis because hydrocarbon storage is a transient behavior and current tests represent steady state. Within vehicle certification tests, however, this hydrocarbon storage capacity is a critical component of the strategy used to meet the regulations. However, the basic, underlying, steady state behavior is the important part within the framework of the current analysis.

Accounting for the temperature effect on DOC performance requires calculating the DOC inlet temperature produced by the current test conditions. Modern diesel engines, including the production version of the GM 1.7L engine, use a close-coupled DOC mounted directly to the turbocharger exit. The single-cylinder engine does not have a turbocharger, nor a full exhaust manifold, so it is not possible to directly measure a turbocharger outlet temperature (TTO). Exhaust port temperature (EGT) is measured in the single-cylinder engine, but not in the partner multi-cylinder engine. As such, it is not possible to directly correlate EGT and TTO from a single engine. There is matching multi-cylinder engine data of exhaust temperature at the turbine outlet (TTO) at fixed 5 bar IMEP load which can be used to estimate the appropriate catalyst inlet temperature, assuming a characteristic heat loss through the manifold and turbocharger. However, there is no TTO data from the multi-cylinder engine across a load sweep. Generating appropriate estimates of TTO for each load condition requires developing a rough correlation between measurements of EGT (measured only on the single cylinder engine) and TTO (measured only on the multi cylinder engine). There should be a reasonable connection between the two temperatures if the engine is operating at a similar condition, given the similarity of the two engines. Figure 52 shows single-cylinder EGT plotted against multi-cylinder TTO for a timing sweep at a fixed load (5 bar IMEP) using a common fuel (Swedish MK1). Temperatures are plotted against combustion phasing, since both are strong functions of it.

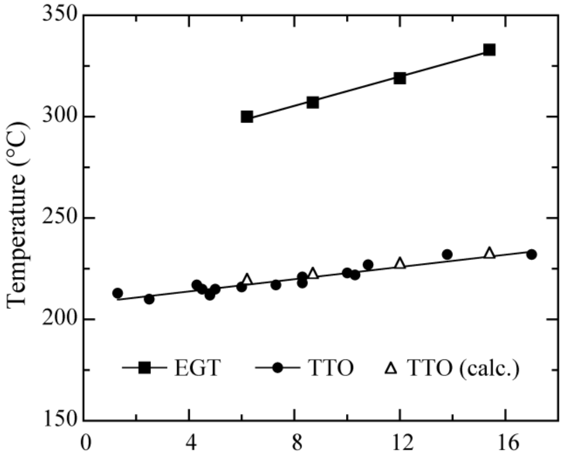


Figure 52: Exhaust gas port temperature (EGT) and turbine outlet temperature (TTO) plotted against combustion phasing. EGT measured on single-cylinder engine, and TTO measured on multi-cylinder engine (multi-cylinder engine data courtesy of Tim Jacobs). ‘TTO (calc)’ uses the correlation given in Equation 12, and is shown calculated for the four EGT levels plotted.

Using this data, a simple correlation between EGT and TTO is developed, as listed in Equation 12 below. This is a very general estimation, whose accuracy is admittedly questionable, but acceptable for the purposes used here.

$$TTO[°C] = 0.4(EGT) + 100 \tag{12}$$

The TTO calculated using this correlation is used as the catalyst inlet temperature to estimate temperature dependent conversion efficiencies using light-off or light-down curves for a selected catalyst. The derived TTO is shown against load for the different fuels in Figure 53.

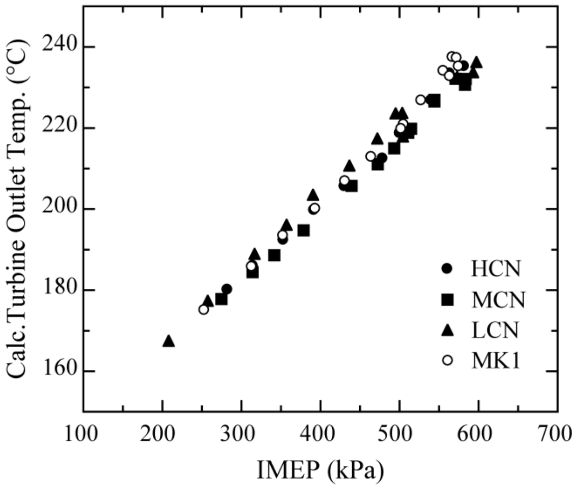
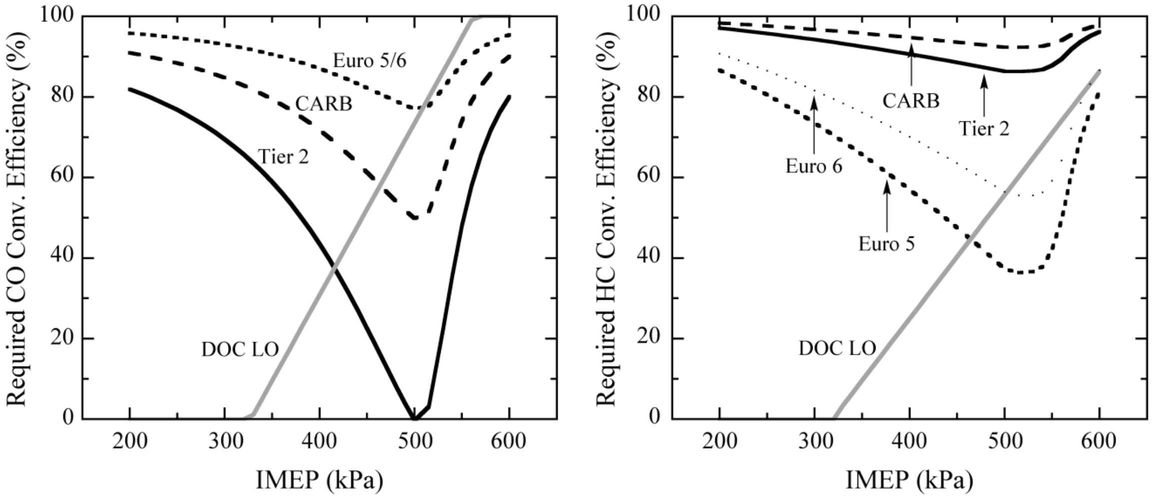


Figure 53: Calculated turbine outlet temperature (TTO) versus engine load for the four test fuels.

The estimated TTOs fall within the range of DOC light-off/light-down hysteresis for the modeled catalysts (reference Figure 51 for light-off and light-down curves). The light down curve nearly covers all operating conditions, but the light-off curve runs through the range of calculated TTOs. Using the derived TTOs (load averaged across the fuels) and representative light-off curves from Knafl, the estimated DOC conversion efficiencies (DOC LO) are calculated and displayed in Figure 54 against the conversion efficiencies required to meet the varying emissions laws as calculated prior.



a. b.

Figure 54: Required DOC conversion efficiency versus engine load along with estimated temperature-dependent catalyst light-off performance. (a) Required CO conversion efficiency (Euro 5 and Euro 6 specify the same maximum CO levels), (b) Required HC conversion efficiency. ‘DOC LO’ represents estimated delivered DOC conversion efficiency.

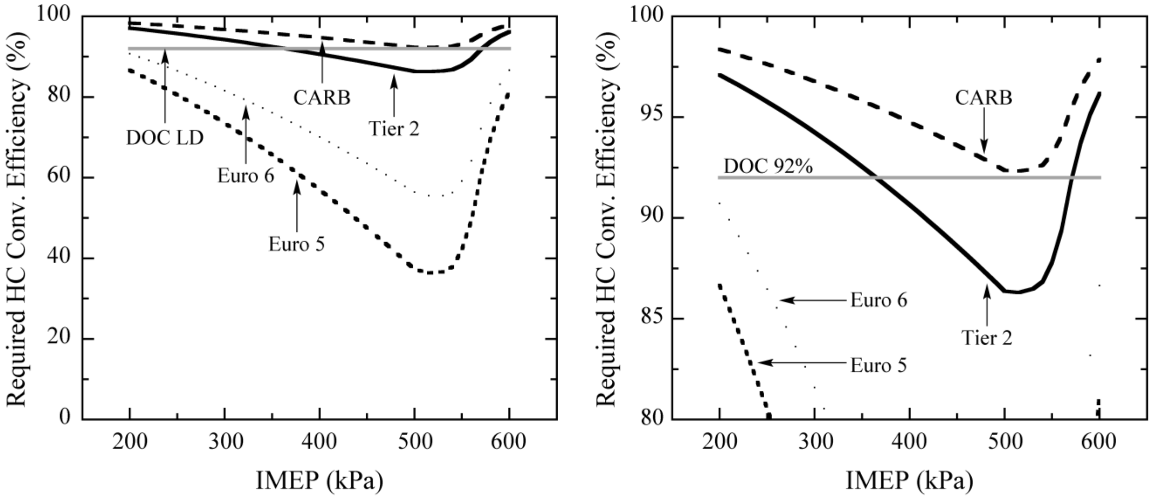
This demonstrates a clear concern with the emission levels produced across the load sweep. The exhaust temperature is likely not sufficient to create the required steady-state conversion efficiency if the catalyst is not fully active. At light loads, not only is the temperature insufficient, but the CO/HC emissions are very high. There will be little conversion at a time when maximum conversion is required. Avoiding this range would restrict this particular premixed combustion mode to a very narrow range of higher loads. This infers a restriction on the operating range of this combustion strategy when the DOC is not fully warmed. Otherwise, improvements to the DOC or operating strategy will likely be required to yield acceptable emissions which meet US and European emissions standards. Shifting the lightoff curve to lower temperatures would increase the operating range size. Additionally, reducing the output level of CO and especially HC emissions would enhance the operating range and utility of the combustion mode according to the current analysis.

Operating Range Restrictions – Full Conversion Efficiency

One of the principal weaknesses of the preceding analysis is analyzing catalyst efficiencies based on a derived temperature – one with questionable accuracy and yet substantial bearing on the results. Also, it only accounts for catalyst behavior in light-off conditions where the catalyst was not already up to operating temperatures. There are several issues with this: (1) the catalyst will frequently be at full operating temperature since engine operation is transient and other engine conditions yield exhaust temperatures sufficient for catalyst light-off, (2) if premixed diesel combustion operation with the DOC in light-off conditions is as problematic as indicated, production engines will have aggressive strategies to insure the catalyst reaches operating temperatures rapidly to insure maximum pollutant conversion in the DOC.

With the light-down curves used, only one test condition would not yield full conversion efficiency. The TTO for this point is fractionally below the assumed cutoff point for catalyst activity. Given the uncertainty limitations of the calculated TTO, it is inappropriate to assert this is a reliable and distinct point for discussion. Further, it occurred at a very low load, where other constraints such as operation stability may prevent operation. As such, examination of cases where the DOC starts at full operational temperature will assume maximum DOC conversion efficiency of CO and HC for all conditions. The fully operational conversion efficiencies for the model catalyst examined here, ‘Reference + Ceria’ from Knafl (2007), were 100% for CO and 92% for HC.

A 100% CO conversion efficiency indicates complete eradication of CO emissions – which would therefore not restrict the operating range. However, the 92% HC conversion efficiency does still indicate a restriction of the usable load range within this analysis. The required HC conversion efficiency is very high at certain conditions, and in excess of what is delivered by the modeled DOC. Figure 55 shows the required HC conversion efficiencies from Figure 50 with the addition of a line representing the 92% DOC conversion efficiency yielded by the selected DOC.



a. b.

Figure 55: Required DOC conversion efficiency versus engine load along with 92% DOC conversion level indicated. (a) Full view, (b) Close up of high conversion range.

The modeled 92% HC conversion efficiency is substantial enough that exit HC emissions for all load conditions tested are less than the level indicated as necessary to meet Euro 5 and Euro 6 emissions standards based on the current analysis. However, this level of modeled conversion is less than the indicated level required for the CARB standards. With regards to Tier 2 standards, the conversion from the modeled DOC is comparable to the required level. So while all loads are not excluded, there is some restriction on operating range. Adequate conversion is only reached for loads between 350 kPa and 570 kPa IMEP, which excludes the low and high load range where the engine-out HC emissions are very high. This is not a severe restriction on operating range, as loads falling outside of this range are very much on the borderline of acceptable operation – the high loads are polluting heavily (with accompanying efficiency problems) and the low loads have borderline combustion stability (high COV).

6.4 Summary and Conclusions

All four test fuels behave similarly, encountering the same load limits and producing comparable emissions trends. The usable load range for all the fuels operating in the tested combustion mode is limited to IMEP values between 250 and 580 kPa. Trends and magnitudes of CO, HC, and soot emissions are identical for all four test fuels.

Changes to injection timing or injection pressure do not increase the peak usable load. Varying injection timing or injection pressure can reduce emissions at a specific load, but the overall peak load value is not affected.

The high load range of the tested combustion mode is primarily limited by equivalence ratio. As the overall equivalence ratio approaches stoichiometric, emissions of smoke, CO, and hydrocarbons all increase sharply due to locations of localized rich regions becoming increasingly prevalent. Increasing intake manifold pressure increases the maximum load limit by increasing the quantity of fuel which can be injected at the limiting equivalence ratio, notwithstanding the increased volumetric efficiency due to the higher inlet pressures.

High DOC conversion efficiencies are required to reduce engine-out CO and HC emissions levels to ranges which would be acceptable for European and US emissions requirements. Using a simplified analysis and DOC behavior modeled from a specific catalyst used in prior testing, basic catalyst behavior is examined. When the modeled DOC is at operational temperatures, the resulting 100% CO conversion should be adequate for all load levels. The 92% conversion efficiency of the modeled catalyst should yield acceptable performance with regards to European emissions standards (Euro 5, Euro 6), but may restrict operating range if trying to meet US standards (Tier 2, and especially CARB ULEV). When the modeled DOC is not at full operational temperature, it has insufficient conversion to reduce the emissions levels produced to meet most emissions standards. Different catalyst formulations, precious metal loadings, and physical designs may be required for vehicle implementation – issues that fall more within the scope of product engineering.

CHAPTER 7

SUMMARY, CONCLUSIONS, AND FUTURE RESEARCH DIRECTION

7.1 Project Summary

This study sought to illuminate the effects of fuel properties on a low-temperature premixed diesel combustion mode. Accordingly, the combustion mode studied was a single-injection 'late' premixed diesel combustion strategy which was the center point of several related preceding studies on a comparable engine. Test fuels represented a variation of properties of interest, with cetane number the primary variable. A secondary closed study of 2-ethylhexyl nitrate behavior was also conducted. Further, the effects (or lack thereof) of other fuel variables including volatility, density, and hydrocarbon composition were inferred but not explicitly studied. The overall spread of the test fuels across a cetane number scale is shown in Figure 56.

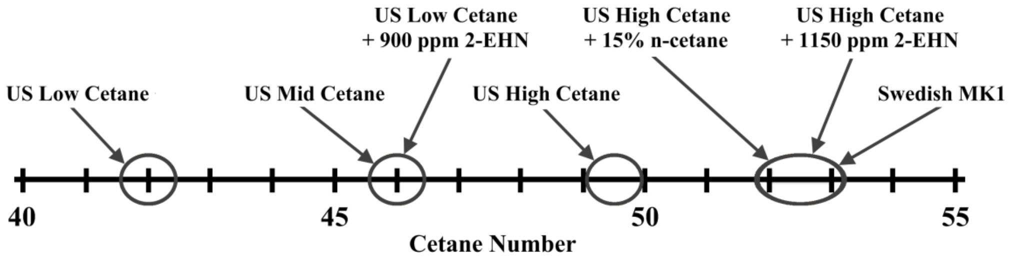


Figure 56: Summary of test fuels used in this study.

With these different test fuels, and within constraints of the selected combustion mode, engine parameters were swept, including EGR level, injection pressure, and engine load. The fuel effects were quantified at these different conditions to examine any secondary parameter interaction. A summary of the parameter changes is shown in Figure 57.

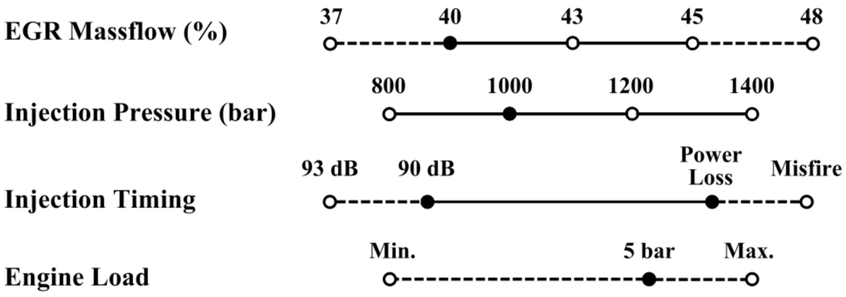


Figure 57: Summary of test conditions used in this study. Solid points are primary conditions. Solid lines represent primary variation levels, with dashed lines being variations outside main region of investigation.

Fuel specific combustion behavior was fully evaluated in response to these parameter changes. During the course of the study, additional engine state effects were also noted, but since they were not primary research variables, their impact was not fully isolated, but rather eliminated with subsequent experimental procedures.

7.2 Research Conclusions

While numerous conclusions can (and were) drawn from the results of tests conducted within this study, for brevity and influence, only the most significant results bear summary here.

For premixed diesel combustion, the principal characteristic property is cetane number. While not systematically varied, changes in other fuel properties including distillation characteristics, aromatic content, and exact fuel hydrocarbon composition, did not substantiate distinct changes in combustion or emissions. It must be acknowledged that it is still possible for these properties to have an effect if varied grossly beyond the bounds of what was tested within this study, but such a fuel would likely be very dissimilar to currently used diesel fuels.

Gaseous emissions, particularly NO_x, resulting from this premixed diesel combustion strategy are principally a function of the cooled EGR fraction and the combustion phasing. Fuel cetane number does not directly impact these emissions. Rather, changes in cetane number alter the main ignition delay, shifting the combustion phasing – the corresponding shift in bulk combustion behavior alters the gaseous emissions. If injection timing is adjusted to counteract the combustion phasing shift due to fuel cetane number, the resulting combustion phasing is matched and gaseous emissions remain constant.

There is no injection timing which gives acceptable behavior subject to the specified criteria for fuels over a ten-point range of cetane number, the range of cetane number expected in commercially available fuels. Using cylinder-pressure feedback to provide combustion phasing control (rather than using fixed injection timing) is highly recommended: by controlling to a fixed combustion phasing the effect of varying cetane number is eliminated.

The presence of 2-EHN within the fuel introduces a new fuel-borne NO_x formation mechanism into the combustion process, which significantly increases NO_x emissions in a premixed diesel combustion mode. The increase in emissions is not reported by prior researchers due to their use of a conventional combustion mode and the high level of NO_x emissions in their tests, both of which lead to other effects overshadowing the NO_x formed by the EHN decomposition. The NO_x emissions levels resulting from premixed diesel combustion are low enough to reveal a consistent increase in NO_x emissions that is directly tied to the addition of 2-EHN to the test fuel. For the tested EHN concentrations (900 ppm, 1150 ppm), the increase in NO_x emissions is around 0.1 g/kg-fuel – an increase of 20-50% (varying with EGR level and combustion phasing) over fuels not containing the additive. Finally, the use of 2-ethylhexyl nitrate appeared to cause significantly worse injector fouling under the specified test conditions than the fuels lacking the additive.

Variations in fuel cetane number impacted neither the operating load limits nor emissions behavior across a range of loads. Trends and magnitudes of soot, CO, and HC emissions are identical for all tested fuels. High DOC conversion efficiencies will be required to reduce the CO and HC emissions to levels which meet US and European emissions requirements.

The high load limit of the tested premixed diesel combustion mode is primarily limited by equivalence ratio. As bulk cylinder equivalence ratio nears stoichiometric, soot, CO, and HC emissions become excessive and load reaches a maximum level, establishing the combustion mode’s high load limit. Varying injection timing or injection pressure can reduce emissions at the peak load condition, but do not increase the load limit of the combustion mode. Increasing intake manifold pressure does increase the load limit by increasing the quantity of fuel which can be fully combusted at the limiting equivalence ratio, notwithstanding the increased volumetric efficiency due to the higher inlet pressures.

7.3 Recommended Future Research Direction

Research begets research. The current investigation has answered a few questions, but has also created the opportunity for, and identified areas for, further exploration and future work.

7.3.1 Expanded Fuel Matrix

Within this study, the fuel cetane number was varied over a range that was consistent with commercially available fuels. However, this is not inclusive of all fuels which future engines will operate on. Already ongoing is a study into one of the currently politically-correct future fuels, biodiesel. More expansive testing of biofuels and other petroleum-alternative fuels should be conducted. Within the petroleum fuels, there should be motivation to study synthetic fuels, both derived from biological material and from natural gas, as there is significant public policy driven motivation to implement these fuels in the future.

7.3.2 Enhanced Particulate Matter Investigation

Measurements of particulates (PM) in this study were limited to soot measurements taken with a smokemeter. This does not provide highly accurate results in the range that is produced by premixed diesel combustion modes. Additionally, smoke measurements only measure the carbon soot portion of PM emissions, and not any of the soluble organic fraction (SOF). While soot emissions did not vary with the different fuel compositions, it is entirely possible that the SOF would vary, along with the overall mass of particulates. More detailed research should be conducted into what impact the fuel type has on particulates, and the related implications this has on a diesel particulate filter (DPF) which will almost certainly be employed on future vehicles.

7.3.3 Expanding the Premixed Diesel Combustion Load Range

One of the findings of this work was that the premixed diesel combustion operating range was limited by the air-handling capabilities of the engine. Increasing the intake boost range was noted to significantly increase the peak load that was available from the premixed combustion mode. The capabilities of the single-cylinder test cell lend themselves handily to further research in this area. The air handling system for the engine, with a few upgrades, could easily supply very high levels of boost and EGR for a study on expanding the operating range. Increasing the range where it is possible to operate in the premixed diesel combustion mode is of substantial utility, and with the capabilities of the test cell, should be investigated further.

7.3.4 Diesel Oxidation Catalyst Behavior

Central to both studies on operating limits (injection timing range, load range) was the behavior of a diesel oxidation catalyst. Accordingly, future work in this field should centrally include examination of the behavior and characteristics of this device. Within this work, it was assumed that a DOC will oxidize all hydrocarbon emissions with matching efficiency. However, different fuels may produce different hydrocarbon species, which may display different oxidation behavior in a DOC. Future work in this direction should focus on the following areas:

1. Fuel specific effects on the DOC conversion behavior
2. Effect of different exhaust hydrocarbon species on the DOC
3. Improved DOC performance, through new formulations and improved models

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